Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2023 – 02:36 PM EST

PDB ID	:	1YRQ
Title	:	Structure of the ready oxidized form of [NiFe]-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Cavazza, C.; Matho, M.; Faber, B.W.; Roseboom, W.; Albracht, S.P.; Garcin, E.; Rousset, M.; Fontecilla-Camps, J.C.
Deposited on	:	2005-02-04
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

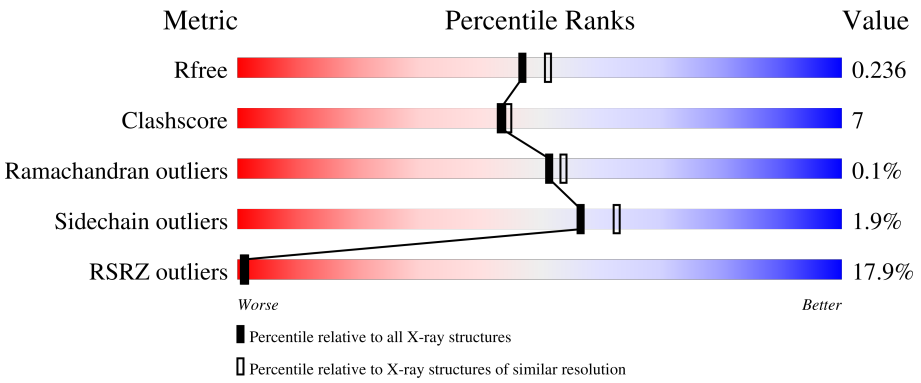
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	264	2% 80% 19%
1	1-B	264	15% 83% 16%
1	1-C	264	% 86% 11%
1	1-D	264	% 83% 17%
1	1-F	264	2% 84% 14%

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Mol	Chain	Length	Quality of chain
1	1-G	264	95% 67% 31%
1	2-A	264	2% 81% 19%
1	2-B	264	15% 83% 16%
1	2-C	264	% 86% 11%
1	2-D	264	% 83% 17%
1	2-F	264	2% 83% 15%
1	2-G	264	95% 66% 32%
2	1-H	549	2% 84% 14%
2	1-I	549	5% 85% 14%
2	1-J	549	3% 82% 16%
2	1-K	549	% 83% 15%
2	1-M	549	3% 81% 17%
2	1-N	549	91% 81% 17%
2	2-H	549	2% 84% 14%
2	2-I	549	5% 85% 14%
2	2-J	549	3% 82% 16%
2	2-K	549	% 83% 15%
2	2-M	549	3% 81% 17%
2	2-N	549	91% 81% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FCO	1-N	550	-	-	X	-
7	FCO	2-N	550	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 77694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	262	1970	1254	330	371	15	0	0	0
1	2-A	262	1970	1254	330	371	15	0	0	0
1	1-B	262	1971	1255	330	371	15	0	0	0
1	2-B	262	1971	1255	330	371	15	0	0	0
1	1-C	260	1952	1243	325	369	15	0	0	0
1	2-C	260	1952	1243	325	369	15	0	0	0
1	1-D	262	1971	1255	330	371	15	0	0	0
1	2-D	262	1971	1255	330	371	15	0	0	0
1	1-F	260	1952	1243	325	369	15	0	0	0
1	2-F	260	1952	1243	325	369	15	0	0	0
1	1-G	262	1970	1254	330	371	15	0	0	0
1	2-G	262	1970	1254	330	371	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	SER	GLU	conflict	UNP P18187
B	171	SER	GLU	conflict	UNP P18187
C	171	SER	GLU	conflict	UNP P18187
D	171	SER	GLU	conflict	UNP P18187
F	171	SER	GLU	conflict	UNP P18187

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Chain	Residue	Modelled	Actual	Comment	Reference
G	171	SER	GLU	conflict	UNP P18187

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1-H	545	4167	2654	725	766	22	0	0	0
2	2-H	545	4167	2654	725	766	22	0	0	0
2	1-I	545	4166	2653	725	766	22	0	0	0
2	2-I	545	4166	2653	725	766	22	0	0	0
2	1-J	544	4162	2651	724	765	22	0	0	0
2	2-J	544	4162	2651	724	765	22	0	0	0
2	1-K	544	4162	2651	724	765	22	0	0	0
2	2-K	544	4162	2651	724	765	22	0	0	0
2	1-M	545	4166	2653	725	766	22	0	0	0
2	2-M	545	4166	2653	725	766	22	0	0	0
2	1-N	545	4167	2654	725	766	22	4	0	0
2	2-N	545	4167	2654	725	766	22	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	198	ASN	ASP	conflict	UNP P18188
H	303	SER	GLU	conflict	UNP P18188
I	198	ASN	ASP	conflict	UNP P18188
I	303	SER	GLU	conflict	UNP P18188
J	198	ASN	ASP	conflict	UNP P18188
J	303	SER	GLU	conflict	UNP P18188
K	198	ASN	ASP	conflict	UNP P18188
K	303	SER	GLU	conflict	UNP P18188
M	198	ASN	ASP	conflict	UNP P18188

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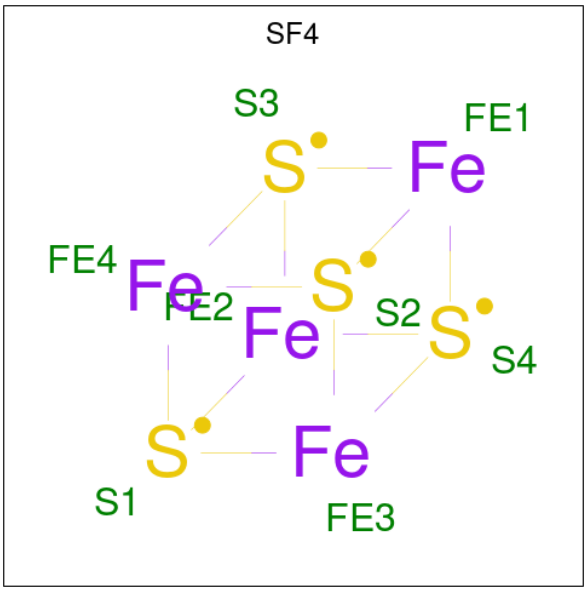
Chain	Residue	Modelled	Actual	Comment	Reference
M	303	SER	GLU	conflict	UNP P18188
N	198	ASN	ASP	conflict	UNP P18188
N	303	SER	GLU	conflict	UNP P18188

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	1-A	1	8	4	4	0	0
3	2-A	1	8	4	4	0	0
3	1-A	1	8	4	4	0	0
3	2-A	1	8	4	4	0	0
3	1-B	1	8	4	4	0	0
3	2-B	1	8	4	4	0	0
3	1-B	1	8	4	4	0	0
3	2-B	1	8	4	4	0	0
3	1-C	1	8	4	4	0	0
3	2-C	1	8	4	4	0	0

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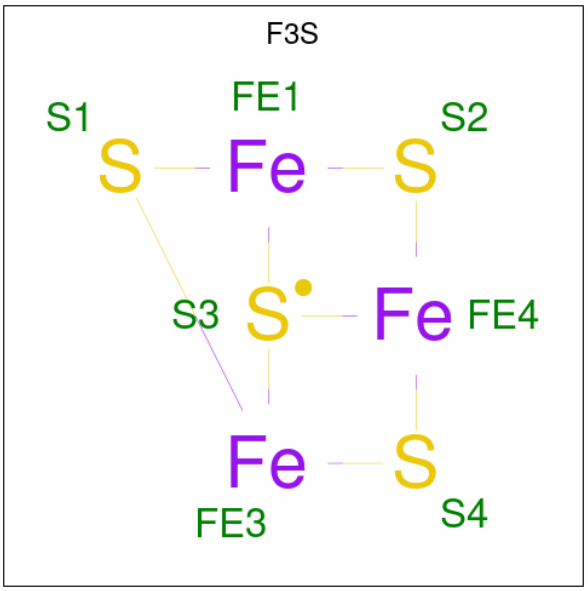
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	1-C	1	8	4	4	0	0
3	2-C	1	8	4	4	0	0
3	1-D	1	8	4	4	0	0
3	2-D	1	8	4	4	0	0
3	1-D	1	8	4	4	0	0
3	2-D	1	8	4	4	0	0
3	1-F	1	8	4	4	0	0
3	2-F	1	8	4	4	0	0
3	1-F	1	8	4	4	0	0
3	2-F	1	8	4	4	0	0
3	1-G	1	8	4	4	0	0
3	2-G	1	8	4	4	0	0
3	1-G	1	8	4	4	0	0
3	2-G	1	8	4	4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
4	1-A	1	7	3	4		0	0
4	2-A	1	7	3	4		0	0
4	1-B	1	7	3	4		0	0
4	2-B	1	7	3	4		0	0
4	1-C	1	7	3	4		0	0
4	2-C	1	7	3	4		0	0
4	1-D	1	7	3	4		0	0
4	2-D	1	7	3	4		0	0
4	1-F	1	7	3	4		0	0
4	2-F	1	7	3	4		0	0
4	1-G	1	7	3	4		0	0
4	2-G	1	7	3	4		0	0

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
5	1-H	1	1	1	0	0
5	2-H	1	1	1	0	0
5	1-I	1	1	1	0	0
5	2-I	1	1	1	0	0
5	1-J	1	1	1	0	0
5	2-J	1	1	1	0	0
5	1-K	1	1	1	0	0
5	2-K	1	1	1	0	0
5	1-M	1	1	1	0	0
5	2-M	1	1	1	0	0
5	1-N	1	1	1	0	0
5	2-N	1	1	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	1-H	1	1	1	0	0
6	2-H	1	1	1	0	0
6	1-I	1	1	1	0	0
6	2-I	1	1	1	0	0
6	1-J	1	1	1	0	0
6	2-J	1	1	1	0	0
6	1-K	1	1	1	0	0
6	2-K	1	1	1	0	0

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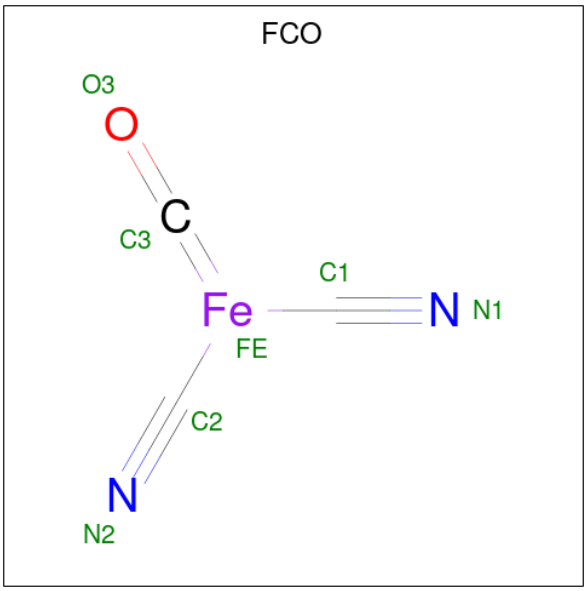
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	1-M	1	1	1	0	0
			Total	Mg		
6	2-M	1	1	1	0	0
			Total	Mg		
6	1-N	1	1	1	0	0
			Total	Mg		
6	2-N	1	1	1	0	0

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	1-H	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	2-H	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	1-I	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	2-I	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	1-J	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	2-J	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
7	1-K	1	7	3	1	2	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	2-K	1	7	3	1	2	1	0	0
7	1-M	1	7	3	1	2	1	0	0
7	2-M	1	7	3	1	2	1	0	0
7	1-N	1	7	3	1	2	1	0	0
7	2-N	1	7	3	1	2	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	1-A	122	122	122	0	0
8	2-A	122	122	122	0	0
8	1-H	245	245	245	0	0
8	2-H	245	245	245	0	0
8	1-B	83	83	83	0	0
8	2-B	84	84	84	0	0
8	1-I	218	218	218	0	0
8	2-I	218	218	218	0	0
8	1-C	120	120	120	0	0
8	2-C	120	120	120	0	0
8	1-J	208	208	208	0	0
8	2-J	208	208	208	0	0
8	1-D	149	149	149	0	0
8	2-D	148	148	148	0	0

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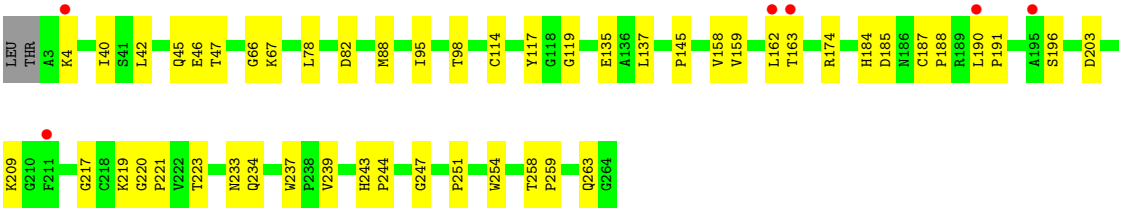
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	1-K	253	253	253	0	0
			Total	O		
8	2-K	253	253	253	0	0
			Total	O		
8	1-F	108	108	108	0	0
			Total	O		
8	2-F	109	109	109	0	0
			Total	O		
8	1-M	183	183	183	0	0
			Total	O		
8	2-M	183	183	183	0	0
			Total	O		
8	1-G	59	59	59	0	0
			Total	O		
8	2-G	58	58	58	0	0
			Total	O		
8	1-N	138	138	138	0	0
			Total	O		
8	2-N	124	124	124	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

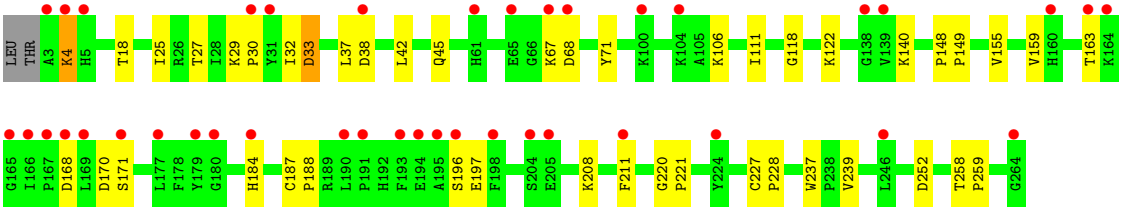
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-A:



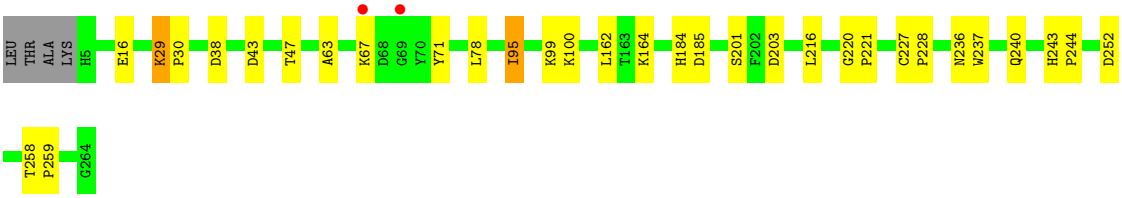
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-B:



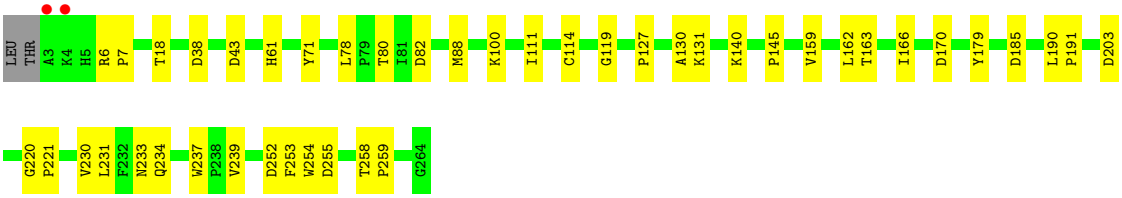
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-C:



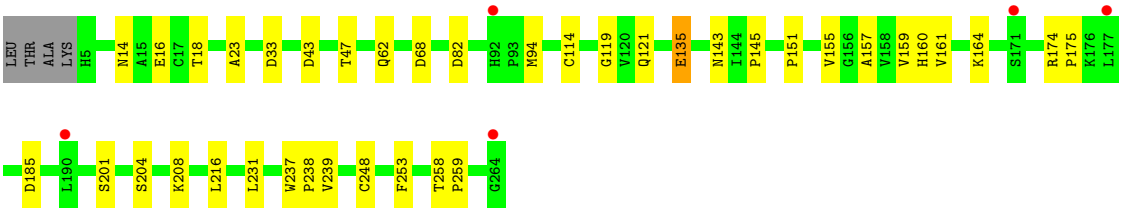
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-D:



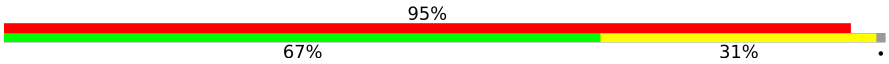
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

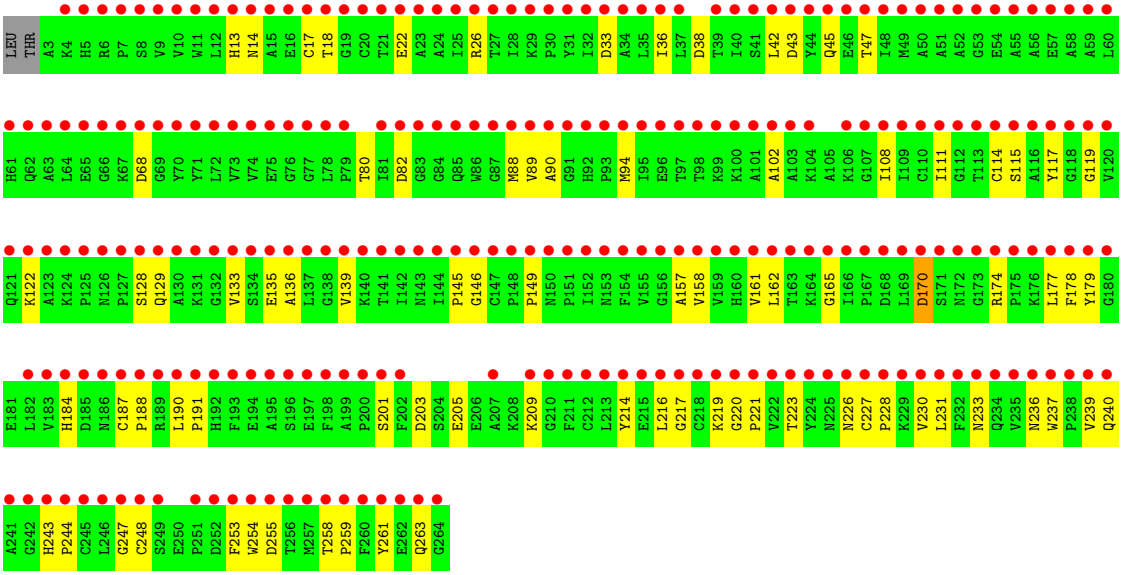
Chain 1-F:



• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

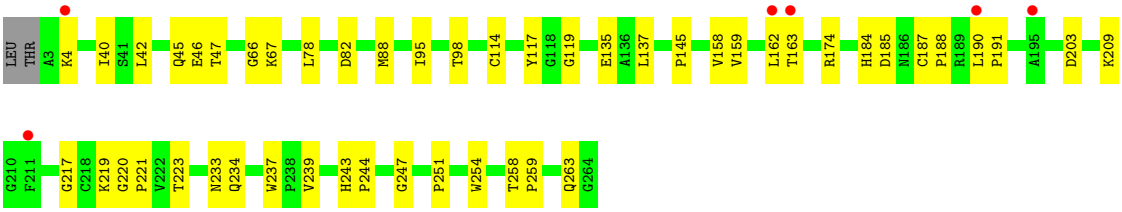
Chain 1-G:





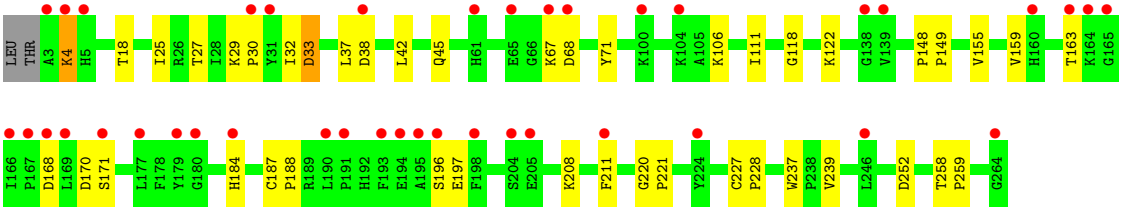
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-A:



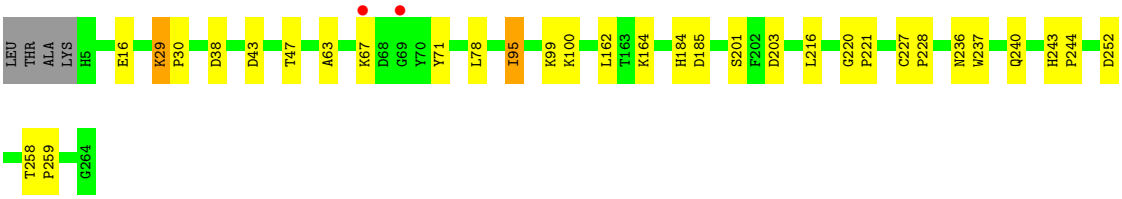
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-B:



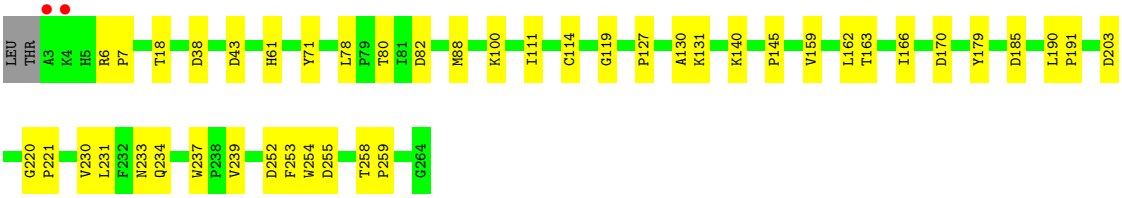
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-C:



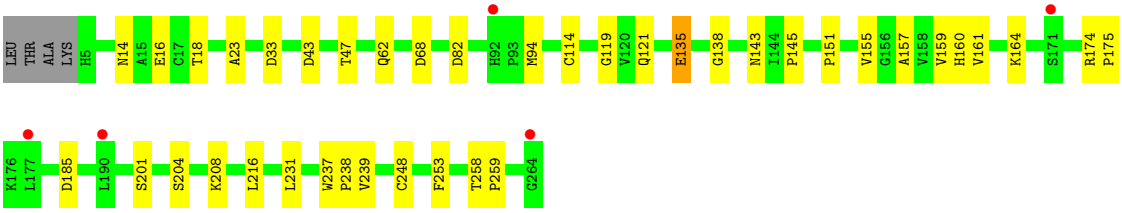
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-D:



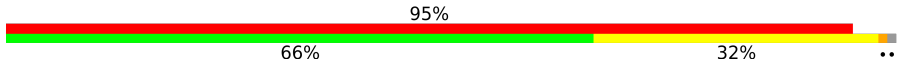
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

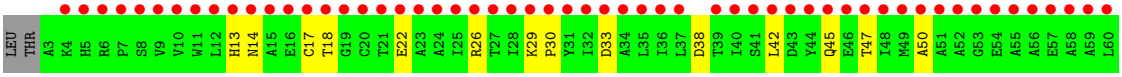
Chain 2-F:

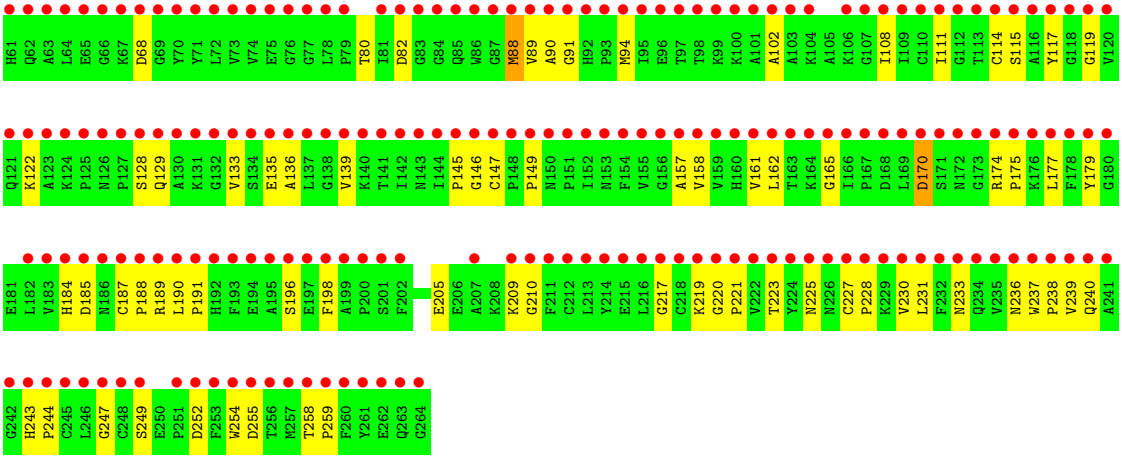


• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-G:

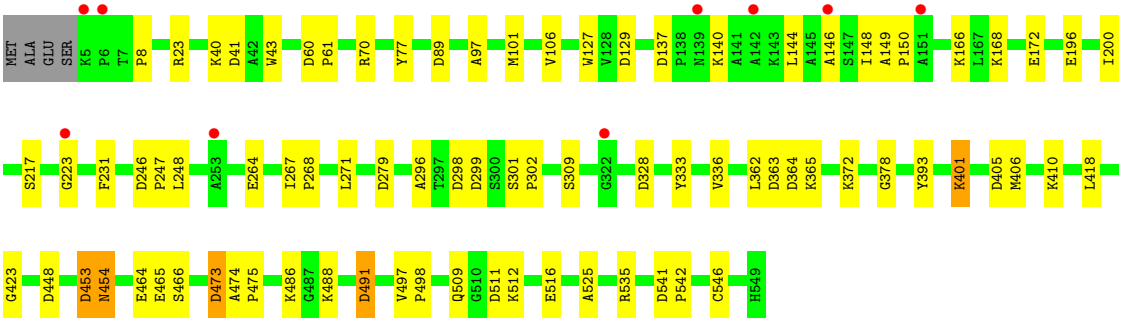






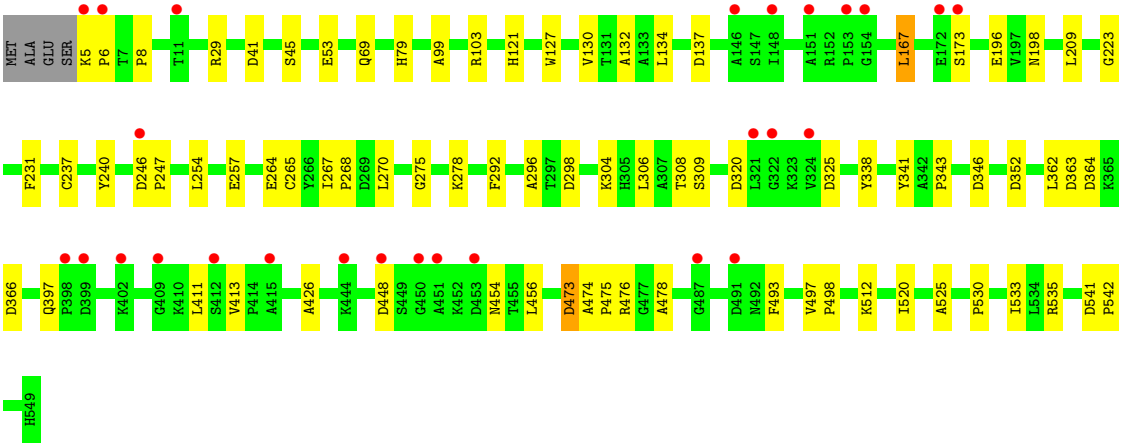
- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-H:



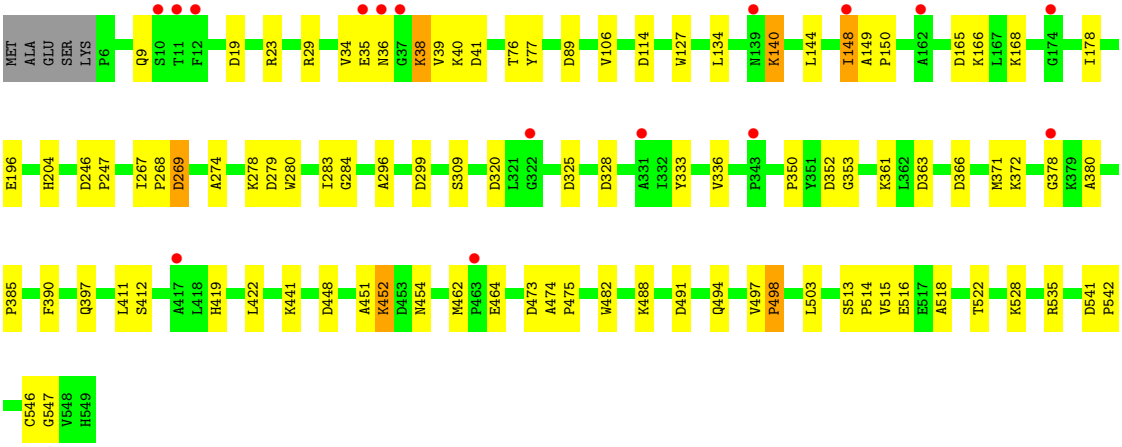
- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-I:



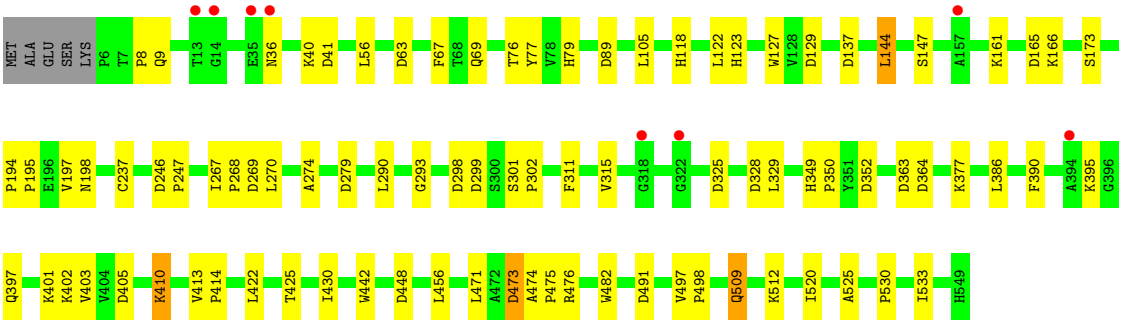
- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-J:



