Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 05:41 pm BST

PDB ID	:	8RTF / pdb_00008rtf
Title	:	Crystal structure of Trypanosoma congolense pyruvate kinase in complex with a single-domain antibody (TcoPYK-sdAb42)
Authors	:	Sterckx, Y.G.-J.
Deposited on	:	2024-01-26
Resolution	:	2.80 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 ⓘ 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 ⓘ) were used in the production of this report:

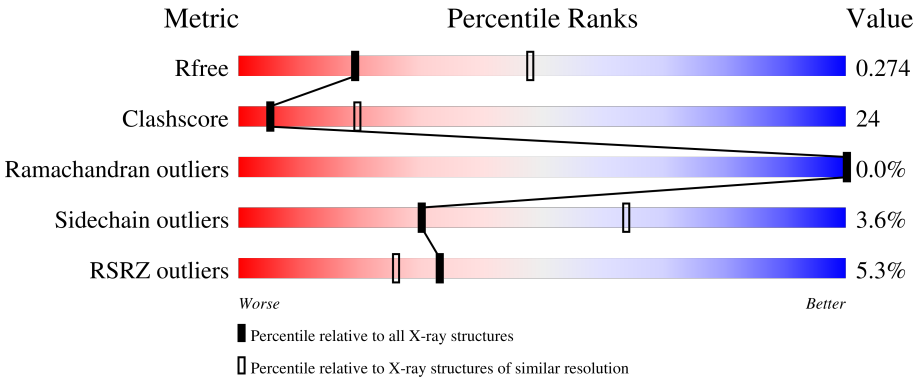
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	A	514	3% 66% 30%
1	B	514	% 50% 27% 21%
1	C	514	4% 61% 34%
1	D	514	2% 61% 33%
1	E	514	5% 46% 28% 23%

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Mol	Chain	Length	Quality of chain
1	F	514	12% 39% 33% 22%
2	G	149	65% 21% 13%
2	H	149	% 61% 23% 13%
2	I	149	3% 46% 32% 7% 13%
2	J	149	% 50% 34% 12%
2	K	149	17% 42% 36% 9% 13%
2	L	149	6% 42% 35% 10% 13%

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
3	GOL	A	601	-	X	-	-
3	GOL	B	701	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25898 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3687	2298	650	713	26			
1	B	404	Total	C	N	O	S	0	0	0
			2996	1859	537	577	23			
1	C	499	Total	C	N	O	S	0	1	0
			3672	2287	654	705	26			
1	D	499	Total	C	N	O	S	0	1	0
			3691	2300	654	711	26			
1	E	395	Total	C	N	O	S	0	0	0
			2920	1807	525	565	23			
1	F	399	Total	C	N	O	S	0	0	0
			2901	1802	515	562	22			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	515	GLU	-	expression tag	UNP G0UYF4
C	516	ASN	-	expression tag	UNP G0UYF4
C	517	LEU	-	expression tag	UNP G0UYF4
C	518	TYR	-	expression tag	UNP G0UYF4
C	519	PHE	-	expression tag	UNP G0UYF4
C	520	GLN	-	expression tag	UNP G0UYF4
C	521	SER	-	expression tag	UNP G0UYF4
C	522	GLY	-	expression tag	UNP G0UYF4
C	523	GLY	-	expression tag	UNP G0UYF4
C	524	HIS	-	expression tag	UNP G0UYF4
C	525	HIS	-	expression tag	UNP G0UYF4
C	526	HIS	-	expression tag	UNP G0UYF4
C	527	HIS	-	expression tag	UNP G0UYF4
C	528	HIS	-	expression tag	UNP G0UYF4
C	529	HIS	-	expression tag	UNP G0UYF4
D	515	GLU	-	expression tag	UNP G0UYF4
D	516	ASN	-	expression tag	UNP G0UYF4
D	517	LEU	-	expression tag	UNP G0UYF4
D	518	TYR	-	expression tag	UNP G0UYF4
D	519	PHE	-	expression tag	UNP G0UYF4
D	520	GLN	-	expression tag	UNP G0UYF4
D	521	SER	-	expression tag	UNP G0UYF4
D	522	GLY	-	expression tag	UNP G0UYF4
D	523	GLY	-	expression tag	UNP G0UYF4
D	524	HIS	-	expression tag	UNP G0UYF4
D	525	HIS	-	expression tag	UNP G0UYF4
D	526	HIS	-	expression tag	UNP G0UYF4
D	527	HIS	-	expression tag	UNP G0UYF4
D	528	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	529	HIS	-	expression tag	UNP G0UYF4
E	500	GLU	-	expression tag	UNP G0UYF4
E	501	ASN	-	expression tag	UNP G0UYF4
E	502	LEU	-	expression tag	UNP G0UYF4
E	503	TYR	-	expression tag	UNP G0UYF4
E	504	PHE	-	expression tag	UNP G0UYF4
E	505	GLN	-	expression tag	UNP G0UYF4
E	506	SER	-	expression tag	UNP G0UYF4
E	507	GLY	-	expression tag	UNP G0UYF4
E	508	GLY	-	expression tag	UNP G0UYF4
E	509	HIS	-	expression tag	UNP G0UYF4
E	510	HIS	-	expression tag	UNP G0UYF4
E	511	HIS	-	expression tag	UNP G0UYF4
E	512	HIS	-	expression tag	UNP G0UYF4
E	513	HIS	-	expression tag	UNP G0UYF4
E	514	HIS	-	expression tag	UNP G0UYF4
F	500	GLU	-	expression tag	UNP G0UYF4
F	501	ASN	-	expression tag	UNP G0UYF4
F	502	LEU	-	expression tag	UNP G0UYF4
F	503	TYR	-	expression tag	UNP G0UYF4
F	504	PHE	-	expression tag	UNP G0UYF4
F	505	GLN	-	expression tag	UNP G0UYF4
F	506	SER	-	expression tag	UNP G0UYF4
F	507	GLY	-	expression tag	UNP G0UYF4
F	508	GLY	-	expression tag	UNP G0UYF4
F	509	HIS	-	expression tag	UNP G0UYF4
F	510	HIS	-	expression tag	UNP G0UYF4
F	511	HIS	-	expression tag	UNP G0UYF4
F	512	HIS	-	expression tag	UNP G0UYF4
F	513	HIS	-	expression tag	UNP G0UYF4
F	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is a protein called Camelid single-domain antibody 42 (sdAb42).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	130	Total	C	N	O	S	0	0	0
			995	622	173	197	3			
2	H	130	