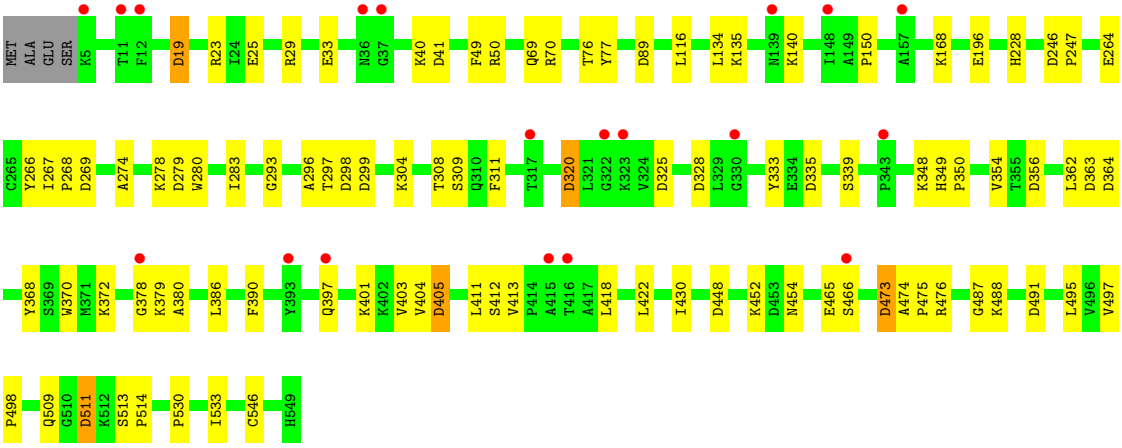
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-K:



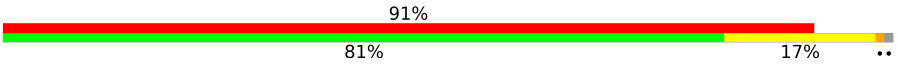
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

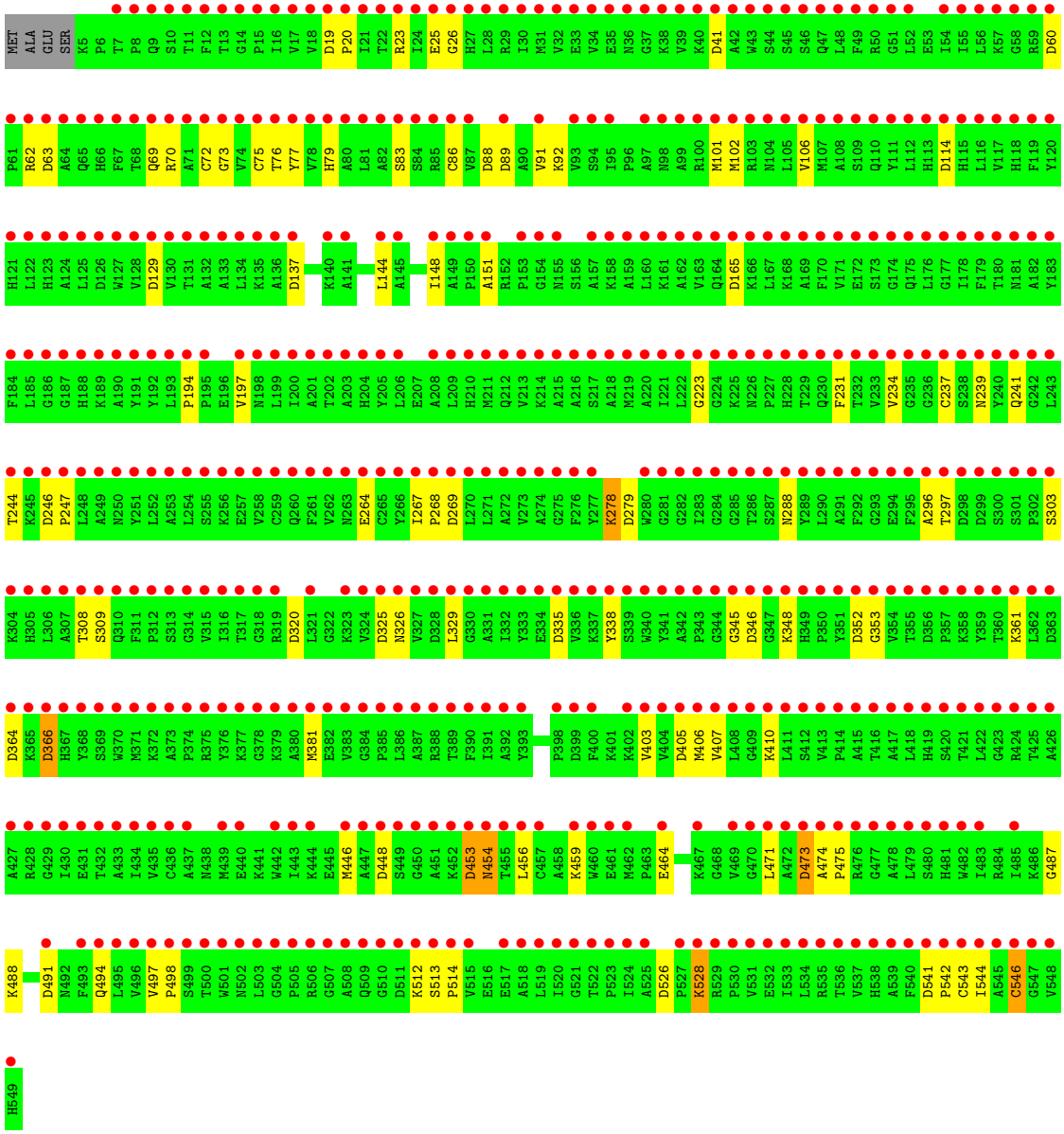
Chain 1-M:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

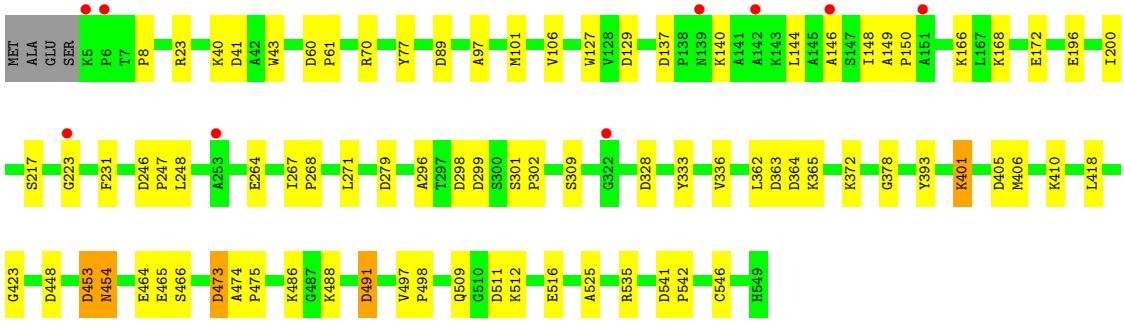
Chain 1-N:





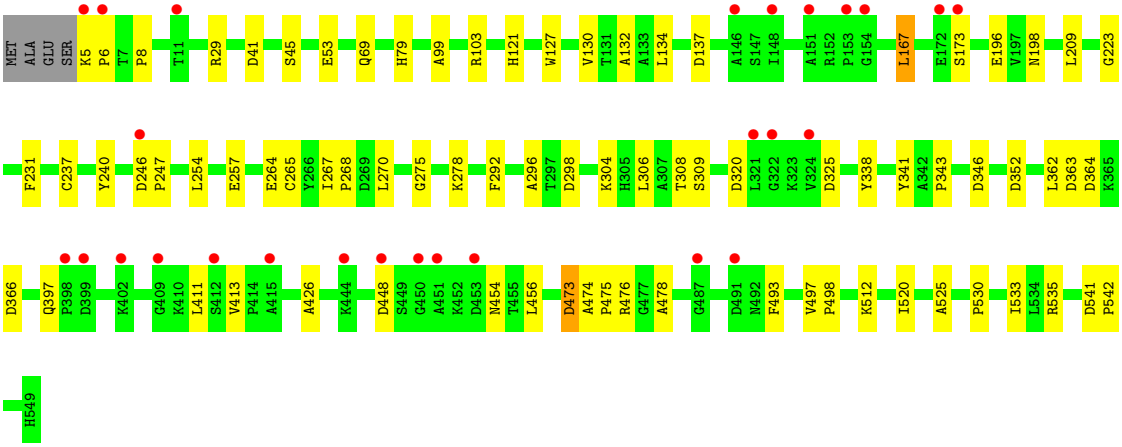
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-H:



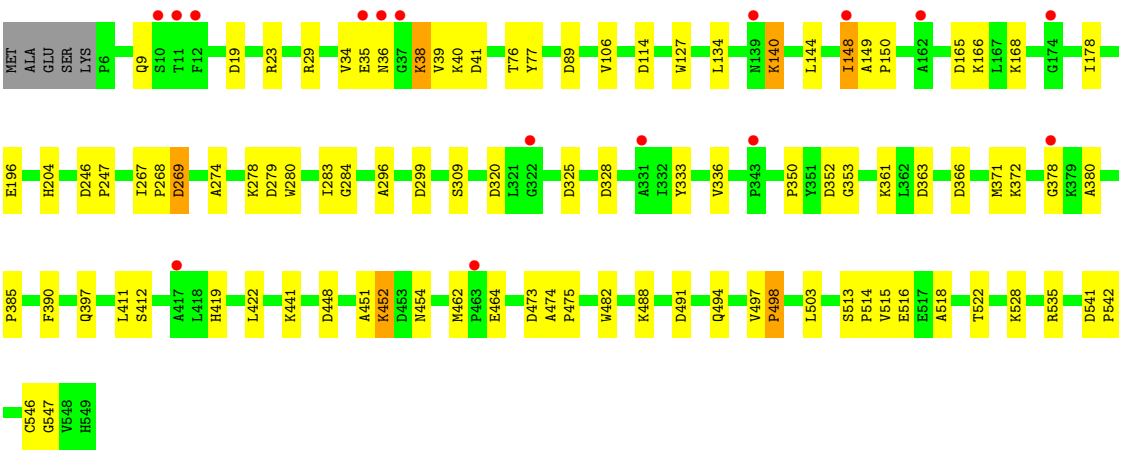
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-I:



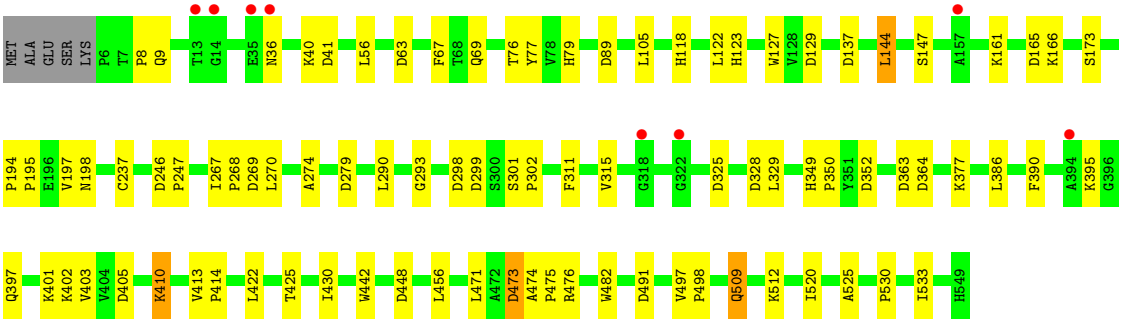
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-J:



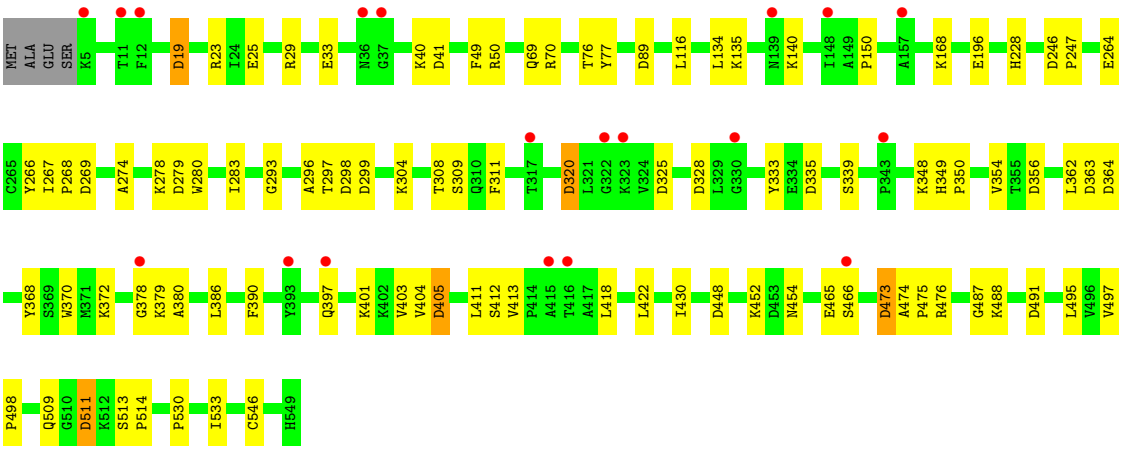
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-K:



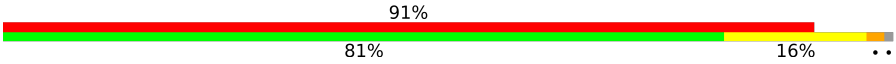
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

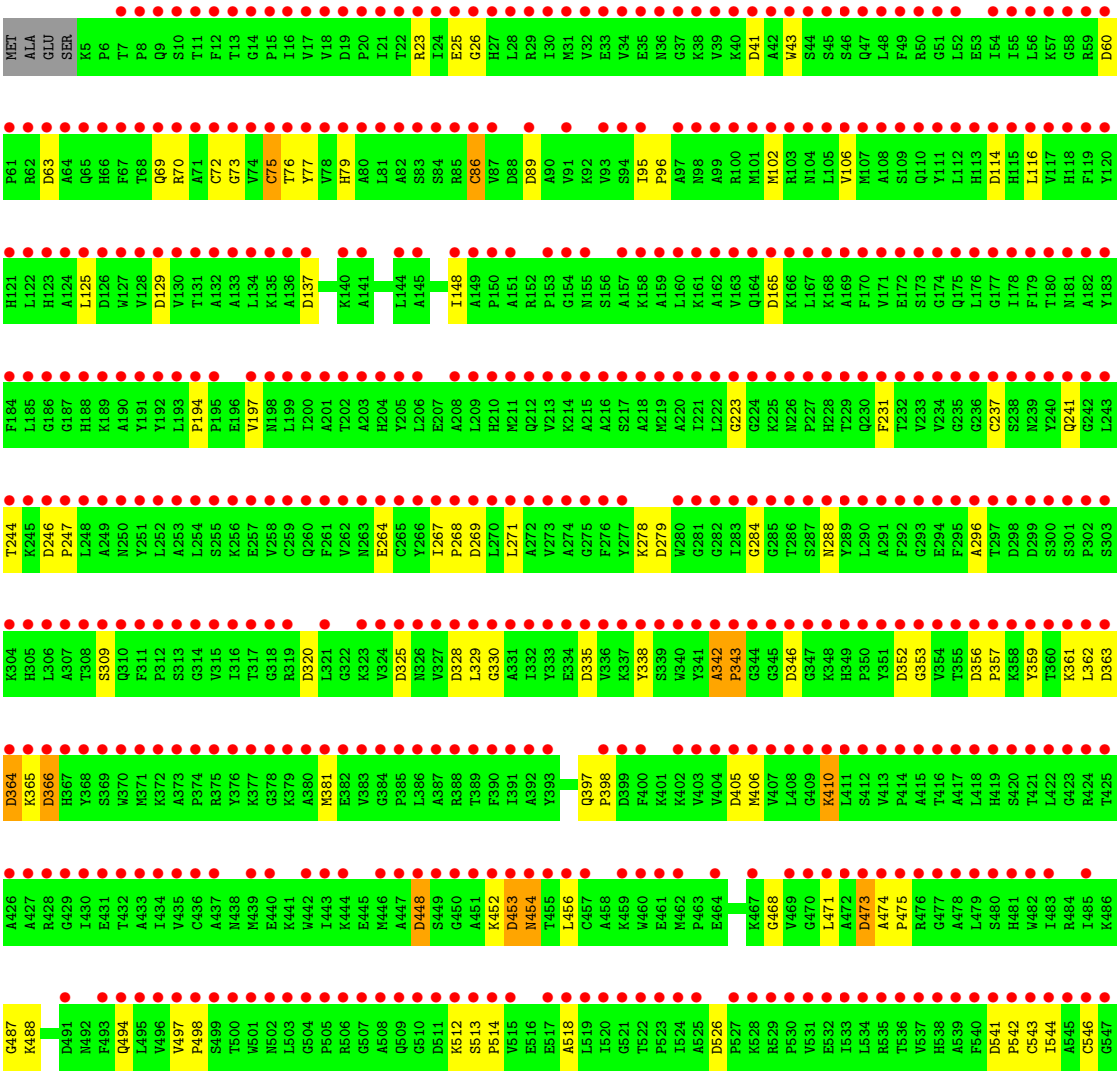
Chain 2-M:



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-N:





V548
H549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.50Å 99.70Å 183.20Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 29.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.10) 87.7 (29.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.171 , 0.220 0.192 , 0.236	Depositor DCC
R_{free} test set	11812 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.59 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	77694	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3614e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FCO, MG, NI, F3S, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	1-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	1-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	1-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	1-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	1-G	0.31	0/2024	0.63	8/2755 (0.3%)
1	2-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	2-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	2-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	2-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	2-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	2-G	0.27	0/2024	0.61	8/2755 (0.3%)
2	1-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	1-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	1-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	1-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	1-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	1-N	0.39	2/4272 (0.0%)	0.69	25/5800 (0.4%)
2	2-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	2-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	2-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	2-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	2-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	2-N	0.30	1/4272 (0.0%)	0.68	22/5800 (0.4%)
All	All	0.51	3/75456 (0.0%)	0.76	269/102532 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-N	361	LYS	CB-CG	10.38	1.80	1.52
2	1-N	459	LYS	C-O	5.89	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-N	75	CYS	CB-SG	5.08	1.90	1.82

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
1	2-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
2	1-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	2-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	1-K	129	ASP	CB-CG-OD2	8.00	125.50	118.30
2	2-K	129	ASP	CB-CG-OD2	8.00	125.50	118.30
2	1-H	89	ASP	CB-CG-OD2	7.94	125.45	118.30
2	2-H	89	ASP	CB-CG-OD2	7.94	125.45	118.30
2	1-H	129	ASP	CB-CG-OD2	7.83	125.34	118.30
2	2-H	129	ASP	CB-CG-OD2	7.83	125.34	118.30
2	1-M	89	ASP	CB-CG-OD2	7.77	125.29	118.30
2	2-M	89	ASP	CB-CG-OD2	7.77	125.29	118.30
2	1-K	165	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-K	165	ASP	CB-CG-OD2	7.24	124.82	118.30
2	1-I	364	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-I	364	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-N	86	CYS	CA-CB-SG	-7.23	100.98	114.00
1	1-D	170	ASP	CB-CG-OD2	7.05	124.65	118.30
1	2-D	170	ASP	CB-CG-OD2	7.05	124.65	118.30
1	1-A	82	ASP	CB-CG-OD2	7.01	124.61	118.30
1	2-A	82	ASP	CB-CG-OD2	7.01	124.61	118.30
2	1-N	361	LYS	CA-CB-CG	-6.99	98.02	113.40
2	1-I	448	ASP	CB-CG-OD2	6.90	124.51	118.30
2	2-I	448	ASP	CB-CG-OD2	6.90	124.51	118.30
1	1-B	252	ASP	CB-CG-OD2	6.87	124.48	118.30
1	2-B	252	ASP	CB-CG-OD2	6.87	124.48	118.30
2	1-K	137	ASP	CB-CG-OD2	6.77	124.39	118.30
2	2-K	137	ASP	CB-CG-OD2	6.77	124.39	118.30
1	1-G	255	ASP	CB-CG-OD2	6.76	124.38	118.30
1	1-D	82	ASP	CB-CG-OD2	6.75	124.38	118.30
1	2-D	82	ASP	CB-CG-OD2	6.75	124.38	118.30
2	1-H	41	ASP	CB-CG-OD2	6.59	124.23	118.30
2	2-H	41	ASP	CB-CG-OD2	6.59	124.23	118.30
2	1-K	473	ASP	CB-CG-OD2	6.57	124.22	118.30
2	2-K	473	ASP	CB-CG-OD2	6.57	124.22	118.30
2	1-J	366	ASP	CB-CG-OD2	6.55	124.20	118.30
2	2-J	366	ASP	CB-CG-OD2	6.55	124.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-I	320	ASP	CB-CG-OD2	6.47	124.12	118.30
2	2-I	320	ASP	CB-CG-OD2	6.47	124.12	118.30
2	1-H	328	ASP	CB-CG-OD2	6.45	124.10	118.30
2	2-H	328	ASP	CB-CG-OD2	6.45	124.10	118.30
1	1-B	33	ASP	CB-CG-OD2	6.44	124.10	118.30
1	2-B	33	ASP	CB-CG-OD2	6.44	124.10	118.30
2	1-J	279	ASP	CB-CG-OD2	6.41	124.07	118.30
2	2-J	279	ASP	CB-CG-OD2	6.41	124.07	118.30
2	1-K	448	ASP	CB-CG-OD2	6.41	124.07	118.30
2	2-K	448	ASP	CB-CG-OD2	6.41	124.07	118.30
2	1-I	473	ASP	CB-CG-OD2	6.37	124.03	118.30
2	2-I	473	ASP	CB-CG-OD2	6.37	124.03	118.30
2	1-J	320	ASP	CB-CG-OD2	6.36	124.02	118.30
2	2-J	320	ASP	CB-CG-OD2	6.36	124.02	118.30
2	1-J	325	ASP	CB-CG-OD2	6.33	123.99	118.30
2	2-J	325	ASP	CB-CG-OD2	6.33	123.99	118.30
2	1-H	363	ASP	CB-CG-OD2	6.32	123.99	118.30
2	2-H	363	ASP	CB-CG-OD2	6.32	123.99	118.30
2	1-K	279	ASP	CB-CG-OD2	6.31	123.97	118.30
2	2-K	279	ASP	CB-CG-OD2	6.31	123.97	118.30
2	1-K	328	ASP	CB-CG-OD2	6.30	123.97	118.30
2	2-K	328	ASP	CB-CG-OD2	6.30	123.97	118.30
2	1-M	279	ASP	CB-CG-OD2	6.28	123.95	118.30
2	2-M	279	ASP	CB-CG-OD2	6.28	123.95	118.30
2	1-M	405	ASP	CB-CG-OD2	6.24	123.92	118.30
2	2-M	405	ASP	CB-CG-OD2	6.24	123.92	118.30
2	1-M	320	ASP	CB-CG-OD2	6.19	123.87	118.30
2	2-M	320	ASP	CB-CG-OD2	6.19	123.87	118.30
2	1-H	491	ASP	CB-CG-OD2	6.16	123.84	118.30
2	2-H	491	ASP	CB-CG-OD2	6.16	123.84	118.30
2	1-N	114	ASP	CB-CG-OD2	6.15	123.83	118.30
2	1-K	41	ASP	CB-CG-OD2	6.13	123.82	118.30
2	2-K	41	ASP	CB-CG-OD2	6.13	123.82	118.30
2	1-J	165	ASP	CB-CG-OD2	6.13	123.81	118.30
2	2-J	165	ASP	CB-CG-OD2	6.13	123.81	118.30
1	1-B	68	ASP	CB-CG-OD2	6.12	123.80	118.30
1	2-B	68	ASP	CB-CG-OD2	6.12	123.80	118.30
2	1-J	363	ASP	CB-CG-OD2	6.11	123.80	118.30
2	2-J	363	ASP	CB-CG-OD2	6.11	123.80	118.30
2	1-N	335	ASP	CB-CG-OD2	6.10	123.79	118.30
2	1-H	137	ASP	CB-CG-OD2	6.05	123.75	118.30
2	2-H	137	ASP	CB-CG-OD2	6.05	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-N	279	ASP	CB-CG-OD2	6.05	123.75	118.30
2	1-N	279	ASP	CB-CG-OD2	6.04	123.73	118.30
2	1-N	269	ASP	CB-CG-OD2	6.03	123.72	118.30
2	1-N	366	ASP	CB-CG-OD2	6.03	123.72	118.30
1	2-G	82	ASP	CB-CG-OD2	6.01	123.71	118.30
1	1-D	43	ASP	CB-CG-OD2	5.98	123.68	118.30
1	2-D	43	ASP	CB-CG-OD2	5.98	123.68	118.30
2	1-M	299	ASP	CB-CG-OD2	5.96	123.66	118.30
2	2-M	299	ASP	CB-CG-OD2	5.96	123.66	118.30
2	1-J	299	ASP	CB-CG-OD2	5.94	123.64	118.30
2	2-J	299	ASP	CB-CG-OD2	5.94	123.64	118.30
2	1-J	89	ASP	CB-CG-OD2	5.93	123.64	118.30
2	2-J	89	ASP	CB-CG-OD2	5.93	123.64	118.30
1	1-A	203	ASP	CB-CG-OD2	5.93	123.64	118.30
1	2-A	203	ASP	CB-CG-OD2	5.93	123.64	118.30
2	1-H	298	ASP	CB-CG-OD2	5.90	123.61	118.30
2	2-H	298	ASP	CB-CG-OD2	5.90	123.61	118.30
2	1-I	325	ASP	CB-CG-OD2	5.90	123.61	118.30
2	2-I	325	ASP	CB-CG-OD2	5.90	123.61	118.30
2	1-N	137	ASP	CB-CG-OD2	5.88	123.59	118.30
2	1-K	325	ASP	CB-CG-OD2	5.85	123.57	118.30
2	2-K	325	ASP	CB-CG-OD2	5.85	123.57	118.30
1	2-G	255	ASP	CB-CG-OD2	5.83	123.55	118.30
2	2-N	269	ASP	CB-CG-OD2	5.82	123.54	118.30
1	1-F	185	ASP	CB-CG-OD2	5.82	123.54	118.30
1	2-F	185	ASP	CB-CG-OD2	5.82	123.54	118.30
1	1-G	170	ASP	CB-CG-OD2	5.82	123.54	118.30
1	2-G	170	ASP	CB-CG-OD2	5.79	123.51	118.30
2	2-N	114	ASP	CB-CG-OD2	5.78	123.50	118.30
1	1-D	38	ASP	CB-CG-OD2	5.78	123.50	118.30
1	2-D	38	ASP	CB-CG-OD2	5.78	123.50	118.30
1	1-G	82	ASP	CB-CG-OD2	5.77	123.49	118.30
2	2-N	335	ASP	CB-CG-OD2	5.75	123.48	118.30
2	1-N	320	ASP	CB-CG-OD2	5.75	123.47	118.30
2	1-M	356	ASP	CB-CG-OD2	5.74	123.46	118.30
2	2-M	356	ASP	CB-CG-OD2	5.74	123.46	118.30
2	1-K	298	ASP	CB-CG-OD2	5.72	123.45	118.30
2	2-K	298	ASP	CB-CG-OD2	5.72	123.45	118.30
2	1-N	448	ASP	CB-CG-OD2	5.71	123.44	118.30
2	1-N	325	ASP	CB-CG-OD2	5.69	123.42	118.30
2	1-N	364	ASP	CB-CG-OD2	5.67	123.40	118.30
2	1-M	473	ASP	CB-CG-OD2	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-M	473	ASP	CB-CG-OD2	5.66	123.39	118.30
2	2-N	473	ASP	CB-CG-OD2	5.66	123.39	118.30
1	2-G	38	ASP	CB-CG-OD2	5.65	123.38	118.30
2	1-I	137	ASP	CB-CG-OD2	5.64	123.38	118.30
2	2-I	137	ASP	CB-CG-OD2	5.64	123.38	118.30
1	1-F	43	ASP	CB-CG-OD2	5.64	123.37	118.30
1	2-F	43	ASP	CB-CG-OD2	5.64	123.37	118.30
2	1-H	364	ASP	CB-CG-OD2	5.63	123.37	118.30
1	1-B	168	ASP	CB-CG-OD2	5.63	123.37	118.30
2	2-H	364	ASP	CB-CG-OD2	5.63	123.37	118.30
1	2-B	168	ASP	CB-CG-OD2	5.63	123.37	118.30
2	2-N	352	ASP	CB-CG-OD2	5.63	123.36	118.30
1	1-D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
1	2-D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
2	2-N	63	ASP	CB-CG-OD2	5.62	123.36	118.30
2	1-N	129	ASP	CB-CG-OD2	5.61	123.35	118.30
2	1-J	114	ASP	CB-CG-OD2	5.59	123.33	118.30
2	2-J	114	ASP	CB-CG-OD2	5.59	123.33	118.30
2	2-N	405	ASP	CB-CG-OD2	5.54	123.28	118.30
2	1-N	346	ASP	CB-CG-OD2	5.51	123.26	118.30
2	1-H	405	ASP	CB-CG-OD2	5.51	123.26	118.30
2	2-H	405	ASP	CB-CG-OD2	5.51	123.26	118.30
2	1-J	41	ASP	CB-CG-OD2	5.50	123.25	118.30
2	2-J	41	ASP	CB-CG-OD2	5.50	123.25	118.30
2	1-N	89	ASP	CB-CG-OD2	5.49	123.24	118.30
2	2-N	165	ASP	CB-CG-OD2	5.47	123.23	118.30
2	1-K	363	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-K	363	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-N	325	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-N	137	ASP	CB-CG-OD2	5.45	123.20	118.30
1	2-G	33	ASP	CB-CG-OD2	5.45	123.20	118.30
2	1-I	346	ASP	CB-CG-OD2	5.45	123.20	118.30
2	2-I	346	ASP	CB-CG-OD2	5.45	123.20	118.30
2	2-N	320	ASP	CB-CG-OD2	5.44	123.19	118.30
2	1-J	491	ASP	CB-CG-OD2	5.44	123.19	118.30
2	2-J	491	ASP	CB-CG-OD2	5.44	123.19	118.30
2	1-H	448	ASP	CB-CG-OD2	5.43	123.19	118.30
2	2-H	448	ASP	CB-CG-OD2	5.43	123.19	118.30
2	1-H	299	ASP	CB-CG-OD2	5.41	123.17	118.30
2	1-M	335	ASP	CB-CG-OD2	5.41	123.17	118.30
2	2-H	299	ASP	CB-CG-OD2	5.41	123.17	118.30
2	2-M	335	ASP	CB-CG-OD2	5.41	123.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-G	185	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1-C	252	ASP	CB-CG-OD2	5.39	123.15	118.30
1	2-C	252	ASP	CB-CG-OD2	5.39	123.15	118.30
1	1-C	43	ASP	CB-CG-OD2	5.38	123.14	118.30
1	2-C	43	ASP	CB-CG-OD2	5.38	123.14	118.30
1	2-G	252	ASP	CB-CG-OD2	5.38	123.14	118.30
2	1-M	363	ASP	CB-CG-OD2	5.38	123.14	118.30
2	2-M	363	ASP	CB-CG-OD2	5.38	123.14	118.30
1	1-B	38	ASP	CB-CG-OD2	5.37	123.14	118.30
1	2-B	38	ASP	CB-CG-OD2	5.37	123.14	118.30
2	1-M	511	ASP	CB-CG-OD2	5.35	123.12	118.30
2	2-M	511	ASP	CB-CG-OD2	5.35	123.12	118.30
2	1-H	473	ASP	CB-CG-OD2	5.35	123.11	118.30
2	2-H	473	ASP	CB-CG-OD2	5.35	123.11	118.30
1	1-B	170	ASP	CB-CG-OD2	5.34	123.11	118.30
1	2-B	170	ASP	CB-CG-OD2	5.34	123.11	118.30
2	2-N	129	ASP	CB-CG-OD2	5.34	123.10	118.30
2	2-N	41	ASP	CB-CG-OD2	5.33	123.10	118.30
1	1-C	185	ASP	CB-CG-OD2	5.33	123.10	118.30
1	2-C	185	ASP	CB-CG-OD2	5.33	123.10	118.30
2	1-K	269	ASP	CB-CG-OD2	5.32	123.09	118.30
2	2-K	269	ASP	CB-CG-OD2	5.32	123.09	118.30
1	1-G	38	ASP	CB-CG-OD2	5.31	123.08	118.30
1	1-C	38	ASP	CB-CG-OD2	5.30	123.07	118.30
1	2-C	38	ASP	CB-CG-OD2	5.30	123.07	118.30
2	1-N	473	ASP	CB-CG-OD2	5.29	123.06	118.30
2	1-N	41	ASP	CB-CG-OD2	5.28	123.06	118.30
1	1-G	203	ASP	CB-CG-OD2	5.27	123.05	118.30
2	1-H	453	ASP	CB-CG-OD2	5.27	123.04	118.30
2	2-H	453	ASP	CB-CG-OD2	5.27	123.04	118.30
1	1-G	43	ASP	CB-CG-OD2	5.27	123.04	118.30
2	1-N	453	ASP	CB-CG-OD2	5.26	123.04	118.30
2	1-N	352	ASP	CB-CG-OD2	5.26	123.03	118.30
2	1-M	328	ASP	CB-CG-OD2	5.25	123.03	118.30
2	2-M	328	ASP	CB-CG-OD2	5.25	123.03	118.30
2	1-J	328	ASP	CB-CG-OD2	5.25	123.02	118.30
2	2-J	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	1-F	68	ASP	CB-CG-OD2	5.23	123.01	118.30
1	2-F	68	ASP	CB-CG-OD2	5.23	123.01	118.30
2	1-I	352	ASP	CB-CG-OD2	5.23	123.00	118.30
2	1-K	89	ASP	CB-CG-OD2	5.23	123.00	118.30
2	2-I	352	ASP	CB-CG-OD2	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-K	89	ASP	CB-CG-OD2	5.23	123.00	118.30
1	2-G	68	ASP	CB-CG-OD2	5.22	123.00	118.30
2	1-M	448	ASP	CB-CG-OD2	5.22	122.99	118.30
2	1-M	491	ASP	CB-CG-OD2	5.22	122.99	118.30
2	2-M	448	ASP	CB-CG-OD2	5.22	122.99	118.30
2	2-M	491	ASP	CB-CG-OD2	5.22	122.99	118.30
1	1-D	203	ASP	CB-CG-OD2	5.21	122.99	118.30
1	2-D	203	ASP	CB-CG-OD2	5.21	122.99	118.30
2	2-N	526	ASP	CB-CG-OD2	5.20	122.98	118.30
2	2-N	453	ASP	CB-CG-OD2	5.20	122.98	118.30
1	1-G	33	ASP	CB-CG-OD2	5.20	122.98	118.30
2	1-K	299	ASP	CB-CG-OD2	5.19	122.97	118.30
2	2-K	299	ASP	CB-CG-OD2	5.19	122.97	118.30
2	1-N	60	ASP	CB-CG-OD2	5.19	122.97	118.30
2	1-M	325	ASP	CB-CG-OD2	5.18	122.96	118.30
2	2-M	325	ASP	CB-CG-OD2	5.18	122.96	118.30
2	1-N	405	ASP	CB-CG-OD2	5.18	122.96	118.30
2	1-K	352	ASP	CB-CG-OD2	5.16	122.95	118.30
2	2-K	352	ASP	CB-CG-OD2	5.16	122.95	118.30
2	2-N	89	ASP	CB-CG-OD2	5.16	122.94	118.30
2	1-K	491	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-K	491	ASP	CB-CG-OD2	5.15	122.94	118.30
2	1-J	269	ASP	CB-CG-OD2	5.15	122.94	118.30
1	1-G	68	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-J	269	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-N	448	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-N	346	ASP	CB-CG-OD2	5.13	122.92	118.30
1	1-F	33	ASP	CB-CG-OD2	5.13	122.92	118.30
1	2-F	33	ASP	CB-CG-OD2	5.13	122.92	118.30
2	1-N	526	ASP	CB-CG-OD2	5.12	122.91	118.30
2	1-M	298	ASP	CB-CG-OD2	5.12	122.91	118.30
2	2-M	298	ASP	CB-CG-OD2	5.12	122.91	118.30
2	2-N	363	ASP	CB-CG-OD2	5.12	122.91	118.30
2	1-N	165	ASP	CB-CG-OD2	5.12	122.90	118.30
2	2-N	60	ASP	CB-CG-OD2	5.11	122.90	118.30
2	1-H	511	ASP	CB-CG-OD2	5.11	122.90	118.30
2	2-H	511	ASP	CB-CG-OD2	5.11	122.90	118.30
2	1-I	363	ASP	CB-CG-OD2	5.11	122.90	118.30
2	2-I	363	ASP	CB-CG-OD2	5.11	122.90	118.30
1	1-D	252	ASP	CB-CG-OD2	5.10	122.89	118.30
2	1-N	88	ASP	CB-CG-OD2	5.10	122.89	118.30
1	2-D	252	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-K	364	ASP	CB-CG-OD2	5.09	122.88	118.30
2	1-N	491	ASP	CB-CG-OD2	5.09	122.88	118.30
2	2-K	364	ASP	CB-CG-OD2	5.09	122.88	118.30
2	1-K	405	ASP	CB-CG-OD2	5.07	122.86	118.30
2	1-M	19	ASP	CB-CG-OD2	5.07	122.86	118.30
2	2-K	405	ASP	CB-CG-OD2	5.07	122.86	118.30
2	2-M	19	ASP	CB-CG-OD2	5.07	122.86	118.30
1	1-C	203	ASP	CB-CG-OD2	5.06	122.86	118.30
1	2-C	203	ASP	CB-CG-OD2	5.06	122.86	118.30
2	1-M	41	ASP	CB-CG-OD2	5.06	122.85	118.30
2	1-N	63	ASP	CB-CG-OD2	5.06	122.85	118.30
2	2-M	41	ASP	CB-CG-OD2	5.06	122.85	118.30
2	1-I	41	ASP	CB-CG-OD2	5.05	122.85	118.30
2	2-I	41	ASP	CB-CG-OD2	5.05	122.85	118.30
2	1-M	269	ASP	CB-CG-OD2	5.02	122.82	118.30
2	2-M	269	ASP	CB-CG-OD2	5.02	122.82	118.30
1	1-D	255	ASP	CB-CG-OD2	5.01	122.81	118.30
1	2-D	255	ASP	CB-CG-OD2	5.01	122.81	118.30
2	1-I	298	ASP	CB-CG-OD2	5.00	122.80	118.30
2	1-K	63	ASP	CB-CG-OD2	5.00	122.80	118.30
2	2-I	298	ASP	CB-CG-OD2	5.00	122.80	118.30
2	2-K	63	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1970	0	1910	30	1
1	1-B	1971	0	1914	22	0
1	1-C	1952	0	1891	14	0
1	1-D	1971	0	1914	26	0
1	1-F	1952	0	1891	25	0
1	1-G	1970	0	1910	62	0
1	2-A	1970	0	1910	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-B	1971	0	1914	21	0
1	2-C	1952	0	1891	14	0
1	2-D	1971	0	1914	26	0
1	2-F	1952	0	1891	28	0
1	2-G	1970	0	1910	67	0
2	1-H	4167	0	4140	52	0
2	1-I	4166	0	4139	45	0
2	1-J	4162	0	4139	57	0
2	1-K	4162	0	4139	52	0
2	1-M	4166	0	4139	57	0
2	1-N	4167	0	4140	60	1
2	2-H	4167	0	4140	52	0
2	2-I	4166	0	4139	45	0
2	2-J	4162	0	4139	57	0
2	2-K	4162	0	4139	52	0
2	2-M	4166	0	4139	57	0
2	2-N	4167	0	4140	80	0
3	1-A	16	0	0	0	0
3	1-B	16	0	0	0	0
3	1-C	16	0	0	0	0
3	1-D	16	0	0	0	0
3	1-F	16	0	0	0	0
3	1-G	16	0	0	0	0
3	2-A	16	0	0	0	0
3	2-B	16	0	0	0	0
3	2-C	16	0	0	0	0
3	2-D	16	0	0	0	0
3	2-F	16	0	0	0	0
3	2-G	16	0	0	1	0
4	1-A	7	0	0	0	0
4	1-B	7	0	0	0	0
4	1-C	7	0	0	0	0
4	1-D	7	0	0	0	0
4	1-F	7	0	0	0	0
4	1-G	7	0	0	0	0
4	2-A	7	0	0	0	0
4	2-B	7	0	0	0	0
4	2-C	7	0	0	0	0
4	2-D	7	0	0	0	0
4	2-F	7	0	0	0	0
4	2-G	7	0	0	0	0
5	1-H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-I	1	0	0	0	0
5	1-J	1	0	0	0	0
5	1-K	1	0	0	0	0
5	1-M	1	0	0	0	0
5	1-N	1	0	0	0	0
5	2-H	1	0	0	0	0
5	2-I	1	0	0	0	0
5	2-J	1	0	0	0	0
5	2-K	1	0	0	0	0
5	2-M	1	0	0	0	0
5	2-N	1	0	0	0	0
6	1-H	1	0	0	0	0
6	1-I	1	0	0	0	0
6	1-J	1	0	0	0	0
6	1-K	1	0	0	0	0
6	1-M	1	0	0	0	0
6	1-N	1	0	0	0	0
6	2-H	1	0	0	0	0
6	2-I	1	0	0	0	0
6	2-J	1	0	0	0	0
6	2-K	1	0	0	0	0
6	2-M	1	0	0	0	0
6	2-N	1	0	0	0	0
7	1-H	7	0	0	0	0
7	1-I	7	0	0	0	0
7	1-J	7	0	0	0	0
7	1-K	7	0	0	0	0
7	1-M	7	0	0	1	0
7	1-N	7	0	0	2	0
7	2-H	7	0	0	0	0
7	2-I	7	0	0	0	0
7	2-J	7	0	0	0	0
7	2-K	7	0	0	0	0
7	2-M	7	0	0	1	0
7	2-N	7	0	0	3	0
8	1-A	122	0	0	3	0
8	1-B	83	0	0	1	0
8	1-C	120	0	0	1	0
8	1-D	149	0	0	4	0
8	1-F	108	0	0	2	0
8	1-G	59	0	0	10	0
8	1-H	245	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1-I	218	0	0	3	0
8	1-J	208	0	0	3	0
8	1-K	253	0	0	6	0
8	1-M	183	0	0	2	0
8	1-N	138	0	0	1	0
8	2-A	122	0	0	3	0
8	2-B	84	0	0	1	0
8	2-C	120	0	0	1	0
8	2-D	148	0	0	4	0
8	2-F	109	0	0	2	0
8	2-G	58	0	0	8	0
8	2-H	245	0	0	2	0
8	2-I	218	0	0	3	0
8	2-J	208	0	0	3	0
8	2-K	253	0	0	6	0
8	2-M	183	0	0	2	0
8	2-N	124	0	0	2	0
All	All	77694	0	72532	977	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:342:ALA:HB1	2:N:343:PRO:CD	1.55	1.33
1:G:177:LEU:HD23	1:G:178:PHE:CE2	1.78	1.17
1:G:177:LEU:HD23	1:G:178:PHE:CZ	1.79	1.16
2:N:342:ALA:CB	2:N:343:PRO:HD2	1.79	1.12
2:N:43:TRP:CZ2	2:N:365:LYS:HE2	1.84	1.10
2:N:342:ALA:O	8:N:5596:HOH:O	1.77	1.02
2:J:448:ASP:O	2:J:452:LYS:HE3	1.62	0.99
2:J:448:ASP:O	2:J:452:LYS:HE3	1.62	0.99
2:N:342:ALA:CB	2:N:343:PRO:CD	2.37	0.99
2:N:342:ALA:HB1	2:N:343:PRO:HD2	1.02	0.99
2:N:497:VAL:HG11	2:N:546:CYS:SG	2.07	0.95
1:G:88:MET:CE	2:N:362:LEU:HD13	2.01	0.91
1:D:61:HIS:HE1	1:D:100:LYS:NZ	1.69	0.89
1:D:61:HIS:HE1	1:D:100:LYS:NZ	1.69	0.89
2:J:497:VAL:CG1	2:J:498:PRO:HD2	2.05	0.86
2:J:497:VAL:CG1	2:J:498:PRO:HD2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:497:VAL:CG1	2:I:498:PRO:HD2	2.06	0.85
2:I:497:VAL:CG1	2:I:498:PRO:HD2	2.06	0.85
1:F:135:GLU:HA	2:N:328:ASP:CG	1.97	0.85
1:G:135:GLU:OE1	8:G:5276:HOH:O	1.95	0.85
2:N:543:CYS:SG	2:N:546:CYS:HB2	2.18	0.83
2:J:448:ASP:O	2:J:452:LYS:CE	2.26	0.83
2:J:448:ASP:O	2:J:452:LYS:CE	2.26	0.83
1:G:177:LEU:CD2	1:G:178:PHE:CZ	2.62	0.82
2:J:497:VAL:HG13	2:J:498:PRO:HD2	1.60	0.82
1:G:135:GLU:OE1	8:G:5276:HOH:O	1.97	0.82
2:J:497:VAL:HG13	2:J:498:PRO:HD2	1.60	0.82
2:J:178:ILE:HG23	8:J:695:HOH:O	1.80	0.82
2:J:178:ILE:HG23	8:J:2690:HOH:O	1.80	0.82
2:H:406:MET:HE3	2:H:410:LYS:HG3	1.62	0.81
2:H:406:MET:HE3	2:H:410:LYS:HG3	1.62	0.81
2:N:342:ALA:HB1	2:N:343:PRO:HD3	1.60	0.80
2:K:497:VAL:CG1	2:K:498:PRO:HD2	2.12	0.79
2:K:497:VAL:CG1	2:K:498:PRO:HD2	2.12	0.79
1:G:88:MET:HE2	2:N:362:LEU:HD13	1.63	0.79
1:D:140:LYS:HE3	8:D:3422:HOH:O	1.83	0.79
1:D:140:LYS:HE3	8:D:3422:HOH:O	1.83	0.79
1:G:115:SER:O	1:G:133:VAL:HG23	1.82	0.78
2:N:497:VAL:CG1	2:N:498:PRO:HD2	2.13	0.78
2:I:5:LYS:N	2:I:6:PRO:HD2	2.00	0.77
2:I:5:LYS:N	2:I:6:PRO:HD2	2.00	0.77
2:N:43:TRP:CZ2	2:N:365:LYS:CE	2.66	0.76
1:G:115:SER:O	1:G:133:VAL:HG23	1.86	0.76
2:N:497:VAL:CG1	2:N:498:PRO:HD2	2.15	0.76
1:G:136:ALA:O	8:G:5287:HOH:O	2.03	0.76
1:F:14:ASN:ND2	1:F:94:MET:HB3	2.01	0.76
1:F:14:ASN:ND2	1:F:94:MET:HB3	2.01	0.76
2:J:333:TYR:OH	2:J:378:GLY:HA2	1.87	0.75
2:J:333:TYR:OH	2:J:378:GLY:HA2	1.87	0.75
1:G:177:LEU:CD2	1:G:178:PHE:CE2	2.66	0.75
1:G:217:GLY:O	1:G:219:LYS:HD3	1.87	0.74
2:J:267:ILE:HB	2:J:268:PRO:HD3	1.70	0.73
2:J:267:ILE:HB	2:J:268:PRO:HD3	1.70	0.73
2:N:25:GLU:OE1	2:N:543:CYS:SG	2.46	0.73
2:I:497:VAL:HG13	2:I:498:PRO:HD2	1.69	0.73
2:I:497:VAL:HG13	2:I:498:PRO:HD2	1.69	0.73
2:M:497:VAL:CG1	2:M:498:PRO:HD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:VAL:CG1	2:M:498:PRO:HD2	2.18	0.73
2:J:353:GLY:HA3	2:J:494:GLN:HG3	1.71	0.73
2:J:353:GLY:HA3	2:J:494:GLN:HG3	1.71	0.73
2:J:134:LEU:HD22	2:J:168:LYS:HG3	1.71	0.72
2:J:134:LEU:HD22	2:J:168:LYS:HG3	1.71	0.72
2:N:497:VAL:HG13	2:N:498:PRO:HD2	1.69	0.72
1:A:223:THR:HG21	1:A:247:GLY:HA2	1.71	0.72
1:A:223:THR:HG21	1:A:247:GLY:HA2	1.71	0.72
1:F:135:GLU:OE1	8:F:4279:HOH:O	2.06	0.71
1:F:135:GLU:OE1	8:F:4279:HOH:O	2.06	0.71
1:D:61:HIS:HE1	1:D:100:LYS:HZ2	1.37	0.71
1:D:61:HIS:HE1	1:D:100:LYS:HZ2	1.37	0.71
2:K:497:VAL:HG12	2:K:498:PRO:HD2	1.72	0.70
2:K:497:VAL:HG12	2:K:498:PRO:HD2	1.72	0.70
2:N:497:VAL:HG13	2:N:498:PRO:HD2	1.71	0.70
1:F:135:GLU:HG2	2:N:328:ASP:HB2	1.72	0.70
1:G:236:ASN:OD1	1:G:240:GLN:HB3	1.91	0.69
2:N:364:ASP:OD2	2:N:366:ASP:N	2.26	0.69
1:G:128:SER:OG	8:G:5272:HOH:O	2.11	0.68
2:M:19:ASP:OD2	2:M:29:ARG:HD2	1.93	0.68
2:M:19:ASP:OD2	2:M:29:ARG:HD2	1.93	0.68
1:G:136:ALA:O	8:G:5287:HOH:O	2.11	0.68
1:G:145:PRO:HG3	1:G:174:ARG:CD	2.24	0.68
2:H:406:MET:CE	2:H:410:LYS:HG3	2.23	0.68
2:H:406:MET:CE	2:H:410:LYS:HG3	2.23	0.68
1:D:61:HIS:HE1	1:D:100:LYS:HZ1	1.40	0.68
1:D:61:HIS:HE1	1:D:100:LYS:HZ1	1.40	0.68
2:K:144:LEU:HD23	2:K:144:LEU:O	1.94	0.67
2:K:144:LEU:HD23	2:K:144:LEU:O	1.94	0.67
2:N:72:CYS:HB3	2:N:75:CYS:SG	2.35	0.67
2:N:271:LEU:HD13	2:N:410:LYS:HD3	1.77	0.67
1:D:61:HIS:CE1	1:D:100:LYS:NZ	2.59	0.67
1:D:61:HIS:CE1	1:D:100:LYS:NZ	2.59	0.67
2:H:497:VAL:CG1	2:H:498:PRO:HD2	2.24	0.66
2:H:497:VAL:CG1	2:H:498:PRO:HD2	2.24	0.66
2:M:497:VAL:HG12	2:M:498:PRO:HD2	1.78	0.66
2:M:497:VAL:HG12	2:M:498:PRO:HD2	1.78	0.66
2:I:497:VAL:HG12	2:I:498:PRO:HD2	1.78	0.65
2:I:497:VAL:HG12	2:I:498:PRO:HD2	1.78	0.65
2:I:5:LYS:N	2:I:6:PRO:CD	2.59	0.65
2:I:5:LYS:N	2:I:6:PRO:CD	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:PRO:HG3	1:G:174:ARG:CD	2.25	0.65
2:N:497:VAL:CG1	2:N:546:CYS:SG	2.83	0.65
2:H:223:GLY:HA2	2:H:231:PHE:CD2	2.32	0.64
2:H:223:GLY:HA2	2:H:231:PHE:CD2	2.32	0.64
8:I:655:HOH:O	2:K:410:LYS:HE3	1.97	0.64
1:G:13:HIS:ND1	8:G:5316:HOH:O	2.30	0.64
1:G:237:TRP:CZ2	1:G:239:VAL:HB	2.33	0.64
8:I:1650:HOH:O	2:K:410:LYS:HE3	1.97	0.64
2:N:72:CYS:SG	2:N:75:CYS:SG	2.96	0.63
1:G:214:TYR:CE2	1:G:263:GLN:NE2	2.67	0.63
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.33	0.62
2:J:127:TRP:CZ2	2:J:535:ARG:HG2	2.34	0.62
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.33	0.62
2:J:127:TRP:CZ2	2:J:535:ARG:HG2	2.34	0.62
2:M:530:PRO:HB2	2:M:533:ILE:HD12	1.81	0.62
2:M:530:PRO:HB2	2:M:533:ILE:HD12	1.81	0.62
2:K:395:LYS:HE3	8:K:797:HOH:O	2.00	0.62
2:K:395:LYS:HE3	8:K:3787:HOH:O	2.00	0.62
2:N:364:ASP:OD2	2:N:364:ASP:C	2.38	0.62
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.82	0.61
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.82	0.61
2:M:411:LEU:O	2:M:413:VAL:HG13	1.99	0.61
2:M:411:LEU:O	2:M:413:VAL:HG13	1.99	0.61
1:F:157:ALA:O	1:F:161:VAL:HG23	2.00	0.61
1:G:258:THR:HA	1:G:259:PRO:C	2.19	0.61
1:F:157:ALA:O	1:F:161:VAL:HG23	2.00	0.61
2:J:497:VAL:HG12	2:J:498:PRO:HD2	1.83	0.61
2:J:497:VAL:HG12	2:J:498:PRO:HD2	1.83	0.61
2:M:511:ASP:HA	8:M:731:HOH:O	1.99	0.61
1:G:205:GLU:O	1:G:209:LYS:HG3	2.00	0.61
2:M:511:ASP:HA	8:M:4721:HOH:O	1.99	0.61
2:K:270:LEU:HD11	2:K:425:THR:HG22	1.83	0.61
2:K:497:VAL:HG13	2:K:498:PRO:HD2	1.83	0.61
1:G:220:GLY:N	1:G:221:PRO:CD	2.64	0.61
2:K:270:LEU:HD11	2:K:425:THR:HG22	1.83	0.61
2:K:497:VAL:HG13	2:K:498:PRO:HD2	1.83	0.61
2:H:393:TYR:CE1	2:H:401:LYS:HD3	2.36	0.61
2:H:393:TYR:CE1	2:H:401:LYS:HD3	2.36	0.61
2:H:454:ASN:H	2:H:454:ASN:HD22	1.49	0.60
2:H:454:ASN:H	2:H:454:ASN:HD22	1.49	0.60
2:H:127:TRP:CZ3	2:H:535:ARG:HD3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:278:LYS:NZ	2:N:278:LYS:HB3	2.16	0.60
2:H:127:TRP:CZ3	2:H:535:ARG:HD3	2.36	0.60
1:G:258:THR:HA	1:G:259:PRO:C	2.21	0.60
1:G:220:GLY:N	1:G:221:PRO:CD	2.63	0.60
1:D:61:HIS:CE1	1:D:100:LYS:HZ2	2.19	0.60
1:D:61:HIS:CE1	1:D:100:LYS:HZ2	2.19	0.60
2:I:474:ALA:HB1	2:I:475:PRO:HD2	1.84	0.60
2:I:474:ALA:HB1	2:I:475:PRO:HD2	1.84	0.60
1:G:18:THR:O	1:G:18:THR:HG22	2.02	0.60
1:F:138:GLY:HA2	2:N:330:GLY:N	2.16	0.60
2:H:97:ALA:O	2:H:101:MET:HG3	2.02	0.59
2:H:97:ALA:O	2:H:101:MET:HG3	2.02	0.59
1:G:128:SER:OG	8:G:5272:HOH:O	2.17	0.59
1:G:18:THR:O	1:G:18:THR:HG22	2.02	0.59
1:G:13:HIS:ND1	8:G:5316:HOH:O	2.31	0.59
1:G:227:CYS:N	1:G:228:PRO:HD2	2.18	0.59
2:K:386:LEU:HD11	2:K:390:PHE:CE1	2.37	0.59
2:M:69:GLN:OE1	2:M:228:HIS:HA	2.03	0.59
2:K:386:LEU:HD11	2:K:390:PHE:CE1	2.37	0.59
2:M:69:GLN:OE1	2:M:228:HIS:HA	2.03	0.59
2:M:386:LEU:HD11	2:M:390:PHE:CE1	2.37	0.59
2:M:386:LEU:HD11	2:M:390:PHE:CE1	2.37	0.59
2:I:304:LYS:O	2:I:308:THR:HG23	2.02	0.59
2:I:304:LYS:O	2:I:308:THR:HG23	2.02	0.59
2:N:72:CYS:CB	2:N:75:CYS:SG	2.91	0.59
2:N:101:MET:HB2	2:N:446:MET:HG3	1.84	0.58
2:I:246:ASP:HB2	2:I:247:PRO:HD3	1.86	0.58
1:F:135:GLU:OE2	2:N:326:ASN:ND2	2.37	0.58
2:I:246:ASP:HB2	2:I:247:PRO:HD3	1.86	0.58
1:G:157:ALA:O	1:G:161:VAL:HG23	2.03	0.58
1:A:254:TRP:HH2	2:H:70:ARG:HD3	1.68	0.58
2:H:149:ALA:HB1	2:H:150:PRO:CD	2.34	0.58
2:N:403:VAL:O	2:N:407:VAL:HG23	2.03	0.58
1:A:254:TRP:HH2	2:H:70:ARG:HD3	1.68	0.58
2:H:149:ALA:HB1	2:H:150:PRO:CD	2.34	0.58
1:A:135:GLU:OE1	8:A:279:HOH:O	2.17	0.58
2:J:296:ALA:HA	2:J:309:SER:HA	1.85	0.58
2:M:140:LYS:HG2	2:M:196:GLU:HG2	1.85	0.58
2:M:296:ALA:HA	2:M:309:SER:HA	1.84	0.58
1:A:135:GLU:OE1	8:A:279:HOH:O	2.17	0.58
2:J:296:ALA:HA	2:J:309:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:140:LYS:HG2	2:M:196:GLU:HG2	1.85	0.58
2:M:296:ALA:HA	2:M:309:SER:HA	1.84	0.58
1:G:230:VAL:O	1:G:231:LEU:HB2	2.04	0.58
2:I:275:GLY:O	2:I:278:LYS:HG3	2.03	0.58
2:I:275:GLY:O	2:I:278:LYS:HG3	2.03	0.58
2:K:274:ALA:CB	2:K:422:LEU:HD11	2.34	0.58
2:K:274:ALA:HB1	2:K:422:LEU:HD11	1.86	0.58
1:G:17:CYS:HB2	2:N:73:GLY:N	2.19	0.58
2:K:274:ALA:CB	2:K:422:LEU:HD11	2.34	0.58
2:K:274:ALA:HB1	2:K:422:LEU:HD11	1.86	0.58
1:F:135:GLU:HA	2:N:328:ASP:OD2	2.04	0.58
2:I:29:ARG:HB3	2:I:45:SER:HB3	1.85	0.57
2:I:29:ARG:HB3	2:I:45:SER:HB3	1.85	0.57
1:D:61:HIS:CE1	1:D:100:LYS:HZ1	2.20	0.57
1:G:157:ALA:O	1:G:161:VAL:HG23	2.03	0.57
1:D:61:HIS:CE1	1:D:100:LYS:HZ1	2.20	0.57
2:H:336:VAL:HG12	2:H:372:LYS:HG2	1.86	0.57
2:J:451:ALA:HB3	2:J:452:LYS:HE2	1.85	0.57
2:H:336:VAL:HG12	2:H:372:LYS:HG2	1.86	0.57
2:J:451:ALA:HB3	2:J:452:LYS:HE2	1.85	0.57
2:H:140:LYS:NZ	2:J:464:GLU:OE1	2.38	0.57
2:M:474:ALA:HB1	2:M:475:PRO:HD2	1.87	0.57
2:H:140:LYS:NZ	2:J:464:GLU:OE1	2.38	0.57
2:M:474:ALA:HB1	2:M:475:PRO:HD2	1.87	0.57
1:G:88:MET:CE	2:N:362:LEU:CD1	2.78	0.57
2:I:530:PRO:HB2	2:I:533:ILE:HD12	1.85	0.57
2:I:530:PRO:HB2	2:I:533:ILE:HD12	1.85	0.57
2:N:246:ASP:HB2	2:N:247:PRO:HD3	1.87	0.57
1:A:223:THR:CG2	1:A:247:GLY:HA2	2.35	0.57
2:H:144:LEU:C	2:H:144:LEU:HD23	2.25	0.57
1:A:223:THR:CG2	1:A:247:GLY:HA2	2.35	0.57
2:H:144:LEU:C	2:H:144:LEU:HD23	2.25	0.57
1:G:139:VAL:HG11	8:G:5293:HOH:O	2.03	0.57
2:H:246:ASP:HB2	2:H:247:PRO:HD3	1.86	0.57
2:H:246:ASP:HB2	2:H:247:PRO:HD3	1.86	0.57
1:G:225:ASN:HD22	1:G:249:SER:HB3	1.70	0.57
1:G:227:CYS:N	1:G:228:PRO:HD2	2.19	0.57
1:B:4:LYS:O	1:B:4:LYS:HD3	2.05	0.56
1:B:140:LYS:NZ	2:N:151:ALA:HB2	2.20	0.56
1:G:237:TRP:CD1	1:G:240:GLN:HB2	2.40	0.56
1:B:4:LYS:O	1:B:4:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:454:ASN:HD22	2:N:454:ASN:H	1.53	0.56
2:M:134:LEU:HD22	2:M:168:LYS:HG3	1.88	0.56
2:M:349:HIS:ND1	2:M:350:PRO:HD2	2.21	0.56
2:N:246:ASP:HB2	2:N:247:PRO:HD3	1.87	0.56
2:M:134:LEU:HD22	2:M:168:LYS:HG3	1.88	0.56
2:M:349:HIS:ND1	2:M:350:PRO:HD2	2.21	0.56
2:J:462:MET:O	2:J:488:LYS:HE3	2.05	0.56
2:J:462:MET:O	2:J:488:LYS:HE3	2.05	0.56
1:G:223:THR:HG21	1:G:247:GLY:HA2	1.85	0.56
2:H:149:ALA:HB1	2:H:150:PRO:HD2	1.86	0.56
2:K:246:ASP:HB2	2:K:247:PRO:HD3	1.87	0.56
2:M:497:VAL:HG13	2:M:498:PRO:HD2	1.86	0.56
2:H:149:ALA:HB1	2:H:150:PRO:HD2	1.86	0.56
2:K:246:ASP:HB2	2:K:247:PRO:HD3	1.87	0.56
2:M:497:VAL:HG13	2:M:498:PRO:HD2	1.86	0.56
2:K:166:LYS:HE3	8:K:751:HOH:O	2.05	0.56
2:K:166:LYS:HE3	8:K:3741:HOH:O	2.05	0.56
1:F:47:THR:O	2:M:23:ARG:HA	2.05	0.55
1:F:47:THR:O	2:M:23:ARG:HA	2.05	0.55
2:J:144:LEU:O	2:J:148:ILE:HG12	2.05	0.55
2:N:72:CYS:HB3	2:N:75:CYS:SG	2.46	0.55
2:J:144:LEU:O	2:J:148:ILE:HG12	2.05	0.55
2:I:267:ILE:N	2:I:267:ILE:HD13	2.22	0.55
1:G:17:CYS:HB2	2:N:72:CYS:HA	1.88	0.55
2:I:267:ILE:N	2:I:267:ILE:HD13	2.22	0.55
1:G:117:TYR:HE2	1:G:145:PRO:HB3	1.71	0.55
2:I:474:ALA:HB1	2:I:475:PRO:CD	2.37	0.55
2:M:401:LYS:NZ	2:M:405:ASP:OD2	2.40	0.55
2:I:474:ALA:HB1	2:I:475:PRO:CD	2.37	0.55
2:M:401:LYS:NZ	2:M:405:ASP:OD2	2.40	0.55
2:N:264:GLU:O	2:N:268:PRO:HG2	2.07	0.55
2:I:265:CYS:C	2:I:268:PRO:HD2	2.27	0.55
1:D:145:PRO:HD2	1:D:179:TYR:CZ	2.40	0.55
2:I:265:CYS:C	2:I:268:PRO:HD2	2.27	0.55
1:D:145:PRO:HD2	1:D:179:TYR:CZ	2.40	0.55
2:H:497:VAL:HG13	2:H:498:PRO:HD2	1.87	0.55
2:H:497:VAL:HG13	2:H:498:PRO:HD2	1.87	0.55
1:G:17:CYS:HB2	2:N:73:GLY:N	2.22	0.55
2:M:380:ALA:HB1	2:M:514:PRO:HD3	1.87	0.55
2:M:380:ALA:HB1	2:M:514:PRO:HD3	1.87	0.55
2:N:474:ALA:HB1	2:N:475:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:TYR:HE2	1:G:145:PRO:HB3	1.72	0.55
2:M:349:HIS:CE1	2:M:350:PRO:HD2	2.43	0.54
2:M:349:HIS:CE1	2:M:350:PRO:HD2	2.43	0.54
1:G:254:TRP:HH2	2:N:70:ARG:HD3	1.71	0.54
1:G:189:ARG:HD3	1:G:210:GLY:O	2.06	0.54
2:J:77:TYR:CD2	2:J:106:VAL:HG12	2.43	0.54
1:F:18:THR:OG1	2:M:25:GLU:HG2	2.07	0.54
2:J:77:TYR:CD2	2:J:106:VAL:HG12	2.43	0.54
1:F:18:THR:OG1	2:M:25:GLU:HG2	2.07	0.54
2:N:338:TYR:HA	2:N:366:ASP:O	2.08	0.54
2:N:474:ALA:HB1	2:N:475:PRO:HD2	1.88	0.54
2:I:8:PRO:HB2	2:I:525:ALA:HB2	1.89	0.54
2:J:353:GLY:HA3	2:J:494:GLN:CG	2.38	0.54
2:I:8:PRO:HB2	2:I:525:ALA:HB2	1.89	0.54
2:J:353:GLY:HA3	2:J:494:GLN:CG	2.38	0.54
1:A:258:THR:HA	1:A:259:PRO:C	2.29	0.54
1:A:258:THR:HA	1:A:259:PRO:C	2.29	0.54
2:N:239:ASN:OD1	8:N:590:HOH:O	2.18	0.53
1:G:190:LEU:N	1:G:191:PRO:CD	2.71	0.53
1:C:47:THR:O	2:J:23:ARG:HA	2.08	0.53
2:K:267:ILE:HB	2:K:268:PRO:HD3	1.89	0.53
1:C:47:THR:O	2:J:23:ARG:HA	2.08	0.53
2:K:267:ILE:HB	2:K:268:PRO:HD3	1.89	0.53
2:K:329:LEU:HD11	2:K:471:LEU:HD11	1.91	0.53
1:G:14:ASN:ND2	1:G:94:MET:HB3	2.23	0.53
2:K:329:LEU:HD11	2:K:471:LEU:HD11	1.91	0.53
1:B:118:GLY:HA3	1:B:122:LYS:HD3	1.90	0.53
1:G:17:CYS:HB2	2:N:73:GLY:H	1.73	0.53
1:B:118:GLY:HA3	1:B:122:LYS:HD3	1.90	0.53
2:K:144:LEU:C	2:K:144:LEU:CD2	2.77	0.53
2:K:144:LEU:C	2:K:144:LEU:CD2	2.77	0.53
1:B:208:LYS:HG2	2:I:240:TYR:CE1	2.44	0.53
1:B:208:LYS:HG2	2:I:240:TYR:CE1	2.44	0.53
2:N:448:ASP:O	2:N:452:LYS:HG3	2.08	0.53
1:B:258:THR:HA	1:B:259:PRO:C	2.29	0.53
2:I:541:ASP:N	2:I:542:PRO:HD3	2.23	0.53
2:M:267:ILE:HB	2:M:268:PRO:HD3	1.91	0.53
2:M:372:LYS:NZ	8:M:606:HOH:O	2.31	0.53
2:M:403:VAL:HG12	2:M:430:ILE:HG23	1.90	0.53
1:B:258:THR:HA	1:B:259:PRO:C	2.29	0.53
2:I:541:ASP:N	2:I:542:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:267:ILE:HB	2:M:268:PRO:HD3	1.91	0.53
2:M:372:LYS:NZ	8:M:4592:HOH:O	2.31	0.53
2:M:403:VAL:HG12	2:M:430:ILE:HG23	1.90	0.53
1:A:66:GLY:O	8:A:287:HOH:O	2.18	0.53
1:G:243:HIS:CG	1:G:244:PRO:HD2	2.44	0.53
1:A:66:GLY:O	8:A:287:HOH:O	2.18	0.53
1:G:91:GLY:HA2	2:N:362:LEU:HD21	1.90	0.53
2:M:348:LYS:HG3	2:M:354:VAL:HG23	1.90	0.52
2:M:348:LYS:HG3	2:M:354:VAL:HG23	1.90	0.52
2:I:223:GLY:HA2	2:I:231:PHE:CD2	2.45	0.52
1:D:78:LEU:O	1:D:130:ALA:HA	2.10	0.52
2:I:223:GLY:HA2	2:I:231:PHE:CD2	2.45	0.52
1:D:78:LEU:O	1:D:130:ALA:HA	2.10	0.52
2:H:144:LEU:HD23	2:H:144:LEU:O	2.10	0.52
2:H:144:LEU:HD23	2:H:144:LEU:O	2.10	0.52
1:G:42:LEU:HD21	1:G:45:GLN:HG3	1.91	0.52
1:D:159:VAL:O	1:D:163:THR:HG23	2.09	0.52
1:D:258:THR:HA	1:D:259:PRO:C	2.30	0.52
1:G:226:ASN:O	1:G:230:VAL:HG22	2.09	0.52
1:D:159:VAL:O	1:D:163:THR:HG23	2.09	0.52
1:D:258:THR:HA	1:D:259:PRO:C	2.30	0.52
1:B:220:GLY:N	1:B:221:PRO:CD	2.73	0.52
1:C:258:THR:HA	1:C:259:PRO:C	2.30	0.52
1:B:220:GLY:N	1:B:221:PRO:CD	2.73	0.52
1:C:258:THR:HA	1:C:259:PRO:C	2.30	0.52
2:H:146:ALA:HB2	8:H:716:HOH:O	2.08	0.52
2:H:497:VAL:HG12	2:H:498:PRO:HD2	1.92	0.52
2:H:146:ALA:HB2	8:H:718:HOH:O	2.08	0.52
2:H:497:VAL:HG12	2:H:498:PRO:HD2	1.92	0.52
2:I:254:LEU:O	2:I:257:GLU:HB3	2.09	0.52
2:I:254:LEU:O	2:I:257:GLU:HB3	2.09	0.52
1:G:114:CYS:HA	1:G:119:GLY:HA3	1.91	0.51
2:K:8:PRO:HB2	2:K:525:ALA:HB2	1.93	0.51
2:N:267:ILE:HB	2:N:268:PRO:HD3	1.93	0.51
2:N:454:ASN:HD22	2:N:454:ASN:H	1.58	0.51
2:K:8:PRO:HB2	2:K:525:ALA:HB2	1.93	0.51
1:G:114:CYS:HA	1:G:119:GLY:HA3	1.91	0.51
2:M:513:SER:HB2	2:M:514:PRO:HD2	1.93	0.51
2:M:513:SER:HB2	2:M:514:PRO:HD2	1.93	0.51
1:G:139:VAL:HG11	8:G:5293:HOH:O	2.10	0.51
1:F:135:GLU:CG	2:N:328:ASP:HB2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:ASN:OD1	1:G:240:GLN:HB3	2.11	0.51
2:J:390:PHE:CZ	2:J:419:HIS:CE1	2.99	0.51
2:J:390:PHE:CZ	2:J:419:HIS:CE1	2.99	0.51
1:A:217:GLY:O	1:A:219:LYS:HD3	2.11	0.51
1:A:233:ASN:HB3	2:H:217:SER:HA	1.92	0.51
2:N:101:MET:CB	2:N:446:MET:HG3	2.40	0.51
1:A:217:GLY:O	1:A:219:LYS:HD3	2.11	0.51
1:A:233:ASN:HB3	2:H:217:SER:HA	1.92	0.51
1:C:63:ALA:O	8:C:2311:HOH:O	2.19	0.51
2:M:76:THR:O	2:M:77:TYR:HB3	2.11	0.51
2:N:498:PRO:HG2	7:N:550:FCO:N1	2.25	0.51
1:C:63:ALA:O	8:C:2311:HOH:O	2.19	0.51
2:M:76:THR:O	2:M:77:TYR:HB3	2.11	0.51
1:G:145:PRO:HG3	1:G:174:ARG:HD3	1.91	0.51
2:N:513:SER:HB2	2:N:514:PRO:HD2	1.93	0.51
2:J:336:VAL:HG12	2:J:372:LYS:HG2	1.93	0.51
1:G:17:CYS:O	1:G:18:THR:HB	2.11	0.51
2:J:336:VAL:HG12	2:J:372:LYS:HG2	1.93	0.51
2:H:196:GLU:OE1	2:H:196:GLU:N	2.43	0.50
2:M:349:HIS:CG	2:M:350:PRO:HD2	2.46	0.50
2:H:196:GLU:OE1	2:H:196:GLU:N	2.43	0.50
2:M:349:HIS:CG	2:M:350:PRO:HD2	2.46	0.50
2:N:498:PRO:HG2	7:N:550:FCO:N1	2.25	0.50
2:K:350:PRO:HB2	2:K:482:TRP:CG	2.46	0.50
1:F:145:PRO:HG3	1:F:174:ARG:HD3	1.93	0.50
2:K:350:PRO:HB2	2:K:482:TRP:CG	2.46	0.50
1:F:145:PRO:HG3	1:F:174:ARG:HD3	1.93	0.50
1:G:205:GLU:O	1:G:209:LYS:HG3	2.12	0.50
1:F:62:GLN:NE2	8:F:4356:HOH:O	2.39	0.50
2:M:150:PRO:HG2	2:M:264:GLU:HG2	1.92	0.50
2:N:338:TYR:HA	2:N:366:ASP:O	2.11	0.50
1:F:62:GLN:NE2	8:F:4356:HOH:O	2.39	0.50
2:M:150:PRO:HG2	2:M:264:GLU:HG2	1.92	0.50
2:J:77:TYR:CE2	2:J:106:VAL:HG12	2.46	0.50
2:J:77:TYR:CE2	2:J:106:VAL:HG12	2.46	0.50
1:A:145:PRO:HG3	1:A:174:ARG:HD3	1.92	0.50
1:G:233:ASN:HA	8:G:5270:HOH:O	2.12	0.50
1:A:145:PRO:HG3	1:A:174:ARG:HD3	1.92	0.50
2:N:513:SER:HB2	2:N:514:PRO:HD2	1.94	0.50
2:H:406:MET:HE3	2:H:410:LYS:CG	2.37	0.50
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TRP:CH2	1:D:239:VAL:HB	2.47	0.50
2:H:406:MET:HE3	2:H:410:LYS:CG	2.37	0.50
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.46	0.50
1:D:237:TRP:CH2	1:D:239:VAL:HB	2.47	0.50
1:G:17:CYS:HB2	2:N:72:CYS:HA	1.94	0.50
1:D:230:VAL:O	1:D:231:LEU:HB2	2.12	0.50
1:G:146:GLY:O	1:G:149:PRO:HD3	2.12	0.50
1:D:230:VAL:O	1:D:231:LEU:HB2	2.12	0.50
1:G:17:CYS:O	1:G:18:THR:HB	2.11	0.50
2:N:267:ILE:HB	2:N:268:PRO:HD3	1.93	0.50
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.94	0.49
2:K:474:ALA:HB1	2:K:475:PRO:HD2	1.94	0.49
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.94	0.49
2:K:474:ALA:HB1	2:K:475:PRO:HD2	1.94	0.49
1:G:158:VAL:O	1:G:162:LEU:HG	2.12	0.49
1:B:71:TYR:CE1	1:B:106:LYS:HD2	2.47	0.49
8:I:655:HOH:O	2:K:410:LYS:CE	2.57	0.49
2:K:144:LEU:HD23	2:K:144:LEU:C	2.31	0.49
1:G:190:LEU:N	1:G:191:PRO:CD	2.74	0.49
1:B:71:TYR:CE1	1:B:106:LYS:HD2	2.47	0.49
8:I:1650:HOH:O	2:K:410:LYS:CE	2.57	0.49
2:K:144:LEU:HD23	2:K:144:LEU:C	2.31	0.49
2:N:498:PRO:HG2	7:N:550:FCO:C1	2.42	0.49
1:C:201:SER:HA	1:C:216:LEU:HD21	1.94	0.49
1:G:47:THR:O	2:N:23:ARG:HA	2.13	0.49
1:C:201:SER:HA	1:C:216:LEU:HD21	1.94	0.49
1:B:208:LYS:HG2	2:I:240:TYR:CZ	2.47	0.49
1:G:42:LEU:HD21	1:G:45:GLN:HG3	1.94	0.49
2:N:264:GLU:O	2:N:268:PRO:HG2	2.11	0.49
1:B:208:LYS:HG2	2:I:240:TYR:CZ	2.47	0.49
1:G:102:ALA:HB1	1:G:108:ILE:HD11	1.95	0.49
2:J:497:VAL:CG1	2:J:498:PRO:CD	2.86	0.49
2:K:237:CYS:HB2	2:K:456:LEU:HG	1.93	0.49
2:N:278:LYS:HB3	2:N:278:LYS:HZ2	1.78	0.49
2:N:288:ASN:HB3	2:N:381:MET:CE	2.43	0.49
2:N:296:ALA:HA	2:N:309:SER:HA	1.94	0.49
2:J:497:VAL:CG1	2:J:498:PRO:CD	2.86	0.49
2:K:237:CYS:HB2	2:K:456:LEU:HG	1.93	0.49
2:J:474:ALA:HB1	2:J:475:PRO:HD2	1.94	0.49
2:J:513:SER:HB2	2:J:514:PRO:HD2	1.94	0.49
2:J:474:ALA:HB1	2:J:475:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:513:SER:HB2	2:J:514:PRO:HD2	1.94	0.49
2:I:512:LYS:HE2	2:I:520:ILE:HD11	1.95	0.49
2:N:83:SER:O	2:N:86:CYS:HB3	2.13	0.49
2:I:512:LYS:HE2	2:I:520:ILE:HD11	1.95	0.49
2:K:301:SER:HB2	2:K:302:PRO:HD2	1.95	0.49
1:F:114:CYS:HA	1:F:119:GLY:HA3	1.94	0.49
2:K:301:SER:HB2	2:K:302:PRO:HD2	1.95	0.49
1:F:114:CYS:HA	1:F:119:GLY:HA3	1.94	0.49
1:F:135:GLU:HA	2:N:328:ASP:OD1	2.13	0.49
2:N:237:CYS:HB2	2:N:456:LEU:HG	1.94	0.49
2:N:359:TYR:O	8:N:5637:HOH:O	2.20	0.49
2:H:296:ALA:HA	2:H:309:SER:HA	1.93	0.48
2:H:541:ASP:N	2:H:542:PRO:HD3	2.28	0.48
1:B:159:VAL:O	1:B:163:THR:HG23	2.13	0.48
2:J:38:LYS:HB3	2:J:40:LYS:HE2	1.94	0.48
2:H:296:ALA:HA	2:H:309:SER:HA	1.93	0.48
2:H:541:ASP:N	2:H:542:PRO:HD3	2.28	0.48
1:B:159:VAL:O	1:B:163:THR:HG23	2.13	0.48
2:J:38:LYS:HB3	2:J:40:LYS:HE2	1.94	0.48
2:N:288:ASN:HB3	2:N:381:MET:CE	2.43	0.48
2:M:474:ALA:HB1	2:M:475:PRO:CD	2.43	0.48
1:F:135:GLU:HG2	2:N:328:ASP:CB	2.42	0.48
2:M:474:ALA:HB1	2:M:475:PRO:CD	2.43	0.48
2:H:301:SER:HB2	2:H:302:PRO:HD2	1.95	0.48
2:H:301:SER:HB2	2:H:302:PRO:HD2	1.95	0.48
1:B:18:THR:O	1:B:18:THR:HG22	2.14	0.48
1:B:18:THR:O	1:B:18:THR:HG22	2.14	0.48
1:G:47:THR:O	2:N:23:ARG:HA	2.13	0.48
2:I:121:HIS:CE1	2:I:209:LEU:HD23	2.49	0.48
2:J:140:LYS:HD3	2:J:196:GLU:HG2	1.95	0.48
2:I:121:HIS:CE1	2:I:209:LEU:HD23	2.49	0.48
2:J:140:LYS:HD3	2:J:196:GLU:HG2	1.95	0.48
2:I:130:VAL:HG12	2:I:167:LEU:HD21	1.95	0.48
2:K:301:SER:HB2	2:K:302:PRO:CD	2.44	0.48
2:N:345:GLY:O	2:N:348:LYS:HG2	2.13	0.48
2:I:130:VAL:HG12	2:I:167:LEU:HD21	1.95	0.48
2:K:301:SER:HB2	2:K:302:PRO:CD	2.44	0.48
2:N:43:TRP:CH2	2:N:365:LYS:HE2	2.43	0.48
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.96	0.48
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.96	0.48
2:H:333:TYR:OH	2:H:378:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:454:ASN:HD22	2:H:454:ASN:N	2.10	0.48
2:K:512:LYS:HE2	2:K:520:ILE:HD11	1.96	0.48
1:F:121:GLN:HB3	2:M:50:ARG:HG2	1.96	0.48
1:G:145:PRO:HD2	1:G:179:TYR:CE1	2.49	0.48
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.96	0.48
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.96	0.48
2:H:333:TYR:OH	2:H:378:GLY:HA2	2.13	0.48
2:H:454:ASN:HD22	2:H:454:ASN:N	2.10	0.48
2:K:512:LYS:HE2	2:K:520:ILE:HD11	1.96	0.48
1:F:121:GLN:HB3	2:M:50:ARG:HG2	1.96	0.48
1:C:71:TYR:CE1	1:C:162:LEU:CD2	2.97	0.48
1:C:71:TYR:CE1	1:C:162:LEU:CD2	2.97	0.48
1:A:47:THR:O	2:H:23:ARG:HA	2.14	0.48
2:H:474:ALA:HB1	2:H:475:PRO:HD2	1.95	0.48
2:I:99:ALA:O	2:I:103:ARG:HG3	2.13	0.48
1:F:135:GLU:OE2	2:N:326:ASN:CB	2.62	0.48
1:A:47:THR:O	2:H:23:ARG:HA	2.14	0.48
2:H:474:ALA:HB1	2:H:475:PRO:HD2	1.95	0.48
2:I:99:ALA:O	2:I:103:ARG:HG3	2.13	0.48
2:N:497:VAL:HG12	2:N:498:PRO:HD2	1.95	0.48
1:F:14:ASN:HD22	1:F:94:MET:HB3	1.74	0.48
1:G:254:TRP:HH2	2:N:70:ARG:HD3	1.79	0.48
1:F:14:ASN:HD22	1:F:94:MET:HB3	1.74	0.48
2:N:498:PRO:HG2	7:N:550:FCO:C1	2.44	0.47
1:G:223:THR:CG2	1:G:247:GLY:HA2	2.44	0.47
1:B:33:ASP:O	1:B:37:LEU:HG	2.14	0.47
1:F:160:HIS:CE1	1:F:164:LYS:HB2	2.50	0.47
1:B:33:ASP:O	1:B:37:LEU:HG	2.14	0.47
1:F:160:HIS:CE1	1:F:164:LYS:HB2	2.50	0.47
1:D:114:CYS:HA	1:D:119:GLY:HA3	1.96	0.47
1:F:135:GLU:CD	2:N:326:ASN:HB2	2.33	0.47
2:M:134:LEU:HD22	2:M:168:LYS:CG	2.43	0.47
2:M:274:ALA:CB	2:M:422:LEU:HD11	2.45	0.47
2:M:403:VAL:CG1	2:M:430:ILE:HG23	2.44	0.47
1:D:114:CYS:HA	1:D:119:GLY:HA3	1.96	0.47
2:M:134:LEU:HD22	2:M:168:LYS:CG	2.43	0.47
2:M:274:ALA:CB	2:M:422:LEU:HD11	2.45	0.47
2:M:403:VAL:CG1	2:M:430:ILE:HG23	2.44	0.47
1:G:196:SER:HA	1:G:198:PHE:CZ	2.49	0.47
2:H:166:LYS:NZ	8:H:560:HOH:O	2.35	0.47
2:H:464:GLU:HA	2:H:488:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.47
2:K:530:PRO:HB2	2:K:533:ILE:HD12	1.97	0.47
2:H:166:LYS:NZ	8:H:562:HOH:O	2.35	0.47
2:H:464:GLU:HA	2:H:488:LYS:HG3	1.96	0.47
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.47
2:K:530:PRO:HB2	2:K:533:ILE:HD12	1.97	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.14	0.47
2:H:196:GLU:O	2:H:200:ILE:HG13	2.15	0.47
2:I:69:GLN:HA	2:I:79:HIS:HB2	1.97	0.47
2:N:102:MET:O	2:N:106:VAL:HG23	2.15	0.47
2:N:474:ALA:HB1	2:N:475:PRO:CD	2.45	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.14	0.47
2:H:196:GLU:O	2:H:200:ILE:HG13	2.15	0.47
2:I:69:GLN:HA	2:I:79:HIS:HB2	1.97	0.47
1:G:14:ASN:ND2	1:G:94:MET:HB3	2.29	0.47
1:G:187:CYS:HA	1:G:188:PRO:HD3	1.82	0.47
1:G:145:PRO:HG3	1:G:174:ARG:HD3	1.93	0.47
1:A:78:LEU:HD22	1:A:95:ILE:HA	1.97	0.47
2:I:264:GLU:O	2:I:268:PRO:HG2	2.15	0.47
2:J:34:VAL:HG12	2:J:35:GLU:N	2.29	0.47
1:D:220:GLY:N	1:D:221:PRO:CD	2.77	0.47
1:A:78:LEU:HD22	1:A:95:ILE:HA	1.97	0.47
2:I:264:GLU:O	2:I:268:PRO:HG2	2.15	0.47
2:J:34:VAL:HG12	2:J:35:GLU:N	2.29	0.47
1:D:220:GLY:N	1:D:221:PRO:CD	2.77	0.47
2:N:541:ASP:N	2:N:542:PRO:HD3	2.29	0.47
2:H:127:TRP:CH2	2:H:535:ARG:HD3	2.49	0.47
2:H:267:ILE:HB	2:H:268:PRO:HD3	1.96	0.47
1:G:36:ILE:O	8:G:5282:HOH:O	2.20	0.47
2:H:127:TRP:CH2	2:H:535:ARG:HD3	2.49	0.47
2:H:267:ILE:HB	2:H:268:PRO:HD3	1.96	0.47
2:I:132:ALA:HB3	2:I:198:ASN:ND2	2.29	0.46
2:M:264:GLU:O	2:M:268:PRO:HG2	2.15	0.46
2:N:76:THR:O	2:N:77:TYR:HB3	2.15	0.46
2:I:132:ALA:HB3	2:I:198:ASN:ND2	2.29	0.46
2:M:264:GLU:O	2:M:268:PRO:HG2	2.15	0.46
1:G:50:ALA:HB2	2:N:125:LEU:HD13	1.96	0.46
1:G:243:HIS:CG	1:G:244:PRO:HD2	2.50	0.46
2:M:70:ARG:N	2:M:70:ARG:HD2	2.30	0.46
2:N:541:ASP:N	2:N:542:PRO:HD3	2.29	0.46
2:M:70:ARG:N	2:M:70:ARG:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:ASN:HA	8:G:5270:HOH:O	2.15	0.46
2:N:194:PRO:HG2	2:N:197:VAL:HG23	1.97	0.46
2:J:278:LYS:NZ	2:J:411:LEU:O	2.44	0.46
2:J:284:GLY:HA2	2:J:518:ALA:O	2.16	0.46
1:F:135:GLU:CD	2:N:326:ASN:HD22	2.18	0.46
2:J:278:LYS:NZ	2:J:411:LEU:O	2.44	0.46
2:J:284:GLY:HA2	2:J:518:ALA:O	2.16	0.46
2:N:237:CYS:HB2	2:N:456:LEU:HG	1.96	0.46
2:N:474:ALA:HB1	2:N:475:PRO:CD	2.44	0.46
2:J:371:MET:CE	2:J:547:GLY:HA3	2.46	0.46
2:J:371:MET:CE	2:J:547:GLY:HA3	2.46	0.46
1:B:148:PRO:HB2	1:B:149:PRO:HD2	1.98	0.46
2:J:497:VAL:HG12	2:J:498:PRO:CD	2.45	0.46
1:G:14:ASN:HD22	1:G:94:MET:HB3	1.80	0.46
2:N:69:GLN:HA	2:N:79:HIS:HB2	1.98	0.46
1:B:148:PRO:HB2	1:B:149:PRO:HD2	1.98	0.46
2:J:497:VAL:HG12	2:J:498:PRO:CD	2.45	0.46
1:D:131:LYS:CE	8:D:3421:HOH:O	2.62	0.46
2:M:293:GLY:HA2	2:M:311:PHE:O	2.16	0.46
2:M:497:VAL:CG1	2:M:498:PRO:CD	2.90	0.46
1:D:131:LYS:CE	8:D:3421:HOH:O	2.62	0.46
2:M:293:GLY:HA2	2:M:311:PHE:O	2.16	0.46
2:M:497:VAL:CG1	2:M:498:PRO:CD	2.90	0.46
1:A:190:LEU:HB3	1:A:191:PRO:HD3	1.97	0.46
2:K:509:GLN:HE21	2:K:509:GLN:HB2	1.63	0.46
1:A:190:LEU:HB3	1:A:191:PRO:HD3	1.97	0.46
2:K:509:GLN:HE21	2:K:509:GLN:HB2	1.63	0.46
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.50	0.46
1:B:184:HIS:HB2	1:B:220:GLY:C	2.35	0.46
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.51	0.46
1:G:223:THR:HG21	1:G:247:GLY:HA2	1.98	0.46
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.50	0.46
1:B:184:HIS:HB2	1:B:220:GLY:C	2.35	0.46
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.51	0.46
1:G:136:ALA:HA	8:G:5287:HOH:O	2.15	0.46
2:J:515:VAL:HG13	2:J:516:GLU:N	2.30	0.46
2:M:333:TYR:OH	2:M:378:GLY:HA2	2.16	0.46
2:J:515:VAL:HG13	2:J:516:GLU:N	2.30	0.46
2:M:333:TYR:OH	2:M:378:GLY:HA2	2.16	0.46
1:G:17:CYS:HB2	2:N:73:GLY:H	1.81	0.46
2:J:76:THR:O	2:J:77:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:246:ASP:HB2	2:M:247:PRO:HD3	1.97	0.45
2:J:76:THR:O	2:J:77:TYR:HB3	2.16	0.45
2:M:246:ASP:HB2	2:M:247:PRO:HD3	1.97	0.45
1:D:190:LEU:N	1:D:191:PRO:CD	2.79	0.45
1:D:190:LEU:N	1:D:191:PRO:CD	2.79	0.45
2:K:413:VAL:HB	2:K:414:PRO:HD2	1.98	0.45
1:F:145:PRO:HG3	1:F:174:ARG:CD	2.46	0.45
1:G:158:VAL:O	1:G:162:LEU:HG	2.15	0.45
2:K:413:VAL:HB	2:K:414:PRO:HD2	1.98	0.45
1:F:145:PRO:HG3	1:F:174:ARG:CD	2.46	0.45
1:G:88:MET:HE3	2:N:362:LEU:CD1	2.46	0.45
2:N:296:ALA:HA	2:N:309:SER:HA	1.99	0.45
1:A:159:VAL:O	1:A:163:THR:HG23	2.15	0.45
1:A:159:VAL:O	1:A:163:THR:HG23	2.15	0.45
2:K:118:HIS:HD2	2:K:122:LEU:HD12	1.81	0.45
2:K:118:HIS:HD2	2:K:122:LEU:HD12	1.81	0.45
2:I:476:ARG:HD2	8:I:557:HOH:O	2.16	0.45
2:I:476:ARG:HD2	8:I:552:HOH:O	2.16	0.45
1:G:227:CYS:N	1:G:228:PRO:CD	2.79	0.45
1:A:220:GLY:N	1:A:221:PRO:CD	2.80	0.45
1:C:164:LYS:HB3	1:C:164:LYS:HE3	1.65	0.45
1:C:227:CYS:HB2	1:C:228:PRO:HD3	1.98	0.45
1:G:161:VAL:HA	1:G:165:GLY:O	2.16	0.45
2:N:25:GLU:HB3	2:N:543:CYS:SG	2.56	0.45
1:A:220:GLY:N	1:A:221:PRO:CD	2.80	0.45
1:C:164:LYS:HB3	1:C:164:LYS:HE3	1.65	0.45
1:C:227:CYS:HB2	1:C:228:PRO:HD3	1.98	0.45
1:B:27:THR:CB	1:B:155:VAL:HG21	2.47	0.45
2:I:292:PHE:CD1	2:I:478:ALA:HB1	2.52	0.45
1:B:27:THR:CB	1:B:155:VAL:HG21	2.47	0.45
2:I:292:PHE:CD1	2:I:478:ALA:HB1	2.52	0.45
2:H:418:LEU:O	2:H:423:GLY:HA3	2.17	0.45
2:H:418:LEU:O	2:H:423:GLY:HA3	2.17	0.45
1:G:220:GLY:N	1:G:221:PRO:HD3	2.32	0.45
2:N:497:VAL:CG1	2:N:498:PRO:CD	2.92	0.45
2:N:487:GLY:O	2:N:488:LYS:HB2	2.17	0.45
1:A:254:TRP:CH2	2:H:70:ARG:HD3	2.50	0.44
2:J:9:GLN:NE2	2:J:36:ASN:O	2.48	0.44
2:M:280:TRP:HA	2:M:283:ILE:HD12	1.99	0.44
2:N:223:GLY:HA2	2:N:231:PHE:CD2	2.52	0.44
1:A:254:TRP:CH2	2:H:70:ARG:HD3	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:9:GLN:NE2	2:J:36:ASN:O	2.48	0.44
2:M:280:TRP:HA	2:M:283:ILE:HD12	1.99	0.44
1:G:146:GLY:O	1:G:149:PRO:HD3	2.17	0.44
1:F:204:SER:O	1:F:208:LYS:HG3	2.17	0.44
1:F:204:SER:O	1:F:208:LYS:HG3	2.17	0.44
1:G:161:VAL:HA	1:G:165:GLY:O	2.16	0.44
1:D:131:LYS:HE2	8:D:3421:HOH:O	2.17	0.44
1:D:131:LYS:HE2	8:D:3421:HOH:O	2.17	0.44
2:H:8:PRO:HB2	2:H:525:ALA:HB2	2.00	0.44
1:B:111:ILE:HG23	1:B:111:ILE:O	2.18	0.44
2:N:497:VAL:HG12	2:N:498:PRO:HD2	1.97	0.44
2:H:8:PRO:HB2	2:H:525:ALA:HB2	2.00	0.44
1:B:111:ILE:HG23	1:B:111:ILE:O	2.18	0.44
2:J:448:ASP:O	2:J:452:LYS:HE2	2.11	0.44
2:J:448:ASP:O	2:J:452:LYS:HE2	2.11	0.44
2:N:512:LYS:HB2	2:N:512:LYS:HE2	1.84	0.44
1:A:190:LEU:N	1:A:191:PRO:CD	2.80	0.44
1:D:18:THR:O	1:D:18:THR:HG22	2.18	0.44
1:G:111:ILE:HG23	1:G:111:ILE:O	2.18	0.44
1:G:261:TYR:CD2	2:N:62:ARG:HB3	2.53	0.44
1:A:190:LEU:N	1:A:191:PRO:CD	2.80	0.44
1:D:18:THR:O	1:D:18:THR:HG22	2.18	0.44
1:G:111:ILE:HG23	1:G:111:ILE:O	2.18	0.44
2:N:329:LEU:HD11	2:N:471:LEU:HD11	1.99	0.44
1:D:80:THR:HG21	1:D:131:LYS:HD2	1.99	0.44
2:K:195:PRO:O	2:K:198:ASN:HB2	2.18	0.44
2:N:487:GLY:O	2:N:488:LYS:HB2	2.18	0.44
1:D:80:THR:HG21	1:D:131:LYS:HD2	1.99	0.44
2:K:195:PRO:O	2:K:198:ASN:HB2	2.18	0.44
1:G:258:THR:HB	1:G:259:PRO:HA	1.98	0.44
2:N:76:THR:O	2:N:77:TYR:HB3	2.17	0.44
2:N:69:GLN:HA	2:N:79:HIS:HB2	1.98	0.44
2:H:474:ALA:HB1	2:H:475:PRO:CD	2.48	0.44
2:H:512:LYS:HD2	2:H:516:GLU:HB3	2.00	0.44
2:J:497:VAL:HG11	2:J:546:CYS:HB3	2.00	0.44
2:K:194:PRO:HG2	2:K:197:VAL:HG23	2.00	0.44
2:M:40:LYS:HA	2:M:40:LYS:HD2	1.85	0.44
2:H:474:ALA:HB1	2:H:475:PRO:CD	2.48	0.44
2:H:512:LYS:HD2	2:H:516:GLU:HB3	2.00	0.44
2:J:497:VAL:HG11	2:J:546:CYS:HB3	2.00	0.44
2:K:194:PRO:HG2	2:K:197:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:40:LYS:HA	2:M:40:LYS:HD2	1.85	0.44
2:J:352:ASP:O	2:J:353:GLY:C	2.55	0.43
2:M:487:GLY:O	2:M:488:LYS:HB2	2.17	0.43
1:G:170:ASP:C	1:G:170:ASP:OD1	2.56	0.43
1:G:187:CYS:HA	1:G:188:PRO:HD3	1.85	0.43
2:J:352:ASP:O	2:J:353:GLY:C	2.55	0.43
2:M:487:GLY:O	2:M:488:LYS:HB2	2.17	0.43
1:G:227:CYS:HB2	1:G:228:PRO:HD3	2.00	0.43
2:J:385:PRO:HD2	8:J:756:HOH:O	2.17	0.43
1:G:80:THR:OG1	1:G:129:GLN:O	2.29	0.43
2:J:385:PRO:HD2	8:J:2751:HOH:O	2.17	0.43
2:H:77:TYR:CD2	2:H:106:VAL:HG12	2.52	0.43
1:C:78:LEU:HD13	1:C:95:ILE:HD12	1.99	0.43
2:K:161:LYS:O	2:K:161:LYS:HG3	2.19	0.43
2:M:49:PHE:HB2	2:M:370:TRP:CD2	2.52	0.43
2:H:77:TYR:CD2	2:H:106:VAL:HG12	2.52	0.43
1:C:78:LEU:HD13	1:C:95:ILE:HD12	1.99	0.43
2:K:161:LYS:O	2:K:161:LYS:HG3	2.19	0.43
2:M:49:PHE:HB2	2:M:370:TRP:CD2	2.52	0.43
2:N:223:GLY:HA2	2:N:231:PHE:CD2	2.53	0.43
2:N:497:VAL:HG12	2:N:498:PRO:CD	2.49	0.43
2:H:150:PRO:HG2	2:H:264:GLU:HA	2.00	0.43
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.77	0.43
2:I:209:LEU:HD23	2:I:209:LEU:HA	1.90	0.43
2:I:362:LEU:HD12	2:I:362:LEU:HA	1.77	0.43
2:K:9:GLN:NE2	2:K:36:ASN:O	2.51	0.43
2:K:293:GLY:HA2	2:K:311:PHE:O	2.18	0.43
2:N:194:PRO:HG2	2:N:197:VAL:HG23	1.99	0.43
2:H:150:PRO:HG2	2:H:264:GLU:HA	2.00	0.43
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.77	0.43
2:I:209:LEU:HD23	2:I:209:LEU:HA	1.90	0.43
2:I:362:LEU:HD12	2:I:362:LEU:HA	1.77	0.43
2:K:9:GLN:NE2	2:K:36:ASN:O	2.51	0.43
2:K:293:GLY:HA2	2:K:311:PHE:O	2.18	0.43
2:H:43:TRP:CE2	2:H:365:LYS:HE2	2.53	0.43
2:I:127:TRP:CZ3	2:I:535:ARG:HD3	2.53	0.43
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.54	0.43
2:K:173:SER:HB2	8:K:681:HOH:O	2.17	0.43
2:K:290:LEU:HD12	2:K:315:VAL:HG22	2.01	0.43
1:F:237:TRP:HB2	1:F:238:PRO:CD	2.48	0.43
2:H:43:TRP:CE2	2:H:365:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:127:TRP:CZ3	2:I:535:ARG:HD3	2.53	0.43
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.54	0.43
2:K:173:SER:HB2	8:K:3670:HOH:O	2.17	0.43
2:K:290:LEU:HD12	2:K:315:VAL:HG22	2.01	0.43
1:F:237:TRP:HB2	1:F:238:PRO:CD	2.48	0.43
1:G:184:HIS:HA	3:G:265:SF4:S1	2.58	0.43
2:N:102:MET:O	2:N:106:VAL:HG23	2.18	0.43
2:M:297:THR:OG1	2:M:308:THR:HB	2.19	0.43
2:M:390:PHE:CZ	2:M:418:LEU:HB2	2.54	0.43
2:N:241:GLN:O	2:N:244:THR:OG1	2.34	0.43
2:M:297:THR:OG1	2:M:308:THR:HB	2.19	0.43
2:M:390:PHE:CZ	2:M:418:LEU:HB2	2.54	0.43
1:G:237:TRP:CZ2	1:G:239:VAL:HB	2.54	0.43
2:J:353:GLY:HA3	2:J:494:GLN:CD	2.39	0.43
2:M:116:LEU:HA	2:M:116:LEU:HD23	1.75	0.43
2:M:404:VAL:HG22	2:M:430:ILE:HD13	2.00	0.43
2:J:353:GLY:HA3	2:J:494:GLN:CD	2.39	0.43
2:M:116:LEU:HA	2:M:116:LEU:HD23	1.75	0.43
2:M:404:VAL:HG22	2:M:430:ILE:HD13	2.00	0.43
1:G:237:TRP:HB2	1:G:238:PRO:HD2	2.00	0.43
2:N:328:ASP:OD1	2:N:328:ASP:C	2.57	0.43
8:G:5321:HOH:O	2:N:234:VAL:HG23	2.18	0.43
2:I:296:ALA:HA	2:I:309:SER:HA	2.01	0.43
2:K:105:LEU:HD21	2:K:442:TRP:HB3	2.00	0.43
2:N:512:LYS:HB2	2:N:512:LYS:HE2	1.87	0.43
2:I:296:ALA:HA	2:I:309:SER:HA	2.01	0.43
2:K:105:LEU:HD21	2:K:442:TRP:HB3	2.00	0.43
1:G:29:LYS:HA	1:G:30:PRO:HA	1.79	0.43
2:I:306:LEU:HD23	2:I:306:LEU:HA	1.90	0.43
2:J:246:ASP:HB2	2:J:247:PRO:HD3	2.00	0.43
2:M:354:VAL:O	2:M:372:LYS:NZ	2.51	0.43
2:I:306:LEU:HD23	2:I:306:LEU:HA	1.90	0.43
2:J:246:ASP:HB2	2:J:247:PRO:HD3	2.00	0.43
2:M:354:VAL:O	2:M:372:LYS:NZ	2.51	0.43
1:G:122:LYS:NZ	8:G:5276:HOH:O	2.36	0.43
1:G:145:PRO:HD2	1:G:179:TYR:CE1	2.54	0.43
2:K:270:LEU:CD1	2:K:425:THR:HG22	2.49	0.42
2:K:377:LYS:CE	8:K:788:HOH:O	2.67	0.42
2:M:364:ASP:O	2:M:368:TYR:HB3	2.19	0.42
2:N:497:VAL:CG1	2:N:498:PRO:CD	2.93	0.42
2:K:270:LEU:CD1	2:K:425:THR:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:377:LYS:CE	8:K:3778:HOH:O	2.67	0.42
2:M:364:ASP:O	2:M:368:TYR:HB3	2.19	0.42
2:H:168:LYS:O	2:H:172:GLU:HG3	2.19	0.42
2:K:123:HIS:CD2	2:K:127:TRP:HE1	2.37	0.42
1:G:89:VAL:O	1:G:90:ALA:HB3	2.19	0.42
2:H:168:LYS:O	2:H:172:GLU:HG3	2.19	0.42
2:K:123:HIS:CD2	2:K:127:TRP:HE1	2.37	0.42
2:J:127:TRP:CH2	2:J:535:ARG:HG2	2.54	0.42
2:J:411:LEU:O	2:J:412:SER:HB2	2.19	0.42
1:G:102:ALA:HB1	1:G:108:ILE:HD11	1.99	0.42
2:J:127:TRP:CH2	2:J:535:ARG:HG2	2.54	0.42
2:J:411:LEU:O	2:J:412:SER:HB2	2.19	0.42
1:G:190:LEU:N	1:G:191:PRO:HD2	2.34	0.42
2:H:271:LEU:HD13	2:H:410:LYS:CE	2.49	0.42
2:I:237:CYS:HB2	2:I:456:LEU:HG	2.02	0.42
2:K:403:VAL:CG1	2:K:430:ILE:HG23	2.49	0.42
1:F:248:CYS:HA	1:F:253:PHE:CD1	2.55	0.42
2:M:465:GLU:O	2:M:466:SER:HB2	2.19	0.42
2:H:271:LEU:HD13	2:H:410:LYS:CE	2.49	0.42
2:I:237:CYS:HB2	2:I:456:LEU:HG	2.02	0.42
2:K:403:VAL:CG1	2:K:430:ILE:HG23	2.49	0.42
1:F:248:CYS:HA	1:F:253:PHE:CD1	2.55	0.42
2:M:465:GLU:O	2:M:466:SER:HB2	2.19	0.42
2:H:362:LEU:HD12	2:H:362:LEU:HA	1.85	0.42
1:B:197:GLU:HB3	1:B:211:PHE:CE1	2.54	0.42
2:I:53:GLU:HG2	2:I:493:PHE:O	2.20	0.42
2:I:343:PRO:HG2	2:K:147:SER:HB3	2.01	0.42
2:J:166:LYS:HE3	2:J:166:LYS:HB2	1.77	0.42
1:D:111:ILE:O	1:D:111:ILE:HG23	2.20	0.42
1:F:258:THR:HA	1:F:259:PRO:C	2.39	0.42
2:N:297:THR:OG1	2:N:308:THR:HB	2.19	0.42
2:H:362:LEU:HD12	2:H:362:LEU:HA	1.85	0.42
1:B:197:GLU:HB3	1:B:211:PHE:CE1	2.54	0.42
2:I:53:GLU:HG2	2:I:493:PHE:O	2.20	0.42
2:I:343:PRO:HG2	2:K:147:SER:HB3	2.01	0.42
2:J:166:LYS:HE3	2:J:166:LYS:HB2	1.77	0.42
1:D:111:ILE:O	1:D:111:ILE:HG23	2.20	0.42
1:F:258:THR:HA	1:F:259:PRO:C	2.39	0.42
1:A:46:GLU:HG3	8:A:289:HOH:O	2.19	0.42
2:K:349:HIS:CG	2:K:350:PRO:HD2	2.55	0.42
2:M:320:ASP:C	2:M:320:ASP:OD1	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:26:GLY:HA3	2:N:544:ILE:HB	2.02	0.42
1:A:46:GLU:HG3	8:A:289:HOH:O	2.19	0.42
2:K:349:HIS:CG	2:K:350:PRO:HD2	2.55	0.42
2:M:320:ASP:C	2:M:320:ASP:OD1	2.58	0.42
2:J:40:LYS:HD3	2:J:40:LYS:HA	1.83	0.42
2:J:350:PRO:HB2	2:J:482:TRP:CG	2.54	0.42
2:J:441:LYS:NZ	8:J:651:HOH:O	2.51	0.42
2:M:495:LEU:N	2:M:495:LEU:HD12	2.35	0.42
2:J:40:LYS:HD3	2:J:40:LYS:HA	1.83	0.42
2:J:350:PRO:HB2	2:J:482:TRP:CG	2.54	0.42
2:J:441:LYS:NZ	8:J:2644:HOH:O	2.51	0.42
2:M:495:LEU:N	2:M:495:LEU:HD12	2.35	0.42
1:A:184:HIS:NE2	1:A:190:LEU:CD1	2.83	0.42
2:H:486:LYS:HB3	2:H:491:ASP:HB2	2.02	0.42
2:K:69:GLN:OE1	2:K:77:TYR:HA	2.19	0.42
2:K:476:ARG:HD2	8:K:557:HOH:O	2.19	0.42
2:N:19:ASP:HA	2:N:20:PRO:HA	1.85	0.42
2:N:91:VAL:O	2:N:92:LYS:HB2	2.20	0.42
1:A:184:HIS:NE2	1:A:190:LEU:CD1	2.83	0.42
2:H:486:LYS:HB3	2:H:491:ASP:HB2	2.02	0.42
2:K:69:GLN:OE1	2:K:77:TYR:HA	2.19	0.42
2:K:476:ARG:HD2	8:K:552:HOH:O	2.19	0.42
2:J:380:ALA:HB1	2:J:514:PRO:HD3	2.02	0.42
2:M:476:ARG:HD2	7:M:550:FCO:C2	2.50	0.42
2:J:380:ALA:HB1	2:J:514:PRO:HD3	2.02	0.42
2:M:476:ARG:HD2	7:M:550:FCO:C2	2.50	0.42
2:N:454:ASN:HD22	2:N:454:ASN:N	2.14	0.42
1:A:40:ILE:HG22	1:A:162:LEU:CD1	2.50	0.42
2:K:76:THR:O	2:K:77:TYR:HB3	2.19	0.42
1:A:40:ILE:HG22	1:A:162:LEU:CD1	2.50	0.42
2:K:76:THR:O	2:K:77:TYR:HB3	2.19	0.42
2:I:411:LEU:O	2:I:413:VAL:HG13	2.20	0.41
2:K:246:ASP:N	2:K:247:PRO:CD	2.83	0.41
2:I:411:LEU:O	2:I:413:VAL:HG13	2.20	0.41
2:K:246:ASP:N	2:K:247:PRO:CD	2.83	0.41
2:N:241:GLN:O	2:N:244:THR:OG1	2.37	0.41
2:N:328:ASP:OD1	2:N:330:GLY:N	2.53	0.41
2:J:515:VAL:CG1	2:J:516:GLU:N	2.83	0.41
2:K:402:LYS:HB2	2:K:402:LYS:HE3	1.85	0.41
1:G:201:SER:HA	1:G:216:LEU:HD21	2.02	0.41
2:J:515:VAL:CG1	2:J:516:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:402:LYS:HB2	2:K:402:LYS:HE3	1.85	0.41
1:G:80:THR:OG1	1:G:129:GLN:O	2.29	0.41
1:C:29:LYS:HA	1:C:30:PRO:HA	1.83	0.41
2:J:274:ALA:CB	2:J:422:LEU:HD11	2.51	0.41
1:G:117:TYR:CE2	1:G:145:PRO:HB3	2.54	0.41
1:G:122:LYS:NZ	8:G:5276:HOH:O	2.41	0.41
1:C:29:LYS:HA	1:C:30:PRO:HA	1.83	0.41
2:J:274:ALA:CB	2:J:422:LEU:HD11	2.51	0.41
1:G:147:CYS:O	1:G:147:CYS:SG	2.78	0.41
2:H:60:ASP:HA	2:H:61:PRO:HD3	1.98	0.41
2:I:196:GLU:OE1	2:I:196:GLU:N	2.50	0.41
2:N:543:CYS:SG	2:N:546:CYS:HB2	2.60	0.41
2:H:60:ASP:HA	2:H:61:PRO:HD3	1.98	0.41
2:I:196:GLU:OE1	2:I:196:GLU:N	2.50	0.41
1:A:233:ASN:O	1:A:234:GLN:HB2	2.21	0.41
1:A:263:GLN:OE1	1:A:263:GLN:HA	2.20	0.41
2:I:134:LEU:HD21	2:I:167:LEU:HB3	2.02	0.41
1:G:223:THR:CG2	1:G:247:GLY:HA2	2.50	0.41
2:N:329:LEU:HD11	2:N:471:LEU:HD11	2.02	0.41
1:A:233:ASN:O	1:A:234:GLN:HB2	2.21	0.41
1:A:263:GLN:OE1	1:A:263:GLN:HA	2.20	0.41
2:I:134:LEU:HD21	2:I:167:LEU:HB3	2.02	0.41
1:G:22:GLU:O	1:G:26:ARG:HG2	2.20	0.41
2:N:26:GLY:HA3	2:N:544:ILE:HB	2.01	0.41
2:J:204:HIS:ND1	2:J:269:ASP:OD2	2.35	0.41
1:D:253:PHE:CZ	1:D:254:TRP:CE2	3.09	0.41
2:M:76:THR:OG1	2:M:228:HIS:N	2.49	0.41
2:N:454:ASN:HD22	2:N:454:ASN:N	2.17	0.41
2:J:204:HIS:ND1	2:J:269:ASP:OD2	2.35	0.41
1:D:253:PHE:CZ	1:D:254:TRP:CE2	3.09	0.41
2:M:76:THR:OG1	2:M:228:HIS:N	2.49	0.41
1:G:237:TRP:CH2	1:G:239:VAL:HB	2.56	0.41
2:H:144:LEU:C	2:H:144:LEU:CD2	2.89	0.41
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.77	0.41
2:H:465:GLU:O	2:H:466:SER:HB2	2.21	0.41
1:C:236:ASN:OD1	1:C:240:GLN:HB3	2.20	0.41
1:D:127:PRO:HD2	8:D:3268:HOH:O	2.20	0.41
2:N:464:GLU:HA	2:N:488:LYS:HG3	2.03	0.41
2:H:144:LEU:C	2:H:144:LEU:CD2	2.89	0.41
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.77	0.41
2:H:465:GLU:O	2:H:466:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASN:OD1	1:C:240:GLN:HB3	2.20	0.41
1:D:127:PRO:HD2	8:D:3268:HOH:O	2.20	0.41
1:G:89:VAL:O	1:G:90:ALA:HB3	2.20	0.41
2:N:284:GLY:HA2	2:N:518:ALA:O	2.21	0.41
2:N:353:GLY:HA3	2:N:494:GLN:HG3	2.02	0.41
1:C:184:HIS:HB2	1:C:220:GLY:C	2.41	0.41
2:K:69:GLN:HA	2:K:79:HIS:HB2	2.03	0.41
2:K:350:PRO:HB2	2:K:482:TRP:CD2	2.55	0.41
2:K:474:ALA:HB1	2:K:475:PRO:CD	2.51	0.41
2:N:497:VAL:HG12	2:N:498:PRO:CD	2.50	0.41
1:C:184:HIS:HB2	1:C:220:GLY:C	2.41	0.41
2:K:69:GLN:HA	2:K:79:HIS:HB2	2.03	0.41
2:K:350:PRO:HB2	2:K:482:TRP:CD2	2.55	0.41
2:K:474:ALA:HB1	2:K:475:PRO:CD	2.51	0.41
1:G:174:ARG:HA	1:G:175:PRO:HD3	1.85	0.41
1:A:187:CYS:HA	1:A:188:PRO:HD3	1.90	0.41
1:A:243:HIS:CG	1:A:244:PRO:HD2	2.56	0.41
2:H:497:VAL:HG11	2:H:546:CYS:HB3	2.02	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.01	0.41
1:B:29:LYS:HA	1:B:30:PRO:HA	1.83	0.41
1:B:227:CYS:N	1:B:228:PRO:HD2	2.35	0.41
2:J:39:VAL:CG2	2:J:522:THR:HB	2.51	0.41
2:J:541:ASP:N	2:J:542:PRO:HD3	2.36	0.41
1:D:6:ARG:HA	1:D:7:PRO:HD3	1.93	0.41
1:D:233:ASN:O	1:D:234:GLN:HB2	2.20	0.41
1:F:155:VAL:O	1:F:159:VAL:HG23	2.21	0.41
1:G:190:LEU:HB3	1:G:191:PRO:HD3	2.02	0.41
1:G:230:VAL:O	1:G:231:LEU:HB2	2.21	0.41
2:N:353:GLY:HA3	2:N:494:GLN:HG3	2.01	0.41
1:A:187:CYS:HA	1:A:188:PRO:HD3	1.90	0.41
1:A:243:HIS:CG	1:A:244:PRO:HD2	2.56	0.41
2:H:497:VAL:HG11	2:H:546:CYS:HB3	2.02	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.01	0.41
1:B:29:LYS:HA	1:B:30:PRO:HA	1.83	0.41
1:B:227:CYS:N	1:B:228:PRO:HD2	2.35	0.41
2:J:39:VAL:CG2	2:J:522:THR:HB	2.51	0.41
2:J:541:ASP:N	2:J:542:PRO:HD3	2.36	0.41
1:D:6:ARG:HA	1:D:7:PRO:HD3	1.93	0.41
1:D:233:ASN:O	1:D:234:GLN:HB2	2.20	0.41
1:F:155:VAL:O	1:F:159:VAL:HG23	2.21	0.41
1:G:170:ASP:C	1:G:170:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:LEU:HB3	1:G:191:PRO:HD3	2.03	0.41
2:I:341:TYR:O	2:I:343:PRO:HD3	2.21	0.41
2:K:56:LEU:HD21	2:K:67:PHE:HB2	2.03	0.41
2:M:349:HIS:CG	2:M:350:PRO:CD	3.04	0.41
2:I:341:TYR:O	2:I:343:PRO:HD3	2.21	0.41
2:K:56:LEU:HD21	2:K:67:PHE:HB2	2.03	0.41
2:M:349:HIS:CG	2:M:350:PRO:CD	3.04	0.41
2:N:75:CYS:CB	7:N:550:FCO:C2	2.99	0.41
1:A:117:TYR:CD2	1:A:251:PRO:HA	2.57	0.40
2:H:509:GLN:HE21	2:H:509:GLN:HB2	1.69	0.40
1:F:23:ALA:O	1:F:151:PRO:HB3	2.20	0.40
1:F:201:SER:HA	1:F:216:LEU:HD21	2.04	0.40
1:G:261:TYR:HD2	2:N:62:ARG:HB3	1.86	0.40
1:A:117:TYR:CD2	1:A:251:PRO:HA	2.57	0.40
2:H:509:GLN:HE21	2:H:509:GLN:HB2	1.69	0.40
1:F:23:ALA:O	1:F:151:PRO:HB3	2.20	0.40
1:F:201:SER:HA	1:F:216:LEU:HD21	2.04	0.40
2:N:95:ILE:HA	2:N:96:PRO:HD3	1.92	0.40
2:N:116:LEU:HD23	2:N:116:LEU:HA	1.97	0.40
2:I:270:LEU:HD21	2:I:426:ALA:HA	2.03	0.40
1:D:71:TYR:CE1	1:D:162:LEU:CD2	3.04	0.40
2:M:267:ILE:N	2:M:268:PRO:CD	2.84	0.40
2:I:270:LEU:HD21	2:I:426:ALA:HA	2.03	0.40
1:D:71:TYR:CE1	1:D:162:LEU:CD2	3.04	0.40
2:M:267:ILE:N	2:M:268:PRO:CD	2.84	0.40
2:N:513:SER:HB2	2:N:514:PRO:CD	2.52	0.40
2:I:246:ASP:N	2:I:247:PRO:CD	2.84	0.40
2:I:338:TYR:HA	2:I:366:ASP:O	2.21	0.40
1:F:143:ASN:O	1:F:175:PRO:HD3	2.21	0.40
2:M:274:ALA:HA	2:M:422:LEU:HD11	2.03	0.40
1:G:136:ALA:HA	8:G:5287:HOH:O	2.21	0.40
1:G:184:HIS:HB2	1:G:220:GLY:C	2.42	0.40
1:G:217:GLY:O	1:G:219:LYS:HD3	2.20	0.40
1:G:248:CYS:HA	1:G:253:PHE:CD2	2.56	0.40
2:I:246:ASP:N	2:I:247:PRO:CD	2.84	0.40
2:I:338:TYR:HA	2:I:366:ASP:O	2.21	0.40
1:F:143:ASN:O	1:F:175:PRO:HD3	2.21	0.40
2:M:274:ALA:HA	2:M:422:LEU:HD11	2.03	0.40
2:N:356:ASP:HA	2:N:357:PRO:HD2	1.93	0.40
8:B:1742:HOH:O	2:I:173:SER:HB2	2.20	0.40
2:J:149:ALA:HB1	2:J:150:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:441:LYS:HE2	2:J:441:LYS:HB3	1.84	0.40
2:M:497:VAL:HG11	2:M:546:CYS:HB3	2.03	0.40
2:N:144:LEU:C	2:N:144:LEU:HD23	2.41	0.40
8:B:1742:HOH:O	2:I:173:SER:HB2	2.20	0.40
2:J:149:ALA:HB1	2:J:150:PRO:HD2	2.03	0.40
2:J:441:LYS:HE2	2:J:441:LYS:HB3	1.84	0.40
2:M:497:VAL:HG11	2:M:546:CYS:HB3	2.03	0.40
1:C:220:GLY:N	1:C:221:PRO:CD	2.84	0.40
2:J:19:ASP:CG	2:J:29:ARG:HB2	2.42	0.40
2:J:280:TRP:HA	2:J:283:ILE:HD12	2.03	0.40
2:K:377:LYS:NZ	8:K:788:HOH:O	2.47	0.40
1:G:22:GLU:O	1:G:26:ARG:HG2	2.21	0.40
1:C:220:GLY:N	1:C:221:PRO:CD	2.84	0.40
2:J:19:ASP:CG	2:J:29:ARG:HB2	2.42	0.40
2:J:280:TRP:HA	2:J:283:ILE:HD12	2.03	0.40
2:K:377:LYS:NZ	8:K:3778:HOH:O	2.47	0.40
2:N:86:CYS:SG	2:N:468:GLY:O	2.80	0.40
2:N:397:GLN:HA	2:N:398:PRO:HD3	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:OG	2:N:528:LYS:NZ[2_656]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	1-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	1-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	1-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	34	32
1	1-G	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	2-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	2-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	2-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	34	32
1	2-G	260/264 (98%)	249 (96%)	11 (4%)	0	100	100
2	1-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	1-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	1-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	1-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	1-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	1-N	543/549 (99%)	524 (96%)	18 (3%)	1 (0%)	47	49
2	2-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	2-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	2-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	2-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	2-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	2-N	543/549 (99%)	521 (96%)	19 (4%)	3 (1%)	25	21
All	All	9624/9756 (99%)	9300 (97%)	318 (3%)	6 (0%)	51	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2-N	343	PRO
2	2-N	342	ALA
1	1-F	231	LEU
1	2-F	231	LEU
2	1-N	148	ILE
2	2-N	148	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	1-B	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	1-C	206/210 (98%)	200 (97%)	6 (3%)	42	46
1	1-D	208/210 (99%)	206 (99%)	2 (1%)	76	82
1	1-F	206/210 (98%)	203 (98%)	3 (2%)	65	71
1	1-G	208/210 (99%)	207 (100%)	1 (0%)	88	92
1	2-A	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	2-B	208/210 (99%)	204 (98%)	4 (2%)	57	63
1	2-C	206/210 (98%)	200 (97%)	6 (3%)	42	46
1	2-D	208/210 (99%)	206 (99%)	2 (1%)	76	82
1	2-F	206/210 (98%)	203 (98%)	3 (2%)	65	71
1	2-G	208/210 (99%)	206 (99%)	2 (1%)	76	82
2	1-H	435/439 (99%)	429 (99%)	6 (1%)	67	73
2	1-I	435/439 (99%)	431 (99%)	4 (1%)	78	84
2	1-J	435/439 (99%)	424 (98%)	11 (2%)	47	52
2	1-K	435/439 (99%)	428 (98%)	7 (2%)	62	69
2	1-M	435/439 (99%)	421 (97%)	14 (3%)	39	41
2	1-N	435/439 (99%)	426 (98%)	9 (2%)	53	59
2	2-H	435/439 (99%)	429 (99%)	6 (1%)	67	73
2	2-I	435/439 (99%)	431 (99%)	4 (1%)	78	84
2	2-J	435/439 (99%)	424 (98%)	11 (2%)	47	52
2	2-K	435/439 (99%)	428 (98%)	7 (2%)	62	69
2	2-M	435/439 (99%)	421 (97%)	14 (3%)	39	41
2	2-N	435/439 (99%)	426 (98%)	9 (2%)	53	59
All	All	7708/7788 (99%)	7565 (98%)	143 (2%)	57	63

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	4	LYS
1	1-A	67	LYS
1	1-A	88	MET
1	1-A	209	LYS
2	1-H	40	LYS
2	1-H	148	ILE
2	1-H	401	LYS
2	1-H	453	ASP
2	1-H	454	ASN
2	1-H	473	ASP
1	1-B	4	LYS
1	1-B	67	LYS
1	1-B	171	SER
1	1-B	196	SER
2	1-I	167	LEU
2	1-I	397	GLN
2	1-I	454	ASN
2	1-I	473	ASP
1	1-C	16	GLU
1	1-C	29	LYS
1	1-C	67	LYS
1	1-C	95	ILE
1	1-C	99	LYS
1	1-C	100	LYS
2	1-J	38	LYS
2	1-J	140	LYS
2	1-J	148	ILE
2	1-J	361	LYS
2	1-J	397	GLN
2	1-J	452	LYS
2	1-J	454	ASN
2	1-J	473	ASP
2	1-J	498	PRO
2	1-J	503	LEU
2	1-J	528	LYS
1	1-D	88	MET
1	1-D	166	ILE
2	1-K	40	LYS
2	1-K	144	LEU
2	1-K	397	GLN
2	1-K	401	LYS
2	1-K	410	LYS
2	1-K	473	ASP

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Mol	Chain	Res	Type
2	1-K	509	GLN
1	1-F	16	GLU
1	1-F	82	ASP
1	1-F	135	GLU
2	1-M	33	GLU
2	1-M	135	LYS
2	1-M	266	TYR
2	1-M	278	LYS
2	1-M	304	LYS
2	1-M	339	SER
2	1-M	362	LEU
2	1-M	379	LYS
2	1-M	397	GLN
2	1-M	412	SER
2	1-M	452	LYS
2	1-M	454	ASN
2	1-M	473	ASP
2	1-M	509	GLN
1	1-G	88	MET
2	1-N	278	LYS
2	1-N	303	SER
2	1-N	406	MET
2	1-N	410	LYS
2	1-N	453	ASP
2	1-N	454	ASN
2	1-N	473	ASP
2	1-N	528	LYS
2	1-N	546	CYS
1	2-A	4	LYS
1	2-A	67	LYS
1	2-A	88	MET
1	2-A	209	LYS
2	2-H	40	LYS
2	2-H	148	ILE
2	2-H	401	LYS
2	2-H	453	ASP
2	2-H	454	ASN
2	2-H	473	ASP
1	2-B	4	LYS
1	2-B	67	LYS
1	2-B	171	SER
1	2-B	196	SER

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Mol	Chain	Res	Type
2	2-I	167	LEU
2	2-I	397	GLN
2	2-I	454	ASN
2	2-I	473	ASP
1	2-C	16	GLU
1	2-C	29	LYS
1	2-C	67	LYS
1	2-C	95	ILE
1	2-C	99	LYS
1	2-C	100	LYS
2	2-J	38	LYS
2	2-J	140	LYS
2	2-J	148	ILE
2	2-J	361	LYS
2	2-J	397	GLN
2	2-J	452	LYS
2	2-J	454	ASN
2	2-J	473	ASP
2	2-J	498	PRO
2	2-J	503	LEU
2	2-J	528	LYS
1	2-D	88	MET
1	2-D	166	ILE
2	2-K	40	LYS
2	2-K	144	LEU
2	2-K	397	GLN
2	2-K	401	LYS
2	2-K	410	LYS
2	2-K	473	ASP
2	2-K	509	GLN
1	2-F	16	GLU
1	2-F	82	ASP
1	2-F	135	GLU
2	2-M	33	GLU
2	2-M	135	LYS
2	2-M	266	TYR
2	2-M	278	LYS
2	2-M	304	LYS
2	2-M	339	SER
2	2-M	362	LEU
2	2-M	379	LYS
2	2-M	397	GLN

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Mol	Chain	Res	Type
2	2-M	412	SER
2	2-M	452	LYS
2	2-M	454	ASN
2	2-M	473	ASP
2	2-M	509	GLN
1	2-G	88	MET
1	2-G	177	LEU
2	2-N	278	LYS
2	2-N	361	LYS
2	2-N	364	ASP
2	2-N	366	ASP
2	2-N	406	MET
2	2-N	410	LYS
2	2-N	453	ASP
2	2-N	454	ASN
2	2-N	473	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	14	ASN
1	1-A	62	GLN
2	1-H	250	ASN
2	1-H	454	ASN
2	1-H	509	GLN
1	1-B	14	ASN
1	1-B	62	GLN
1	1-B	172	ASN
2	1-I	454	ASN
1	1-C	62	GLN
1	1-C	172	ASN
2	1-J	454	ASN
1	1-D	14	ASN
1	1-D	61	HIS
1	1-D	172	ASN
2	1-K	509	GLN
1	1-F	14	ASN
2	1-M	454	ASN
2	1-M	509	GLN
1	1-G	14	ASN
1	1-G	172	ASN
2	1-N	123	HIS

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Mol	Chain	Res	Type
2	1-N	326	ASN
2	1-N	454	ASN
2	1-N	509	GLN
1	2-A	14	ASN
1	2-A	62	GLN
2	2-H	250	ASN
2	2-H	454	ASN
2	2-H	509	GLN
1	2-B	14	ASN
1	2-B	62	GLN
1	2-B	172	ASN
2	2-I	454	ASN
1	2-C	62	GLN
1	2-C	172	ASN
2	2-J	454	ASN
1	2-D	14	ASN
1	2-D	61	HIS
1	2-D	172	ASN
2	2-K	509	GLN
1	2-F	14	ASN
2	2-M	454	ASN
2	2-M	509	GLN
1	2-G	14	ASN
2	2-N	123	HIS
2	2-N	454	ASN
2	2-N	509	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SF4	1-F	267	1	0,12,12	-	-	-		
3	SF4	1-D	265	1	0,12,12	-	-	-		
4	F3S	1-A	266	1	0,9,9	-	-	-		
7	FCO	1-K	550	8,2	0,6,6	-	-	-		
3	SF4	1-F	265	1	0,12,12	-	-	-		
7	FCO	1-N	550	8,2	0,6,6	-	-	-		
4	F3S	2-D	266	1	0,9,9	-	-	-		
4	F3S	1-D	266	1	0,9,9	-	-	-		
3	SF4	2-F	265	1	0,12,12	-	-	-		
3	SF4	1-C	267	1	0,12,12	-	-	-		
7	FCO	2-M	550	8,2	0,6,6	-	-	-		
3	SF4	2-B	267	1	0,12,12	-	-	-		
4	F3S	2-A	266	1	0,9,9	-	-	-		
7	FCO	1-I	550	8,2	0,6,6	-	-	-		
4	F3S	1-B	266	1	0,9,9	-	-	-		
3	SF4	2-B	265	1	0,12,12	-	-	-		
4	F3S	1-C	266	1	0,9,9	-	-	-		
4	F3S	1-G	266	1	0,9,9	-	-	-		
4	F3S	2-B	266	1	0,9,9	-	-	-		
3	SF4	2-A	267	1	0,12,12	-	-	-		
4	F3S	1-F	266	1	0,9,9	-	-	-		
3	SF4	2-A	265	1	0,12,12	-	-	-		
3	SF4	1-B	267	1	0,12,12	-	-	-		
4	F3S	2-C	266	1	0,9,9	-	-	-		
4	F3S	2-G	266	1	0,9,9	-	-	-		
3	SF4	1-G	267	1	0,12,12	-	-	-		
3	SF4	2-D	267	1	0,12,12	-	-	-		
7	FCO	2-N	550	8,2	0,6,6	-	-	-		
7	FCO	2-K	550	8,2	0,6,6	-	-	-		
7	FCO	2-I	550	8,2	0,6,6	-	-	-		
3	SF4	2-F	267	1	0,12,12	-	-	-		
7	FCO	1-J	550	8,2	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FCO	2-J	550	8,2	0,6,6	-	-	-		
3	SF4	1-B	265	1	0,12,12	-	-	-		
3	SF4	2-G	267	1	0,12,12	-	-	-		
3	SF4	1-A	267	1	0,12,12	-	-	-		
3	SF4	1-G	265	1	0,12,12	-	-	-		
7	FCO	1-M	550	8,2	0,6,6	-	-	-		
3	SF4	1-D	267	1	0,12,12	-	-	-		
3	SF4	1-C	265	1	0,12,12	-	-	-		
3	SF4	1-A	265	1	0,12,12	-	-	-		
4	F3S	2-F	266	1	0,9,9	-	-	-		
3	SF4	2-G	265	1	0,12,12	-	-	-		
3	SF4	2-D	265	1	0,12,12	-	-	-		
3	SF4	2-C	267	1	0,12,12	-	-	-		
7	FCO	1-H	550	8,2	0,6,6	-	-	-		
7	FCO	2-H	550	8,2	0,6,6	-	-	-		
3	SF4	2-C	265	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	1-F	267	1	-	-	0/6/5/5
3	SF4	1-D	265	1	-	-	0/6/5/5
4	F3S	1-A	266	1	-	-	0/3/3/3
3	SF4	1-F	265	1	-	-	0/6/5/5
4	F3S	2-D	266	1	-	-	0/3/3/3
4	F3S	1-D	266	1	-	-	0/3/3/3
3	SF4	2-F	265	1	-	-	0/6/5/5
3	SF4	1-C	267	1	-	-	0/6/5/5
3	SF4	2-B	267	1	-	-	0/6/5/5
4	F3S	2-A	266	1	-	-	0/3/3/3
4	F3S	1-B	266	1	-	-	0/3/3/3
3	SF4	2-B	265	1	-	-	0/6/5/5
4	F3S	1-C	266	1	-	-	0/3/3/3
4	F3S	1-G	266	1	-	-	0/3/3/3
4	F3S	2-B	266	1	-	-	0/3/3/3
3	SF4	2-A	267	1	-	-	0/6/5/5
4	F3S	1-F	266	1	-	-	0/3/3/3
3	SF4	2-A	265	1	-	-	0/6/5/5
3	SF4	1-B	267	1	-	-	0/6/5/5
4	F3S	2-C	266	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	2-G	266	1	-	-	0/3/3/3
3	SF4	1-G	267	1	-	-	0/6/5/5
3	SF4	2-D	267	1	-	-	0/6/5/5
3	SF4	2-F	267	1	-	-	0/6/5/5
3	SF4	1-B	265	1	-	-	0/6/5/5
3	SF4	2-G	267	1	-	-	0/6/5/5
3	SF4	1-A	267	1	-	-	0/6/5/5
3	SF4	1-G	265	1	-	-	0/6/5/5
3	SF4	1-D	267	1	-	-	0/6/5/5
3	SF4	1-C	265	1	-	-	0/6/5/5
3	SF4	1-A	265	1	-	-	0/6/5/5
4	F3S	2-F	266	1	-	-	0/3/3/3
3	SF4	2-G	265	1	-	-	0/6/5/5
3	SF4	2-D	265	1	-	-	0/6/5/5
3	SF4	2-C	267	1	-	-	0/6/5/5
3	SF4	2-C	265	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-N	550	FCO	2	0
7	2-M	550	FCO	1	0
7	2-N	550	FCO	3	0
7	1-M	550	FCO	1	0
3	2-G	265	SF4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1-A	262/264 (99%)	-0.24	6 (2%) 60 65	5, 9, 18, 28	8 (3%)
1	1-B	262/264 (99%)	0.57	40 (15%) 2 3	4, 10, 18, 25	6 (2%)
1	1-C	260/264 (98%)	-0.36	2 (0%) 86 88	4, 9, 16, 23	6 (2%)
1	1-D	262/264 (99%)	-0.48	2 (0%) 86 88	3, 9, 16, 30	5 (1%)
1	1-F	260/264 (98%)	-0.14	5 (1%) 66 71	4, 10, 17, 24	6 (2%)
1	1-G	262/264 (99%)	5.25	251 (95%) 0 0	6, 10, 10, 11	262 (100%)
1	2-A	262/264 (99%)	-0.24	6 (2%) 60 65	5, 9, 18, 28	8 (3%)
1	2-B	262/264 (99%)	0.57	40 (15%) 2 3	4, 10, 18, 25	6 (2%)
1	2-C	260/264 (98%)	-0.36	2 (0%) 86 88	4, 9, 16, 23	6 (2%)
1	2-D	262/264 (99%)	-0.48	2 (0%) 86 88	3, 9, 16, 30	5 (1%)
1	2-F	260/264 (98%)	-0.14	5 (1%) 66 71	4, 10, 17, 24	6 (2%)
1	2-G	262/264 (99%)	5.25	251 (95%) 0 0	6, 10, 10, 11	262 (100%)
2	1-H	545/549 (99%)	-0.25	9 (1%) 70 74	4, 9, 16, 27	11 (2%)
2	1-I	545/549 (99%)	-0.01	27 (4%) 28 34	3, 9, 16, 24	6 (1%)
2	1-J	544/549 (99%)	-0.11	16 (2%) 51 57	4, 9, 17, 23	12 (2%)
2	1-K	544/549 (99%)	-0.23	8 (1%) 73 77	3, 9, 17, 24	12 (2%)
2	1-M	545/549 (99%)	0.03	19 (3%) 44 50	3, 10, 16, 31	12 (2%)
2	1-N	545/549 (99%)	4.35	502 (92%) 0 0	6, 10, 11, 12	545 (100%)
2	2-H	545/549 (99%)	-0.25	9 (1%) 70 74	4, 9, 16, 27	11 (2%)
2	2-I	545/549 (99%)	-0.01	27 (4%) 28 34	3, 9, 16, 24	6 (1%)
2	2-J	544/549 (99%)	-0.11	16 (2%) 51 57	4, 9, 17, 23	12 (2%)
2	2-K	544/549 (99%)	-0.23	8 (1%) 73 77	3, 9, 17, 24	12 (2%)
2	2-M	545/549 (99%)	0.03	19 (3%) 44 50	3, 10, 16, 31	12 (2%)
2	2-N	545/549 (99%)	4.35	502 (92%) 0 0	6, 10, 11, 12	545 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	9672/9756 (99%)	0.67	1774 (18%)	1	1	3, 9, 16, 31	1782 (18%)

All (1774) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-N	171	VAL	15.6
2	2-N	171	VAL	15.6
2	1-N	186	GLY	15.1
2	2-N	186	GLY	15.1
1	1-G	137	LEU	13.5
1	2-G	137	LEU	13.5
2	1-N	185	LEU	12.7
2	2-N	185	LEU	12.7
2	1-N	451	ALA	12.2
2	2-N	451	ALA	12.2
1	1-G	145	PRO	11.8
1	2-G	145	PRO	11.8
1	1-G	196	SER	11.8
1	2-G	196	SER	11.8
1	1-G	254	TRP	11.7
1	2-G	254	TRP	11.7
2	1-N	181	ASN	11.5
2	2-N	181	ASN	11.5
2	1-N	134	LEU	11.0
2	2-N	134	LEU	11.0
2	1-N	247	PRO	11.0
2	2-N	247	PRO	11.0
2	1-N	199	LEU	11.0
2	2-N	199	LEU	11.0
2	1-N	324	VAL	10.9
2	2-N	324	VAL	10.9
1	1-G	79	PRO	10.7
1	2-G	79	PRO	10.7
1	1-G	12	LEU	10.7
1	2-G	12	LEU	10.7
1	1-G	138	GLY	10.6
1	2-G	138	GLY	10.6
1	1-G	114	CYS	10.5
1	2-G	114	CYS	10.5
1	1-G	64	LEU	10.5
1	2-G	64	LEU	10.5
2	1-N	347	GLY	10.4

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Mol	Chain	Res	Type	RSRZ
2	2-N	347	GLY	10.4
1	1-G	169	LEU	10.4
1	2-G	169	LEU	10.4
1	1-G	10	VAL	10.3
1	2-G	10	VAL	10.3
2	1-N	155	ASN	10.3
2	2-N	155	ASN	10.3
2	1-N	49	PHE	10.1
2	2-N	49	PHE	10.1
2	1-N	289	TYR	10.1
2	2-N	289	TYR	10.1
2	1-N	176	LEU	10.1
2	2-N	176	LEU	10.1
2	1-N	154	GLY	10.0
2	2-N	154	GLY	10.0
1	1-G	58	ALA	9.8
1	2-G	58	ALA	9.8
2	1-N	174	GLY	9.7
2	2-N	174	GLY	9.7
2	1-N	341	TYR	9.6
2	2-N	341	TYR	9.6
2	1-N	213	VAL	9.6
2	2-N	213	VAL	9.6
2	1-N	327	VAL	9.6
2	2-N	327	VAL	9.6
2	1-N	175	GLN	9.6
2	2-N	175	GLN	9.6
2	1-N	184	PHE	9.4
2	2-N	184	PHE	9.4
1	1-G	237	TRP	9.3
1	2-G	237	TRP	9.3
1	1-G	213	LEU	9.2
1	2-G	213	LEU	9.2
1	1-G	49	MET	9.1
1	2-G	49	MET	9.1
1	1-G	157	ALA	9.1
1	2-G	157	ALA	9.1
1	1-G	248	CYS	9.1
1	2-G	248	CYS	9.1
1	1-G	74	VAL	8.9
1	2-G	74	VAL	8.9
1	1-G	11	TRP	8.9

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Mol	Chain	Res	Type	RSRZ
1	2-G	11	TRP	8.9
2	1-N	187	GLY	8.9
2	2-N	187	GLY	8.9
2	1-N	246	ASP	8.8
2	2-N	246	ASP	8.8
2	1-N	51	GLY	8.8
2	2-N	51	GLY	8.8
1	1-G	136	ALA	8.8
1	2-G	136	ALA	8.8
2	1-N	178	ILE	8.7
2	2-N	178	ILE	8.7
2	1-N	393	TYR	8.6
2	2-N	393	TYR	8.6
1	1-G	17	CYS	8.5
1	2-G	17	CYS	8.5
2	1-N	180	THR	8.5
2	2-N	180	THR	8.5
2	1-N	177	GLY	8.4
2	2-N	177	GLY	8.4
1	1-G	108	ILE	8.4
1	2-G	108	ILE	8.4
1	1-G	158	VAL	8.4
1	2-G	158	VAL	8.4
1	1-G	110	CYS	8.3
1	2-G	110	CYS	8.3
2	1-N	130	VAL	8.3
2	2-N	130	VAL	8.3
1	1-G	47	THR	8.3
1	2-G	47	THR	8.3
2	1-N	366	ASP	8.2
2	2-N	366	ASP	8.2
1	1-G	168	ASP	8.1
1	2-G	168	ASP	8.1
1	1-G	166	ILE	8.0
1	2-G	166	ILE	8.0
2	1-N	518	ALA	8.0
2	2-N	518	ALA	8.0
1	1-G	190	LEU	8.0
1	2-G	190	LEU	8.0
1	1-G	154	PHE	7.9
1	2-G	154	PHE	7.9
2	1-N	67	PHE	7.9

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Mol	Chain	Res	Type	RSRZ
2	2-N	67	PHE	7.9
1	1-G	72	LEU	7.9
1	2-G	72	LEU	7.9
2	1-N	344	GLY	7.9
2	2-N	344	GLY	7.9
1	1-G	32	ILE	7.8
1	2-G	32	ILE	7.8
2	1-N	131	THR	7.8
2	2-N	131	THR	7.8
2	1-N	377	LYS	7.8
2	2-N	377	LYS	7.8
1	1-G	199	ALA	7.7
1	2-G	199	ALA	7.7
2	1-N	206	LEU	7.7
2	2-N	206	LEU	7.7
2	1-N	54	ILE	7.7
2	2-N	54	ILE	7.7
1	1-G	61	HIS	7.6
1	2-G	61	HIS	7.6
2	1-N	42	ALA	7.6
2	2-N	42	ALA	7.6
1	1-G	52	ALA	7.5
1	2-G	52	ALA	7.5
1	1-G	44	TYR	7.5
1	2-G	44	TYR	7.5
2	1-N	227	PRO	7.4
2	2-N	227	PRO	7.4
2	1-N	370	TRP	7.3
2	2-N	370	TRP	7.3
2	1-N	132	ALA	7.3
2	1-N	182	ALA	7.3
2	1-N	508	ALA	7.3
2	2-N	132	ALA	7.3
2	2-N	182	ALA	7.3
2	2-N	508	ALA	7.3
1	1-G	77	GLY	7.3
1	2-G	77	GLY	7.3
1	1-G	42	LEU	7.3
1	2-G	42	LEU	7.3
2	1-N	359	TYR	7.3
2	2-N	359	TYR	7.3
1	1-G	20	CYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	1-G	133	VAL	7.2
1	2-G	20	CYS	7.2
1	2-G	133	VAL	7.2
1	1-G	109	ILE	7.2
1	2-G	109	ILE	7.2
2	1-N	183	TYR	7.2
2	2-N	183	TYR	7.2
1	1-G	144	ILE	7.2
1	2-G	144	ILE	7.2
1	1-G	261	TYR	7.2
1	2-G	261	TYR	7.2
1	1-G	246	LEU	7.1
1	2-G	246	LEU	7.1
1	1-G	91	GLY	7.1
1	2-G	91	GLY	7.1
1	1-G	45	GLN	7.1
1	2-G	45	GLN	7.1
1	1-G	120	VAL	7.1
1	2-G	120	VAL	7.1
1	1-G	207	ALA	7.1
1	2-G	207	ALA	7.1
1	1-G	15	ALA	7.0
1	2-G	15	ALA	7.0
2	1-N	72	CYS	7.0
2	2-N	72	CYS	7.0
2	1-N	76	THR	7.0
2	2-N	76	THR	7.0
2	1-N	321	LEU	7.0
2	2-N	321	LEU	7.0
1	1-G	62	GLN	7.0
1	2-G	62	GLN	7.0
2	1-N	326	ASN	7.0
2	2-N	326	ASN	7.0
1	1-G	117	TYR	7.0
1	2-G	117	TYR	7.0
2	1-N	106	VAL	7.0
2	2-N	106	VAL	7.0
2	1-N	135	LYS	6.9
2	2-N	135	LYS	6.9
1	1-G	148	PRO	6.9
1	2-G	148	PRO	6.9
2	1-N	254	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
2	2-N	254	LEU	6.9
2	1-N	221	ILE	6.9
2	2-N	221	ILE	6.9
1	1-G	46	GLU	6.9
1	2-G	46	GLU	6.9
1	1-G	118	GLY	6.9
1	2-G	118	GLY	6.9
1	1-G	73	VAL	6.9
1	2-G	73	VAL	6.9
1	1-G	90	ALA	6.9
1	2-G	90	ALA	6.9
2	1-N	330	GLY	6.9
2	2-N	330	GLY	6.9
1	1-G	232	PHE	6.8
1	2-G	232	PHE	6.8
2	1-N	229	THR	6.8
2	2-N	229	THR	6.8
1	1-G	155	VAL	6.8
1	2-G	155	VAL	6.8
1	1-G	262	GLU	6.8
1	2-G	262	GLU	6.8
2	1-N	403	VAL	6.8
2	2-N	403	VAL	6.8
1	1-G	48	ILE	6.7
1	2-G	48	ILE	6.7
2	1-N	228	HIS	6.7
2	2-N	228	HIS	6.7
1	1-G	159	VAL	6.7
1	2-G	159	VAL	6.7
2	1-N	369	SER	6.6
2	2-N	369	SER	6.6
1	1-G	43	ASP	6.6
1	2-G	43	ASP	6.6
1	1-G	149	PRO	6.6
1	2-G	149	PRO	6.6
1	1-G	7	PRO	6.6
1	1-G	239	VAL	6.6
1	2-G	7	PRO	6.6
1	2-G	239	VAL	6.6
1	1-G	171	SER	6.6
1	2-G	171	SER	6.6
2	1-N	172	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
2	2-N	172	GLU	6.6
1	1-G	86	TRP	6.6
1	2-G	86	TRP	6.6
2	1-N	546	CYS	6.6
2	2-N	546	CYS	6.6
1	1-G	260	PHE	6.6
1	2-G	260	PHE	6.6
1	1-G	13	HIS	6.5
1	2-G	13	HIS	6.5
2	1-N	331	ALA	6.5
2	2-N	331	ALA	6.5
2	1-N	99	ALA	6.5
2	2-N	99	ALA	6.5
2	1-N	350	PRO	6.5
2	2-N	350	PRO	6.5
2	1-N	75	CYS	6.5
2	2-N	75	CYS	6.5
2	1-N	376	TYR	6.5
2	2-N	376	TYR	6.5
1	1-G	9	VAL	6.4
1	2-G	9	VAL	6.4
1	1-G	258	THR	6.4
1	2-G	258	THR	6.4
1	1-G	25	ILE	6.4
1	2-G	25	ILE	6.4
2	1-N	336	VAL	6.4
2	2-N	336	VAL	6.4
1	1-G	23	ALA	6.4
1	2-G	23	ALA	6.4
2	1-N	80	ALA	6.3
2	2-N	80	ALA	6.3
2	1-N	543	CYS	6.3
2	2-N	543	CYS	6.3
1	1-G	70	TYR	6.3
1	2-G	70	TYR	6.3
1	1-G	177	LEU	6.3
1	2-G	177	LEU	6.3
1	1-G	253	PHE	6.3
1	2-G	253	PHE	6.3
2	1-N	66	HIS	6.3
2	2-N	66	HIS	6.3
2	1-N	179	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
2	2-N	179	PHE	6.3
1	1-G	53	GLY	6.3
1	2-G	53	GLY	6.3
2	1-N	112	LEU	6.3
2	2-N	112	LEU	6.3
1	1-G	227	CYS	6.3
1	2-G	227	CYS	6.3
1	1-G	21	THR	6.3
1	2-G	21	THR	6.3
2	1-N	410	LYS	6.2
2	2-N	410	LYS	6.2
2	1-N	71	ALA	6.2
2	2-N	71	ALA	6.2
1	1-G	95	ILE	6.2
1	2-G	95	ILE	6.2
1	1-G	24	ALA	6.2
1	2-G	24	ALA	6.2
1	1-G	238	PRO	6.2
1	2-G	238	PRO	6.2
2	1-N	253	ALA	6.2
2	2-N	253	ALA	6.2
2	1-N	125	LEU	6.2
2	1-N	205	TYR	6.2
2	2-N	125	LEU	6.2
2	2-N	205	TYR	6.2
1	1-G	198	PHE	6.2
1	2-G	198	PHE	6.2
2	1-N	77	TYR	6.1
2	2-N	77	TYR	6.1
2	1-N	332	ILE	6.1
2	2-N	332	ILE	6.1
2	1-N	544	ILE	6.1
2	2-N	544	ILE	6.1
2	1-N	149	ALA	6.1
2	2-N	149	ALA	6.1
2	1-N	501	TRP	6.1
2	2-N	501	TRP	6.1
1	1-G	147	CYS	6.0
1	2-G	147	CYS	6.0
1	1-G	229	LYS	6.0
1	2-G	229	LYS	6.0
2	1-N	400	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
2	2-N	400	PHE	6.0
2	1-N	21	ILE	6.0
2	2-N	21	ILE	6.0
2	1-N	329	LEU	6.0
2	2-N	329	LEU	6.0
1	1-G	214	TYR	6.0
1	2-G	214	TYR	6.0
1	1-G	161	VAL	5.9
1	2-G	161	VAL	5.9
2	1-N	333	TYR	5.9
2	2-N	333	TYR	5.9
2	1-N	342	ALA	5.9
2	2-N	342	ALA	5.9
2	1-N	338	TYR	5.9
2	2-N	338	TYR	5.9
1	1-G	215	GLU	5.9
1	2-G	215	GLU	5.9
2	1-N	167	LEU	5.9
2	1-N	418	LEU	5.9
2	2-N	167	LEU	5.9
2	2-N	418	LEU	5.9
1	1-G	67	LYS	5.9
1	2-G	67	LYS	5.9
2	1-N	34	VAL	5.8
2	2-N	34	VAL	5.8
2	1-N	105	LEU	5.8
2	2-N	105	LEU	5.8
1	1-G	179	TYR	5.8
1	2-G	179	TYR	5.8
1	1-G	218	CYS	5.8
1	2-G	218	CYS	5.8
2	1-N	223	GLY	5.8
2	2-N	223	GLY	5.8
2	1-N	74	VAL	5.8
2	2-N	74	VAL	5.8
2	1-N	406	MET	5.8
2	2-N	406	MET	5.8
1	1-G	165	GLY	5.8
1	2-G	165	GLY	5.8
1	1-G	225	ASN	5.7
1	2-G	225	ASN	5.7
2	1-N	281	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
2	2-N	281	GLY	5.7
2	1-N	52	LEU	5.7
2	2-N	52	LEU	5.7
2	1-N	122	LEU	5.7
2	2-N	122	LEU	5.7
2	1-N	340	TRP	5.7
2	2-N	340	TRP	5.7
2	1-N	297	THR	5.7
2	1-N	432	THR	5.7
2	2-N	297	THR	5.7
2	2-N	432	THR	5.7
1	1-G	40	ILE	5.7
1	2-G	40	ILE	5.7
1	1-G	97	THR	5.6
1	2-G	97	THR	5.6
1	1-G	180	GLY	5.6
1	2-G	180	GLY	5.6
2	1-N	291	ALA	5.6
2	2-N	291	ALA	5.6
2	1-N	43	TRP	5.6
2	2-N	43	TRP	5.6
1	1-G	189	ARG	5.6
1	2-G	189	ARG	5.6
1	1-G	163	THR	5.6
1	2-G	163	THR	5.6
2	1-N	443	ILE	5.6
2	2-N	443	ILE	5.6
2	1-N	117	VAL	5.6
2	2-N	117	VAL	5.6
2	1-N	226	ASN	5.6
2	2-N	226	ASN	5.6
2	1-N	73	GLY	5.6
2	2-N	73	GLY	5.6
2	1-N	433	ALA	5.6
2	2-N	433	ALA	5.6
2	1-N	258	VAL	5.6
2	2-N	258	VAL	5.6
2	1-N	209	LEU	5.5
2	2-N	209	LEU	5.5
1	1-G	222	VAL	5.5
1	2-G	222	VAL	5.5
2	1-N	415	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
2	1-N	509	GLN	5.5
2	2-N	415	ALA	5.5
2	2-N	509	GLN	5.5
1	1-G	178	PHE	5.5
1	2-G	178	PHE	5.5
2	1-N	510	GLY	5.5
2	2-N	510	GLY	5.5
2	1-N	69	GLN	5.5
2	1-N	230	GLN	5.5
2	2-N	69	GLN	5.5
2	2-N	230	GLN	5.5
1	1-G	51	ALA	5.4
1	2-G	51	ALA	5.4
2	1-N	343	PRO	5.4
2	1-N	360	THR	5.4
2	2-N	343	PRO	5.4
2	2-N	360	THR	5.4
1	1-G	71	TYR	5.4
1	2-G	71	TYR	5.4
1	1-G	245	CYS	5.4
1	2-G	245	CYS	5.4
1	1-G	54	GLU	5.4
1	2-G	54	GLU	5.4
2	1-N	24	ILE	5.4
2	2-N	24	ILE	5.4
2	1-N	447	ALA	5.4
2	2-N	447	ALA	5.4
1	1-G	4	LYS	5.4
1	2-G	4	LYS	5.4
2	1-N	28	LEU	5.4
2	2-N	28	LEU	5.4
2	1-N	17	VAL	5.4
2	2-N	17	VAL	5.4
2	1-N	220	ALA	5.4
2	2-N	220	ALA	5.4
2	1-N	250	ASN	5.4
2	2-N	250	ASN	5.4
1	1-G	60	LEU	5.4
1	2-G	60	LEU	5.4
2	1-N	456	LEU	5.4
2	2-N	456	LEU	5.4
1	1-G	30	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	2-G	30	PRO	5.4
2	1-N	548	VAL	5.4
2	2-N	548	VAL	5.4
1	1-G	78	LEU	5.4
1	2-G	78	LEU	5.4
2	1-N	290	LEU	5.4
2	2-N	290	LEU	5.4
2	1-N	265	CYS	5.4
2	2-N	265	CYS	5.4
1	1-B	165	GLY	5.4
1	1-G	217	GLY	5.4
1	2-B	165	GLY	5.4
1	2-G	217	GLY	5.4
1	1-G	127	PRO	5.4
1	2-G	127	PRO	5.4
1	1-G	50	ALA	5.4
1	2-G	50	ALA	5.4
2	1-N	435	VAL	5.3
2	2-N	435	VAL	5.3
2	1-N	261	PHE	5.3
2	1-N	390	PHE	5.3
2	2-N	261	PHE	5.3
2	2-N	390	PHE	5.3
2	1-N	11	THR	5.3
2	1-N	417	ALA	5.3
2	2-N	11	THR	5.3
2	2-N	417	ALA	5.3
2	1-N	70	ARG	5.3
2	2-N	70	ARG	5.3
1	1-G	172	ASN	5.3
1	2-G	172	ASN	5.3
1	1-G	18	THR	5.3
1	2-G	18	THR	5.3
2	1-N	354	VAL	5.3
2	2-N	354	VAL	5.3
1	1-G	36	ILE	5.3
1	2-G	36	ILE	5.3
2	1-N	170	PHE	5.3
2	1-N	365	LYS	5.3
2	2-N	170	PHE	5.3
2	2-N	365	LYS	5.3
2	1-N	46	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	2-N	46	SER	5.3
1	1-G	194	GLU	5.3
1	2-G	194	GLU	5.3
1	1-G	216	LEU	5.3
1	2-G	216	LEU	5.3
2	1-N	266	TYR	5.3
2	2-N	266	TYR	5.3
1	1-G	41	SER	5.3
1	2-G	41	SER	5.3
1	1-G	257	MET	5.3
1	2-G	257	MET	5.3
2	1-N	386	LEU	5.3
2	2-N	386	LEU	5.3
1	1-G	150	ASN	5.3
1	2-G	150	ASN	5.3
2	1-N	378	GLY	5.2
2	1-N	389	THR	5.2
2	2-N	378	GLY	5.2
2	2-N	389	THR	5.2
2	1-N	374	PRO	5.2
2	2-N	374	PRO	5.2
2	1-N	457	CYS	5.2
2	2-N	457	CYS	5.2
2	1-N	356	ASP	5.2
2	2-N	356	ASP	5.2
2	1-N	13	THR	5.2
2	2-N	13	THR	5.2
1	1-G	259	PRO	5.2
1	2-G	259	PRO	5.2
1	1-G	92	HIS	5.2
1	2-G	92	HIS	5.2
2	1-N	36	ASN	5.2
2	2-N	36	ASN	5.2
2	1-N	216	ALA	5.2
2	2-N	216	ALA	5.2
2	1-N	150	PRO	5.2
2	2-N	150	PRO	5.2
1	1-G	88	MET	5.2
1	2-G	88	MET	5.2
2	1-N	107	MET	5.2
2	2-N	107	MET	5.2
2	1-N	16	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	2-N	16	ILE	5.2
1	1-G	107	GLY	5.2
1	2-G	107	GLY	5.2
2	1-N	116	LEU	5.2
2	2-N	116	LEU	5.2
2	1-N	232	THR	5.2
2	2-N	232	THR	5.2
2	1-N	316	ILE	5.2
2	2-N	316	ILE	5.2
1	1-G	8	SER	5.2
1	1-G	57	GLU	5.2
1	2-G	8	SER	5.2
1	2-G	57	GLU	5.2
1	1-G	69	GLY	5.2
1	2-G	69	GLY	5.2
1	1-G	231	LEU	5.2
1	2-G	231	LEU	5.2
1	1-G	228	PRO	5.1
1	2-G	228	PRO	5.1
2	1-N	460	TRP	5.1
2	2-N	460	TRP	5.1
2	1-N	430	ILE	5.1
2	2-N	430	ILE	5.1
1	1-G	193	PHE	5.1
1	2-G	193	PHE	5.1
2	1-N	429	GLY	5.1
2	2-N	429	GLY	5.1
2	1-N	65	GLN	5.1
2	2-N	65	GLN	5.1
1	1-G	113	THR	5.1
1	2-G	113	THR	5.1
2	1-N	22	THR	5.1
2	2-N	22	THR	5.1
1	1-G	167	PRO	5.1
1	2-G	167	PRO	5.1
2	1-N	63	ASP	5.1
2	2-N	63	ASP	5.1
1	1-G	55	ALA	5.1
1	1-G	123	ALA	5.1
1	2-G	55	ALA	5.1
1	2-G	123	ALA	5.1
2	1-N	219	MET	5.1

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Mol	Chain	Res	Type	RSRZ
2	2-N	219	MET	5.1
2	1-N	479	LEU	5.1
2	2-N	479	LEU	5.1
1	1-G	132	GLY	5.1
1	2-G	132	GLY	5.1
2	1-N	120	TYR	5.1
2	1-N	533	ILE	5.1
2	2-N	120	TYR	5.1
2	2-N	533	ILE	5.1
1	1-G	244	PRO	5.1
1	2-G	244	PRO	5.1
2	1-N	426	ALA	5.1
2	2-N	426	ALA	5.1
1	1-G	35	LEU	5.1
1	2-G	35	LEU	5.1
2	1-N	231	PHE	5.1
2	2-N	231	PHE	5.1
1	1-G	87	GLY	5.0
1	2-G	87	GLY	5.0
1	1-G	66	GLY	5.0
1	2-G	66	GLY	5.0
2	1-N	286	THR	5.0
2	2-N	286	THR	5.0
2	1-N	346	ASP	5.0
2	2-N	346	ASP	5.0
2	1-N	56	LEU	5.0
2	2-N	56	LEU	5.0
1	1-G	115	SER	5.0
1	2-G	115	SER	5.0
2	1-N	78	VAL	5.0
2	2-N	78	VAL	5.0
1	1-G	76	GLY	5.0
1	2-G	76	GLY	5.0
1	1-G	151	PRO	5.0
1	2-G	151	PRO	5.0
2	1-N	225	LYS	5.0
2	2-N	225	LYS	5.0
2	1-N	68	THR	4.9
2	2-N	68	THR	4.9
2	1-N	482	TRP	4.9
2	2-N	482	TRP	4.9
1	1-G	63	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	1-G	116	ALA	4.9
1	2-G	63	ALA	4.9
1	2-G	116	ALA	4.9
1	1-G	19	GLY	4.9
1	2-G	19	GLY	4.9
2	1-N	30	ILE	4.9
2	2-N	30	ILE	4.9
2	1-N	292	PHE	4.9
2	1-N	295	PHE	4.9
2	2-N	292	PHE	4.9
2	2-N	295	PHE	4.9
2	1-N	81	LEU	4.9
2	2-N	81	LEU	4.9
2	1-N	64	ALA	4.9
2	1-N	163	VAL	4.9
2	2-N	64	ALA	4.9
2	2-N	163	VAL	4.9
2	1-N	530	PRO	4.9
2	2-N	530	PRO	4.9
2	1-N	379	LYS	4.9
2	2-N	379	LYS	4.9
2	1-N	173	SER	4.9
2	2-N	173	SER	4.9
2	1-N	517	GLU	4.9
2	2-N	517	GLU	4.9
2	1-N	514	PRO	4.8
2	2-N	514	PRO	4.8
2	1-N	315	VAL	4.8
2	2-N	315	VAL	4.8
1	1-G	247	GLY	4.8
1	2-G	247	GLY	4.8
1	1-G	104	LYS	4.8
1	2-G	104	LYS	4.8
1	1-G	202	PHE	4.8
1	2-G	202	PHE	4.8
1	1-G	243	HIS	4.8
1	2-G	243	HIS	4.8
2	1-N	251	TYR	4.8
2	2-N	251	TYR	4.8
1	1-G	98	THR	4.8
1	2-G	98	THR	4.8
1	1-B	169	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	2-B	169	LEU	4.8
2	1-N	119	PHE	4.8
2	2-N	119	PHE	4.8
1	1-G	103	ALA	4.8
1	2-G	103	ALA	4.8
2	1-N	367	HIS	4.8
2	2-N	367	HIS	4.8
2	1-N	402	LYS	4.8
2	2-N	402	LYS	4.8
1	1-G	142	ILE	4.8
1	2-G	142	ILE	4.8
2	1-N	240	TYR	4.7
2	1-N	244	THR	4.7
2	2-N	240	TYR	4.7
2	2-N	244	THR	4.7
2	1-N	260	GLN	4.7
2	2-N	260	GLN	4.7
2	1-N	20	PRO	4.7
2	2-N	20	PRO	4.7
2	1-N	128	VAL	4.7
2	2-N	128	VAL	4.7
1	1-G	56	ALA	4.7
1	2-G	56	ALA	4.7
1	1-G	111	ILE	4.7
1	2-G	111	ILE	4.7
2	1-N	547	GLY	4.7
2	2-N	547	GLY	4.7
1	1-G	27	THR	4.7
1	2-G	27	THR	4.7
2	1-N	293	GLY	4.6
2	2-N	293	GLY	4.6
1	1-G	89	VAL	4.6
1	1-G	121	GLN	4.6
1	2-G	89	VAL	4.6
1	2-G	121	GLN	4.6
1	1-G	200	PRO	4.6
1	2-G	200	PRO	4.6
1	1-G	263	GLN	4.6
1	2-G	263	GLN	4.6
1	1-G	226	ASN	4.6
1	2-G	226	ASN	4.6
2	1-N	311	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
2	2-N	311	PHE	4.6
2	1-N	520	ILE	4.6
2	2-N	520	ILE	4.6
2	1-M	322	GLY	4.6
2	2-M	322	GLY	4.6
2	1-N	452	LYS	4.6
2	2-N	452	LYS	4.6
2	1-N	141	ALA	4.6
2	1-N	272	ALA	4.6
2	2-N	141	ALA	4.6
2	2-N	272	ALA	4.6
1	1-G	16	GLU	4.5
1	2-G	16	GLU	4.5
2	1-N	137	ASP	4.5
2	2-N	137	ASP	4.5
2	1-N	27	HIS	4.5
2	1-N	425	THR	4.5
2	2-N	27	HIS	4.5
2	2-N	425	THR	4.5
1	1-G	195	ALA	4.5
1	2-G	195	ALA	4.5
2	1-N	373	ALA	4.5
2	2-N	373	ALA	4.5
1	1-B	67	LYS	4.5
1	2-B	67	LYS	4.5
2	1-N	224	GLY	4.5
2	1-N	539	ALA	4.5
2	2-N	224	GLY	4.5
2	2-N	539	ALA	4.5
2	1-N	113	HIS	4.5
2	2-N	113	HIS	4.5
1	1-G	230	VAL	4.5
1	2-G	230	VAL	4.5
2	1-N	407	VAL	4.5
2	2-N	407	VAL	4.5
2	1-N	348	LYS	4.5
2	1-N	409	GLY	4.5
2	2-N	348	LYS	4.5
2	2-N	409	GLY	4.5
2	1-N	133	ALA	4.5
2	1-N	307	ALA	4.5
2	2-N	133	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
2	2-N	307	ALA	4.5
2	1-N	148	ILE	4.5
2	1-N	160	LEU	4.5
2	1-N	248	LEU	4.5
2	2-N	148	ILE	4.5
2	2-N	160	LEU	4.5
2	2-N	248	LEU	4.5
2	1-N	383	VAL	4.5
2	2-N	383	VAL	4.5
1	1-G	185	ASP	4.5
1	2-G	185	ASP	4.5
1	1-G	251	PRO	4.4
1	2-G	251	PRO	4.4
2	1-N	527	PRO	4.4
2	2-N	527	PRO	4.4
2	1-N	531	VAL	4.4
2	2-N	531	VAL	4.4
1	1-G	264	GLY	4.4
1	2-G	264	GLY	4.4
2	1-N	362	LEU	4.4
2	2-N	362	LEU	4.4
1	1-G	153	ASN	4.4
1	2-G	153	ASN	4.4
2	1-N	521	GLY	4.4
2	2-N	521	GLY	4.4
1	1-G	6	ARG	4.4
1	2-G	6	ARG	4.4
2	1-N	32	VAL	4.4
2	2-N	32	VAL	4.4
1	1-G	135	GLU	4.4
1	2-G	135	GLU	4.4
1	1-G	211	PHE	4.4
1	2-G	211	PHE	4.4
2	1-N	83	SER	4.4
2	1-N	287	SER	4.4
2	2-N	83	SER	4.4
2	2-N	287	SER	4.4
2	1-N	422	LEU	4.4
2	2-N	422	LEU	4.4
1	1-G	81	ILE	4.4
1	2-G	81	ILE	4.4
2	1-N	280	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
2	2-N	280	TRP	4.4
2	1-N	41	ASP	4.4
2	2-N	41	ASP	4.4
2	1-M	415	ALA	4.3
2	2-M	415	ALA	4.3
1	1-G	219	LYS	4.3
1	2-G	219	LYS	4.3
1	1-G	93	PRO	4.3
1	2-G	93	PRO	4.3
2	1-I	153	PRO	4.3
2	2-I	153	PRO	4.3
1	1-G	99	LYS	4.3
1	2-G	99	LYS	4.3
2	1-N	437	ALA	4.3
2	2-N	437	ALA	4.3
2	1-N	499	SER	4.3
2	2-N	499	SER	4.3
1	1-G	235	VAL	4.3
1	2-G	235	VAL	4.3
1	1-G	252	ASP	4.3
1	2-G	252	ASP	4.3
2	1-N	86	CYS	4.3
2	2-N	86	CYS	4.3
2	1-N	208	ALA	4.3
2	2-N	208	ALA	4.3
2	1-N	23	ARG	4.3
2	2-N	23	ARG	4.3
2	1-N	267	ILE	4.3
2	2-N	267	ILE	4.3
1	1-G	256	THR	4.3
1	2-G	256	THR	4.3
2	1-N	368	TYR	4.3
2	2-N	368	TYR	4.3
1	1-G	191	PRO	4.3
1	2-G	191	PRO	4.3
2	1-N	129	ASP	4.3
2	2-N	129	ASP	4.3
1	1-G	223	THR	4.3
1	2-G	223	THR	4.3
2	1-N	108	ALA	4.3
2	2-N	108	ALA	4.3
2	1-N	420	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	2-N	420	SER	4.3
2	1-N	363	ASP	4.3
2	2-N	363	ASP	4.3
2	1-N	111	TYR	4.3
2	2-N	111	TYR	4.3
2	1-N	157	ALA	4.3
2	2-N	157	ALA	4.3
2	1-N	188	HIS	4.3
2	2-N	188	HIS	4.3
2	1-N	211	MET	4.2
2	2-N	211	MET	4.2
2	1-N	222	LEU	4.2
2	2-N	222	LEU	4.2
2	1-N	427	ALA	4.2
2	2-N	427	ALA	4.2
1	1-G	29	LYS	4.2
1	2-G	29	LYS	4.2
2	1-N	202	THR	4.2
2	2-N	202	THR	4.2
2	1-N	361	LYS	4.2
2	2-N	361	LYS	4.2
2	1-N	391	ILE	4.2
2	2-N	391	ILE	4.2
2	1-N	145	ALA	4.2
2	1-N	153	PRO	4.2
2	2-N	145	ALA	4.2
2	2-N	153	PRO	4.2
1	1-G	65	GLU	4.2
1	2-G	65	GLU	4.2
1	1-G	141	THR	4.2
1	2-G	141	THR	4.2
1	1-G	249	SER	4.2
1	2-G	249	SER	4.2
2	1-N	233	VAL	4.2
2	2-N	233	VAL	4.2
2	1-N	242	GLY	4.2
2	2-N	242	GLY	4.2
2	1-N	534	LEU	4.2
2	2-N	534	LEU	4.2
2	1-N	33	GLU	4.2
2	2-N	33	GLU	4.2
2	1-N	237	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	1-N	262	VAL	4.2
2	2-N	237	CYS	4.2
2	2-N	262	VAL	4.2
2	1-N	121	HIS	4.2
2	2-N	121	HIS	4.2
2	1-N	381	MET	4.2
2	2-N	381	MET	4.2
1	1-G	100	LYS	4.2
1	1-G	234	GLN	4.2
1	2-G	100	LYS	4.2
1	2-G	234	GLN	4.2
2	1-N	349	HIS	4.2
2	1-N	419	HIS	4.2
2	2-N	349	HIS	4.2
2	2-N	419	HIS	4.2
1	1-G	31	TYR	4.2
1	2-G	31	TYR	4.2
2	1-N	470	GLY	4.1
2	2-N	470	GLY	4.1
2	1-N	496	VAL	4.1
2	2-N	496	VAL	4.1
2	1-N	472	ALA	4.1
2	2-N	472	ALA	4.1
2	1-N	102	MET	4.1
2	2-N	102	MET	4.1
1	1-G	146	GLY	4.1
1	2-G	146	GLY	4.1
2	1-N	453	ASP	4.1
2	2-N	453	ASP	4.1
2	1-N	39	VAL	4.1
2	2-N	39	VAL	4.1
2	1-N	385	PRO	4.1
2	2-N	385	PRO	4.1
1	1-G	156	GLY	4.1
1	2-G	156	GLY	4.1
2	1-N	296	ALA	4.1
2	1-N	392	ALA	4.1
2	2-N	296	ALA	4.1
2	2-N	392	ALA	4.1
1	1-G	233	ASN	4.1
1	2-G	233	ASN	4.1
1	1-G	112	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	1-G	242	GLY	4.1
1	2-G	112	GLY	4.1
1	2-G	242	GLY	4.1
2	1-N	325	ASP	4.1
2	2-N	325	ASP	4.1
1	1-B	167	PRO	4.1
1	2-B	167	PRO	4.1
1	1-G	125	PRO	4.0
1	2-G	125	PRO	4.0
2	1-N	26	GLY	4.0
2	1-N	48	LEU	4.0
2	2-N	26	GLY	4.0
2	2-N	48	LEU	4.0
1	1-G	14	ASN	4.0
1	1-G	143	ASN	4.0
1	2-G	14	ASN	4.0
1	2-G	143	ASN	4.0
2	1-N	190	ALA	4.0
2	2-N	190	ALA	4.0
1	1-G	175	PRO	4.0
1	2-G	175	PRO	4.0
2	1-N	411	LEU	4.0
2	1-N	519	LEU	4.0
2	2-N	411	LEU	4.0
2	2-N	519	LEU	4.0
2	1-J	36	ASN	4.0
2	2-J	36	ASN	4.0
2	1-N	317	THR	4.0
2	2-N	317	THR	4.0
2	1-N	239	ASN	4.0
2	2-N	239	ASN	4.0
1	1-G	59	ALA	4.0
1	2-G	59	ALA	4.0
2	1-I	322	GLY	4.0
2	2-I	322	GLY	4.0
2	1-N	195	PRO	4.0
2	2-N	195	PRO	4.0
1	1-G	82	ASP	4.0
1	1-G	224	TYR	4.0
1	2-G	82	ASP	4.0
1	2-G	224	TYR	4.0
2	1-N	413	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	2-N	413	VAL	4.0
2	1-N	136	ALA	4.0
2	1-N	387	ALA	4.0
2	2-N	136	ALA	4.0
2	2-N	387	ALA	4.0
2	1-N	243	LEU	4.0
2	2-N	243	LEU	4.0
1	1-G	94	MET	4.0
1	2-G	94	MET	4.0
1	1-G	152	ILE	4.0
1	2-G	152	ILE	4.0
2	1-I	453	ASP	3.9
2	1-N	115	HIS	3.9
2	2-I	453	ASP	3.9
2	2-N	115	HIS	3.9
2	1-N	127	TRP	3.9
2	2-N	127	TRP	3.9
2	1-N	249	ALA	3.9
2	2-N	249	ALA	3.9
2	1-N	31	MET	3.9
2	2-N	31	MET	3.9
2	1-N	306	LEU	3.9
2	1-N	498	PRO	3.9
2	2-N	306	LEU	3.9
2	2-N	498	PRO	3.9
2	1-N	234	VAL	3.9
2	2-N	234	VAL	3.9
2	1-N	428	ARG	3.9
2	2-N	428	ARG	3.9
1	1-G	5	HIS	3.9
1	2-G	5	HIS	3.9
2	1-N	305	HIS	3.9
2	2-N	305	HIS	3.9
2	1-N	62	ARG	3.9
2	2-N	62	ARG	3.9
2	1-N	109	SER	3.9
2	2-N	109	SER	3.9
2	1-N	448	ASP	3.9
2	2-N	448	ASP	3.9
2	1-N	118	HIS	3.9
2	2-N	118	HIS	3.9
2	1-N	201	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	2-N	201	ALA	3.8
2	1-N	495	LEU	3.8
2	2-N	495	LEU	3.8
2	1-N	217	SER	3.8
2	2-N	217	SER	3.8
1	1-G	119	GLY	3.8
1	2-G	119	GLY	3.8
2	1-N	416	THR	3.8
2	2-N	416	THR	3.8
2	1-N	536	THR	3.8
2	2-N	536	THR	3.8
2	1-N	50	ARG	3.8
2	2-N	50	ARG	3.8
2	1-N	203	ALA	3.8
2	1-N	399	ASP	3.8
2	2-N	203	ALA	3.8
2	2-N	399	ASP	3.8
2	1-I	148	ILE	3.7
2	2-I	148	ILE	3.7
2	1-N	312	PRO	3.7
2	2-N	312	PRO	3.7
1	1-G	37	LEU	3.7
1	2-G	37	LEU	3.7
2	1-N	284	GLY	3.7
2	2-N	284	GLY	3.7
1	1-G	183	VAL	3.7
1	2-G	183	VAL	3.7
2	1-N	164	GLN	3.7
2	2-N	164	GLN	3.7
2	1-N	35	GLU	3.7
2	2-N	35	GLU	3.7
2	1-N	538	HIS	3.7
2	2-N	538	HIS	3.7
2	1-N	98	ASN	3.7
2	2-N	98	ASN	3.7
2	1-N	480	SER	3.7
2	2-N	480	SER	3.7
1	1-G	241	ALA	3.7
1	2-G	241	ALA	3.7
2	1-M	378	GLY	3.7
2	1-N	504	GLY	3.7
2	1-N	540	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	2-M	378	GLY	3.7
2	2-N	504	GLY	3.7
2	2-N	540	PHE	3.7
2	1-N	446	MET	3.7
2	2-N	446	MET	3.7
2	1-N	44	SER	3.7
2	2-N	44	SER	3.7
2	1-N	282	GLY	3.7
2	2-N	282	GLY	3.7
2	1-M	343	PRO	3.6
2	1-N	84	SER	3.6
2	2-M	343	PRO	3.6
2	2-N	84	SER	3.6
2	1-N	423	GLY	3.6
2	2-N	423	GLY	3.6
2	1-N	273	VAL	3.6
2	2-N	273	VAL	3.6
2	1-N	114	ASP	3.6
2	2-N	114	ASP	3.6
2	1-N	29	ARG	3.6
2	2-N	29	ARG	3.6
2	1-N	337	LYS	3.6
2	2-N	337	LYS	3.6
2	1-N	18	VAL	3.6
2	1-N	19	ASP	3.6
2	2-N	18	VAL	3.6
2	2-N	19	ASP	3.6
1	1-G	26	ARG	3.6
1	2-G	26	ARG	3.6
2	1-N	473	ASP	3.6
2	2-N	473	ASP	3.6
2	1-N	469	VAL	3.6
2	2-N	469	VAL	3.6
2	1-N	408	LEU	3.6
2	2-N	408	LEU	3.6
2	1-N	388	ARG	3.6
2	2-N	388	ARG	3.6
2	1-N	158	LYS	3.6
2	1-N	256	LYS	3.6
2	2-N	158	LYS	3.6
2	2-N	256	LYS	3.6
1	1-B	194	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	2-B	194	GLU	3.6
2	1-N	87	VAL	3.6
2	1-N	309	SER	3.6
2	2-N	87	VAL	3.6
2	2-N	309	SER	3.6
2	1-N	12	PHE	3.5
2	2-N	12	PHE	3.5
2	1-N	270	LEU	3.5
2	2-N	270	LEU	3.5
2	1-J	37	GLY	3.5
2	1-N	245	LYS	3.5
2	2-J	37	GLY	3.5
2	2-N	245	LYS	3.5
2	1-N	537	VAL	3.5
2	2-N	537	VAL	3.5
1	1-G	101	ALA	3.5
1	2-G	101	ALA	3.5
2	1-N	478	ALA	3.5
2	2-N	478	ALA	3.5
2	1-N	238	SER	3.5
2	2-N	238	SER	3.5
2	1-N	471	LEU	3.5
2	2-N	471	LEU	3.5
2	1-N	328	ASP	3.5
2	2-N	328	ASP	3.5
1	1-G	75	GLU	3.5
1	2-G	75	GLU	3.5
2	1-N	58	GLY	3.5
2	2-N	58	GLY	3.5
2	1-N	271	LEU	3.5
2	2-N	271	LEU	3.5
1	1-G	187	CYS	3.5
1	2-G	187	CYS	3.5
2	1-N	545	ALA	3.5
2	2-N	545	ALA	3.5
2	1-N	475	PRO	3.5
2	2-N	475	PRO	3.5
2	1-H	146	ALA	3.5
2	2-H	146	ALA	3.5
2	1-N	421	THR	3.5
2	2-N	421	THR	3.5
2	1-N	285	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	1-N	300	SER	3.5
2	2-N	285	GLY	3.5
2	2-N	300	SER	3.5
2	1-H	6	PRO	3.4
2	1-N	268	PRO	3.4
2	2-H	6	PRO	3.4
2	2-N	268	PRO	3.4
2	1-N	124	ALA	3.4
2	1-N	274	ALA	3.4
2	2-N	124	ALA	3.4
2	2-N	274	ALA	3.4
2	1-N	384	GLY	3.4
2	2-N	384	GLY	3.4
2	1-N	299	ASP	3.4
2	2-N	299	ASP	3.4
2	1-N	95	ILE	3.4
2	1-N	434	ILE	3.4
2	2-N	95	ILE	3.4
2	2-N	434	ILE	3.4
2	1-N	308	THR	3.4
2	2-N	308	THR	3.4
2	1-N	442	TRP	3.4
2	2-N	442	TRP	3.4
2	1-N	503	LEU	3.4
2	2-N	503	LEU	3.4
2	1-N	497	VAL	3.4
2	2-N	497	VAL	3.4
2	1-N	351	TYR	3.4
2	2-N	351	TYR	3.4
2	1-N	298	ASP	3.4
2	2-N	298	ASP	3.4
2	1-N	193	LEU	3.4
2	2-N	193	LEU	3.4
2	1-N	101	MET	3.4
2	2-N	101	MET	3.4
1	1-G	236	ASN	3.4
1	2-G	236	ASN	3.4
2	1-N	375	ARG	3.4
2	2-N	375	ARG	3.4
2	1-N	61	PRO	3.4
2	2-N	61	PRO	3.4
1	1-A	163	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	2-A	163	THR	3.4
1	1-G	83	GLY	3.4
1	2-G	83	GLY	3.4
1	1-B	61	HIS	3.3
1	2-B	61	HIS	3.3
2	1-N	79	HIS	3.3
2	2-N	79	HIS	3.3
2	1-N	335	ASP	3.3
2	1-N	505	PRO	3.3
2	2-N	335	ASP	3.3
2	2-N	505	PRO	3.3
2	1-N	110	GLN	3.3
2	1-N	144	LEU	3.3
2	2-N	110	GLN	3.3
2	2-N	144	LEU	3.3
2	1-N	529	ARG	3.3
2	2-N	529	ARG	3.3
1	1-B	168	ASP	3.3
1	2-B	168	ASP	3.3
2	1-N	276	PHE	3.3
2	2-N	276	PHE	3.3
1	1-G	39	THR	3.3
1	2-G	39	THR	3.3
2	1-N	198	ASN	3.3
2	1-N	524	ILE	3.3
2	2-N	198	ASN	3.3
2	2-N	524	ILE	3.3
2	1-N	382	GLU	3.3
2	2-N	382	GLU	3.3
2	1-N	259	CYS	3.3
2	2-N	259	CYS	3.3
2	1-J	343	PRO	3.3
2	1-N	215	ALA	3.3
2	2-J	343	PRO	3.3
2	2-N	215	ALA	3.3
2	1-N	191	TYR	3.3
2	2-N	191	TYR	3.3
1	1-G	173	GLY	3.3
1	2-G	173	GLY	3.3
2	1-N	151	ALA	3.3
2	1-N	528	LYS	3.3
2	2-N	151	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	2-N	528	LYS	3.3
2	1-N	318	GLY	3.3
2	2-N	318	GLY	3.3
2	1-N	194	PRO	3.3
2	2-N	194	PRO	3.3
2	1-N	494	GLN	3.3
2	2-N	494	GLN	3.3
2	1-N	439	MET	3.3
2	2-N	439	MET	3.3
1	1-B	139	VAL	3.3
1	2-B	139	VAL	3.3
1	1-B	264	GLY	3.2
1	2-B	264	GLY	3.2
2	1-N	511	ASP	3.2
2	2-N	511	ASP	3.2
2	1-N	549	HIS	3.2
2	2-N	549	HIS	3.2
2	1-N	512	LYS	3.2
2	2-N	512	LYS	3.2
2	1-N	352	ASP	3.2
2	1-N	357	PRO	3.2
2	2-N	352	ASP	3.2
2	2-N	357	PRO	3.2
2	1-N	40	LYS	3.2
2	1-N	502	ASN	3.2
2	2-N	40	LYS	3.2
2	2-N	502	ASN	3.2
1	1-G	85	GLN	3.2
1	2-G	85	GLN	3.2
2	1-I	398	PRO	3.2
2	2-I	398	PRO	3.2
1	1-B	224	TYR	3.2
1	2-B	224	TYR	3.2
2	1-N	450	GLY	3.2
2	1-N	477	GLY	3.2
2	2-N	450	GLY	3.2
2	2-N	477	GLY	3.2
2	1-N	45	SER	3.2
2	2-N	45	SER	3.2
2	1-H	139	ASN	3.2
2	1-N	294	GLU	3.2
2	2-H	139	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	2-N	294	GLU	3.2
1	1-G	128	SER	3.2
1	2-G	128	SER	3.2
2	1-N	542	PRO	3.2
2	2-N	542	PRO	3.2
2	1-N	345	GLY	3.2
2	2-N	345	GLY	3.2
1	1-G	22	GLU	3.2
1	2-G	22	GLU	3.2
1	1-C	67	LYS	3.2
1	2-C	67	LYS	3.2
2	1-J	11	THR	3.2
2	1-N	455	THR	3.2
2	2-J	11	THR	3.2
2	2-N	455	THR	3.2
2	1-N	210	HIS	3.1
2	1-N	507	GLY	3.1
2	2-N	210	HIS	3.1
2	2-N	507	GLY	3.1
2	1-H	151	ALA	3.1
2	1-N	474	ALA	3.1
2	2-H	151	ALA	3.1
2	2-N	474	ALA	3.1
1	1-B	138	GLY	3.1
1	2-B	138	GLY	3.1
2	1-N	9	GLN	3.1
2	1-N	371	MET	3.1
2	2-N	9	GLN	3.1
2	2-N	371	MET	3.1
1	1-G	129	GLN	3.1
1	2-G	129	GLN	3.1
2	1-N	55	ILE	3.1
2	2-N	55	ILE	3.1
2	1-N	449	SER	3.1
2	2-N	449	SER	3.1
1	1-G	212	CYS	3.1
1	2-G	212	CYS	3.1
2	1-I	146	ALA	3.1
2	1-N	436	CYS	3.1
2	2-I	146	ALA	3.1
2	2-N	436	CYS	3.1
2	1-N	60	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	1-N	168	LYS	3.1
2	1-N	304	LYS	3.1
2	2-N	60	ASP	3.1
2	2-N	168	LYS	3.1
2	2-N	304	LYS	3.1
2	1-N	500	THR	3.1
2	2-N	500	THR	3.1
2	1-I	448	ASP	3.1
2	2-I	448	ASP	3.1
2	1-M	148	ILE	3.1
2	2-M	148	ILE	3.1
2	1-I	451	ALA	3.0
2	2-I	451	ALA	3.0
2	1-N	7	THR	3.0
2	1-N	10	SER	3.0
2	2-N	7	THR	3.0
2	2-N	10	SER	3.0
2	1-N	269	ASP	3.0
2	2-N	269	ASP	3.0
2	1-I	6	PRO	3.0
2	2-I	6	PRO	3.0
2	1-N	47	GLN	3.0
2	2-N	47	GLN	3.0
1	1-G	184	HIS	3.0
1	2-G	184	HIS	3.0
2	1-J	162	ALA	3.0
2	2-J	162	ALA	3.0
2	1-N	303	SER	3.0
2	1-N	339	SER	3.0
2	2-N	303	SER	3.0
2	2-N	339	SER	3.0
2	1-N	372	LYS	3.0
2	1-N	459	LYS	3.0
2	2-N	372	LYS	3.0
2	2-N	459	LYS	3.0
2	1-J	148	ILE	3.0
2	2-J	148	ILE	3.0
2	1-N	123	HIS	3.0
2	1-N	212	GLN	3.0
2	2-N	123	HIS	3.0
2	2-N	212	GLN	3.0
2	1-N	541	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	2-N	541	ASP	3.0
1	1-G	102	ALA	3.0
1	2-G	102	ALA	3.0
2	1-K	157	ALA	3.0
2	1-N	162	ALA	3.0
2	1-N	461	GLU	3.0
2	2-K	157	ALA	3.0
2	2-N	162	ALA	3.0
2	2-N	461	GLU	3.0
1	1-G	28	ILE	3.0
1	2-G	28	ILE	3.0
2	1-N	283	ILE	3.0
2	2-N	283	ILE	3.0
2	1-N	288	ASN	3.0
2	2-N	288	ASN	3.0
1	1-G	174	ARG	3.0
1	2-G	174	ARG	3.0
1	1-G	255	ASP	3.0
1	2-G	255	ASP	3.0
2	1-N	313	SER	3.0
2	2-N	313	SER	3.0
1	1-G	106	LYS	2.9
1	1-G	131	LYS	2.9
1	2-G	106	LYS	2.9
1	2-G	131	LYS	2.9
2	1-N	523	PRO	2.9
2	2-N	523	PRO	2.9
1	1-B	166	ILE	2.9
1	2-B	166	ILE	2.9
2	1-N	264	GLU	2.9
2	2-N	264	GLU	2.9
2	1-N	200	ILE	2.9
2	2-N	200	ILE	2.9
2	1-N	334	GLU	2.9
2	2-N	334	GLU	2.9
1	1-B	31	TYR	2.9
1	2-B	31	TYR	2.9
2	1-N	8	PRO	2.9
2	2-N	8	PRO	2.9
2	1-N	364	ASP	2.9
2	2-N	364	ASP	2.9
2	1-N	355	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	2-N	355	THR	2.9
1	1-G	176	LYS	2.9
1	2-G	176	LYS	2.9
1	1-G	201	SER	2.9
1	2-G	201	SER	2.9
2	1-N	25	GLU	2.9
2	2-N	25	GLU	2.9
1	1-A	195	ALA	2.9
1	2-A	195	ALA	2.9
2	1-M	157	ALA	2.9
2	1-N	476	ARG	2.9
2	1-N	506	ARG	2.9
2	2-M	157	ALA	2.9
2	2-N	476	ARG	2.9
2	2-N	506	ARG	2.9
1	1-D	4	LYS	2.9
1	2-D	4	LYS	2.9
1	1-B	5	HIS	2.8
1	2-B	5	HIS	2.8
2	1-N	218	ALA	2.8
2	2-N	218	ALA	2.8
2	1-N	277	TYR	2.8
2	2-N	277	TYR	2.8
2	1-J	378	GLY	2.8
2	2-J	378	GLY	2.8
1	1-G	209	LYS	2.8
1	2-G	209	LYS	2.8
2	1-I	415	ALA	2.8
2	2-I	415	ALA	2.8
2	1-M	37	GLY	2.8
2	2-M	37	GLY	2.8
2	1-N	93	VAL	2.8
2	1-N	197	VAL	2.8
2	2-N	93	VAL	2.8
2	2-N	197	VAL	2.8
1	1-G	34	ALA	2.8
1	2-G	34	ALA	2.8
1	1-B	171	SER	2.8
1	2-B	171	SER	2.8
1	1-G	192	HIS	2.8
1	2-G	192	HIS	2.8
2	1-N	481	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	2-N	481	HIS	2.8
2	1-N	515	VAL	2.8
2	2-N	515	VAL	2.8
2	1-N	103	ARG	2.8
2	1-N	301	SER	2.8
2	1-N	483	ILE	2.8
2	2-N	103	ARG	2.8
2	2-N	301	SER	2.8
2	2-N	483	ILE	2.8
2	1-N	94	SER	2.8
2	2-N	94	SER	2.8
2	1-N	235	GLY	2.8
2	1-N	236	GLY	2.8
2	1-N	314	GLY	2.8
2	2-N	235	GLY	2.8
2	2-N	236	GLY	2.8
2	2-N	314	GLY	2.8
1	1-B	164	LYS	2.8
1	2-B	164	LYS	2.8
2	1-N	522	THR	2.7
2	2-N	522	THR	2.7
2	1-N	85	ARG	2.7
2	2-N	85	ARG	2.7
2	1-I	412	SER	2.7
2	1-N	412	SER	2.7
2	2-I	412	SER	2.7
2	2-N	412	SER	2.7
2	1-M	5	LYS	2.7
2	1-N	59	ARG	2.7
2	1-N	100	ARG	2.7
2	2-M	5	LYS	2.7
2	2-N	59	ARG	2.7
2	2-N	100	ARG	2.7
2	1-N	513	SER	2.7
2	2-N	513	SER	2.7
2	1-H	5	LYS	2.7
2	1-K	35	GLU	2.7
2	2-H	5	LYS	2.7
2	2-K	35	GLU	2.7
2	1-N	169	ALA	2.7
2	2-N	169	ALA	2.7
1	1-G	197	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	2-G	197	GLU	2.7
2	1-N	275	GLY	2.7
2	1-N	380	ALA	2.7
2	2-N	275	GLY	2.7
2	2-N	380	ALA	2.7
1	1-B	190	LEU	2.7
1	1-G	182	LEU	2.7
1	2-B	190	LEU	2.7
1	2-G	182	LEU	2.7
1	1-G	68	ASP	2.7
1	2-G	68	ASP	2.7
2	1-N	255	SER	2.7
2	2-N	255	SER	2.7
1	1-D	3	ALA	2.7
1	2-D	3	ALA	2.7
2	1-M	317	THR	2.7
2	2-M	317	THR	2.7
1	1-G	221	PRO	2.7
1	2-G	221	PRO	2.7
2	1-I	487	GLY	2.7
2	2-I	487	GLY	2.7
2	1-N	444	LYS	2.6
2	2-N	444	LYS	2.6
2	1-I	450	GLY	2.6
2	1-N	37	GLY	2.6
2	2-I	450	GLY	2.6
2	2-N	37	GLY	2.6
2	1-N	405	ASP	2.6
2	2-N	405	ASP	2.6
1	1-B	163	THR	2.6
1	2-B	163	THR	2.6
2	1-I	11	THR	2.6
2	2-I	11	THR	2.6
1	1-G	134	SER	2.6
1	2-G	134	SER	2.6
2	1-N	252	LEU	2.6
2	2-N	252	LEU	2.6
2	1-N	126	ASP	2.6
2	2-N	126	ASP	2.6
1	1-G	188	PRO	2.6
1	2-G	188	PRO	2.6
2	1-N	398	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	2-N	398	PRO	2.6
2	1-N	241	GLN	2.6
2	2-N	241	GLN	2.6
2	1-K	36	ASN	2.6
2	1-M	139	ASN	2.6
2	2-K	36	ASN	2.6
2	2-M	139	ASN	2.6
1	1-G	33	ASP	2.6
1	1-G	240	GLN	2.6
1	2-G	33	ASP	2.6
1	2-G	240	GLN	2.6
2	1-N	263	ASN	2.6
2	2-N	263	ASN	2.6
2	1-N	97	ALA	2.6
2	2-N	97	ALA	2.6
1	1-F	177	LEU	2.6
1	2-F	177	LEU	2.6
2	1-J	10	SER	2.5
2	2-J	10	SER	2.5
2	1-N	192	TYR	2.5
2	2-N	192	TYR	2.5
1	1-G	122	LYS	2.5
1	2-G	122	LYS	2.5
2	1-K	318	GLY	2.5
2	2-K	318	GLY	2.5
1	1-B	3	ALA	2.5
1	2-B	3	ALA	2.5
2	1-N	14	GLY	2.5
2	2-N	14	GLY	2.5
1	1-G	170	ASP	2.5
1	2-G	170	ASP	2.5
1	1-B	104	LYS	2.5
1	1-B	198	PHE	2.5
1	1-B	211	PHE	2.5
1	1-G	140	LYS	2.5
1	2-B	104	LYS	2.5
1	2-B	198	PHE	2.5
1	2-B	211	PHE	2.5
1	2-G	140	LYS	2.5
2	1-N	189	LYS	2.5
2	1-N	214	LYS	2.5
2	2-N	189	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	2-N	214	LYS	2.5
2	1-N	454	ASN	2.5
2	2-N	454	ASN	2.5
1	1-G	220	GLY	2.5
1	2-G	220	GLY	2.5
2	1-I	151	ALA	2.5
2	1-N	82	ALA	2.5
2	2-I	151	ALA	2.5
2	2-N	82	ALA	2.5
1	1-G	124	LYS	2.5
1	2-G	124	LYS	2.5
1	1-G	186	ASN	2.5
1	2-G	186	ASN	2.5
2	1-N	104	ASN	2.5
2	2-N	104	ASN	2.5
2	1-I	409	GLY	2.5
2	2-I	409	GLY	2.5
1	1-G	210	GLY	2.5
1	2-G	210	GLY	2.5
1	1-A	4	LYS	2.5
1	2-A	4	LYS	2.5
2	1-I	5	LYS	2.5
2	1-M	323	LYS	2.5
2	2-I	5	LYS	2.5
2	2-M	323	LYS	2.5
2	1-N	431	GLU	2.4
2	2-N	431	GLU	2.4
1	1-B	180	GLY	2.4
1	2-B	180	GLY	2.4
2	1-H	322	GLY	2.4
2	2-H	322	GLY	2.4
1	1-B	191	PRO	2.4
1	2-B	191	PRO	2.4
2	1-M	11	THR	2.4
2	1-N	424	ARG	2.4
2	1-N	462	MET	2.4
2	2-M	11	THR	2.4
2	2-N	424	ARG	2.4
2	2-N	462	MET	2.4
1	1-B	205	GLU	2.4
1	2-B	205	GLU	2.4
2	1-J	139	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	1-M	36	ASN	2.4
2	2-J	139	ASN	2.4
2	2-M	36	ASN	2.4
2	1-N	57	LYS	2.4
2	2-N	57	LYS	2.4
1	1-B	195	ALA	2.4
1	2-B	195	ALA	2.4
2	1-N	493	PHE	2.4
2	2-N	493	PHE	2.4
2	1-J	322	GLY	2.4
2	2-J	322	GLY	2.4
2	1-I	173	SER	2.4
2	2-I	173	SER	2.4
2	1-J	35	GLU	2.4
2	2-J	35	GLU	2.4
1	1-B	68	ASP	2.4
1	2-B	68	ASP	2.4
1	1-B	179	TYR	2.4
1	2-B	179	TYR	2.4
1	1-G	164	LYS	2.4
1	2-G	164	LYS	2.4
2	1-M	12	PHE	2.4
2	2-M	12	PHE	2.4
2	1-H	142	ALA	2.4
2	2-H	142	ALA	2.4
2	1-N	358	LYS	2.4
2	2-N	358	LYS	2.4
1	1-B	177	LEU	2.3
1	2-B	177	LEU	2.3
2	1-M	397	GLN	2.3
2	2-M	397	GLN	2.3
2	1-N	440	GLU	2.3
2	2-N	440	GLU	2.3
2	1-N	414	PRO	2.3
2	2-N	414	PRO	2.3
2	1-N	319	ARG	2.3
2	2-N	319	ARG	2.3
2	1-N	204	HIS	2.3
2	2-N	204	HIS	2.3
1	1-B	246	LEU	2.3
1	2-B	246	LEU	2.3
2	1-I	321	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	2-I	321	LEU	2.3
2	1-N	165	ASP	2.3
2	2-N	165	ASP	2.3
1	1-G	139	VAL	2.3
1	2-G	139	VAL	2.3
1	1-G	130	ALA	2.3
1	2-G	130	ALA	2.3
2	1-N	257	GLU	2.3
2	1-N	485	ILE	2.3
2	2-N	257	GLU	2.3
2	2-N	485	ILE	2.3
1	1-B	193	PHE	2.3
1	2-B	193	PHE	2.3
1	1-G	126	ASN	2.3
1	2-G	126	ASN	2.3
2	1-H	223	GLY	2.3
2	2-H	223	GLY	2.3
1	1-G	84	GLY	2.2
1	2-G	84	GLY	2.2
2	1-N	15	PRO	2.2
2	2-N	15	PRO	2.2
2	1-I	402	LYS	2.2
2	2-I	402	LYS	2.2
2	1-N	91	VAL	2.2
2	2-N	91	VAL	2.2
1	1-B	204	SER	2.2
1	2-B	204	SER	2.2
2	1-N	166	LYS	2.2
2	2-N	166	LYS	2.2
1	1-B	184	HIS	2.2
1	1-G	160	HIS	2.2
1	2-B	184	HIS	2.2
1	2-G	160	HIS	2.2
2	1-N	302	PRO	2.2
2	1-N	404	VAL	2.2
2	2-N	302	PRO	2.2
2	2-N	404	VAL	2.2
2	1-K	13	THR	2.2
2	2-K	13	THR	2.2
1	1-C	69	GLY	2.2
1	1-F	171	SER	2.2
1	2-C	69	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	2-F	171	SER	2.2
2	1-I	324	VAL	2.2
2	2-I	324	VAL	2.2
1	1-B	100	LYS	2.2
1	2-B	100	LYS	2.2
2	1-N	161	LYS	2.2
2	1-N	467	LYS	2.2
2	2-N	161	LYS	2.2
2	2-N	467	LYS	2.2
2	1-H	253	ALA	2.2
2	2-H	253	ALA	2.2
1	1-B	65	GLU	2.2
1	2-B	65	GLU	2.2
2	1-K	322	GLY	2.2
2	2-K	322	GLY	2.2
1	1-G	162	LEU	2.2
1	2-G	162	LEU	2.2
2	1-N	38	LYS	2.2
2	2-N	38	LYS	2.2
2	1-M	393	TYR	2.2
2	2-M	393	TYR	2.2
2	1-I	491	ASP	2.2
2	1-J	417	ALA	2.2
2	1-N	491	ASP	2.2
2	1-N	525	ALA	2.2
2	2-I	491	ASP	2.2
2	2-J	417	ALA	2.2
2	2-N	491	ASP	2.2
2	2-N	525	ALA	2.2
1	1-A	162	LEU	2.1
1	2-A	162	LEU	2.1
2	1-M	466	SER	2.1
2	1-N	310	GLN	2.1
2	2-M	466	SER	2.1
2	2-N	310	GLN	2.1
2	1-N	323	LYS	2.1
2	2-N	323	LYS	2.1
2	1-N	535	ARG	2.1
2	2-N	535	ARG	2.1
2	1-N	353	GLY	2.1
2	2-N	353	GLY	2.1
1	1-G	96	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	2-G	96	GLU	2.1
2	1-M	416	THR	2.1
2	2-M	416	THR	2.1
2	1-N	89	ASP	2.1
2	2-N	89	ASP	2.1
1	1-F	190	LEU	2.1
1	2-F	190	LEU	2.1
1	1-F	264	GLY	2.1
1	2-F	264	GLY	2.1
2	1-N	140	LYS	2.1
2	2-N	140	LYS	2.1
2	1-N	532	GLU	2.1
2	2-N	532	GLU	2.1
2	1-I	154	GLY	2.1
2	2-I	154	GLY	2.1
2	1-I	444	LYS	2.1
2	2-I	444	LYS	2.1
2	1-K	394	ALA	2.1
2	1-N	159	ALA	2.1
2	2-K	394	ALA	2.1
2	2-N	159	ALA	2.1
2	1-I	246	ASP	2.1
2	2-I	246	ASP	2.1
2	1-M	330	GLY	2.1
2	2-M	330	GLY	2.1
1	1-B	38	ASP	2.1
1	2-B	38	ASP	2.1
2	1-J	12	PHE	2.1
2	2-J	12	PHE	2.1
1	1-B	160	HIS	2.1
1	1-F	92	HIS	2.1
1	2-B	160	HIS	2.1
1	2-F	92	HIS	2.1
2	1-K	14	GLY	2.1
2	2-K	14	GLY	2.1
2	1-I	172	GLU	2.0
2	1-N	464	GLU	2.0
2	2-I	172	GLU	2.0
2	2-N	464	GLU	2.0
1	1-A	190	LEU	2.0
1	2-A	190	LEU	2.0
2	1-J	174	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	2-J	174	GLY	2.0
2	1-J	331	ALA	2.0
2	2-J	331	ALA	2.0
1	1-A	211	PHE	2.0
1	2-A	211	PHE	2.0
1	1-B	196	SER	2.0
1	2-B	196	SER	2.0
1	1-B	30	PRO	2.0
1	2-B	30	PRO	2.0
2	1-J	463	PRO	2.0
2	2-J	463	PRO	2.0
1	1-B	4	LYS	2.0
1	2-B	4	LYS	2.0
2	1-I	399	ASP	2.0
2	2-I	399	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	1-G	265	8/8	0.85	0.32	4,6,7,8	8
3	SF4	2-G	265	8/8	0.85	0.32	8,10,11,12	8
6	MG	1-N	553	1/1	0.86	0.27	8,8,8,8	1
6	MG	2-N	553	1/1	0.86	0.27	8,8,8,8	1
4	F3S	1-G	266	7/7	0.92	0.36	8,9,11,11	7
4	F3S	2-G	266	7/7	0.92	0.36	10,10,11,11	7
6	MG	1-M	553	1/1	0.95	0.13	8,8,8,8	0
6	MG	2-M	553	1/1	0.95	0.13	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	1-G	267	8/8	0.96	0.41	7,10,10,12	8
3	SF4	2-G	267	8/8	0.96	0.41	7,10,10,12	8
6	MG	1-H	553	1/1	0.96	0.06	8,8,8,8	0
6	MG	2-H	553	1/1	0.96	0.06	8,8,8,8	0
6	MG	1-K	553	1/1	0.97	0.07	3,3,3,3	0
6	MG	2-K	553	1/1	0.97	0.07	3,3,3,3	0
3	SF4	1-A	265	8/8	0.97	0.05	7,9,10,12	0
3	SF4	2-A	265	8/8	0.97	0.05	7,9,10,12	0
6	MG	1-J	553	1/1	0.97	0.09	5,5,5,5	0
6	MG	2-J	553	1/1	0.97	0.09	5,5,5,5	0
7	FCO	1-N	550	7/7	0.97	0.37	5,6,7,9	7
7	FCO	2-N	550	7/7	0.97	0.37	5,6,7,9	7
4	F3S	1-D	266	7/7	0.98	0.04	7,8,10,10	0
4	F3S	2-D	266	7/7	0.98	0.04	7,8,10,10	0
4	F3S	1-F	266	7/7	0.98	0.05	7,9,12,12	0
4	F3S	2-F	266	7/7	0.98	0.05	7,9,12,12	0
3	SF4	1-B	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	2-B	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	1-F	265	8/8	0.98	0.06	6,7,10,10	0
3	SF4	2-F	265	8/8	0.98	0.06	6,7,10,10	0
3	SF4	1-F	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	2-F	267	8/8	0.98	0.05	4,8,9,10	0
3	SF4	1-A	267	8/8	0.98	0.05	7,8,10,11	0
3	SF4	2-A	267	8/8	0.98	0.05	7,8,10,11	0
3	SF4	1-B	265	8/8	0.98	0.09	5,6,9,9	0
3	SF4	2-B	265	8/8	0.98	0.09	5,6,9,9	0
4	F3S	1-A	266	7/7	0.98	0.05	6,7,10,13	0
4	F3S	2-A	266	7/7	0.98	0.05	6,7,10,13	0
4	F3S	1-B	266	7/7	0.98	0.06	9,10,10,10	0
4	F3S	2-B	266	7/7	0.98	0.06	9,10,10,10	0
5	NI	1-N	551	1/1	0.99	0.32	13,13,13,13	1
5	NI	2-N	551	1/1	0.99	0.32	12,12,12,12	1
3	SF4	1-C	267	8/8	0.99	0.04	5,9,10,10	0
3	SF4	2-C	267	8/8	0.99	0.04	5,9,10,10	0
6	MG	1-I	553	1/1	0.99	0.07	6,6,6,6	0
6	MG	2-I	553	1/1	0.99	0.07	6,6,6,6	0
4	F3S	1-C	266	7/7	0.99	0.04	9,10,11,12	0
4	F3S	2-C	266	7/7	0.99	0.04	9,10,11,12	0
3	SF4	1-D	265	8/8	0.99	0.03	6,8,9,9	0
3	SF4	2-D	265	8/8	0.99	0.03	6,8,9,9	0
3	SF4	1-D	267	8/8	0.99	0.04	3,7,9,9	0
3	SF4	2-D	267	8/8	0.99	0.04	3,7,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	1-C	265	8/8	0.99	0.04	6,6,8,9	0
3	SF4	2-C	265	8/8	0.99	0.04	6,6,8,9	0
7	FCO	1-H	550	7/7	0.99	0.06	8,9,11,13	0
7	FCO	2-H	550	7/7	0.99	0.06	8,9,11,13	0
7	FCO	1-K	550	7/7	0.99	0.07	6,8,10,12	0
7	FCO	2-K	550	7/7	0.99	0.07	6,8,10,12	0
7	FCO	1-M	550	7/7	0.99	0.10	4,6,7,12	0
7	FCO	2-M	550	7/7	0.99	0.10	4,6,7,12	0
5	NI	1-I	551	1/1	0.99	0.03	10,10,10,10	0
5	NI	2-I	551	1/1	0.99	0.03	10,10,10,10	0
5	NI	1-M	551	1/1	1.00	0.06	8,8,8,8	0
5	NI	2-M	551	1/1	1.00	0.06	8,8,8,8	0
7	FCO	1-I	550	7/7	1.00	0.06	3,5,8,9	0
7	FCO	2-I	550	7/7	1.00	0.06	3,5,8,9	0
7	FCO	1-J	550	7/7	1.00	0.08	7,7,11,12	0
7	FCO	2-J	550	7/7	1.00	0.08	7,7,11,12	0
5	NI	1-H	551	1/1	1.00	0.02	9,9,9,9	0
5	NI	2-H	551	1/1	1.00	0.02	9,9,9,9	0
5	NI	1-J	551	1/1	1.00	0.05	9,9,9,9	0
5	NI	2-J	551	1/1	1.00	0.05	9,9,9,9	0
5	NI	1-K	551	1/1	1.00	0.04	11,11,11,11	0
5	NI	2-K	551	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.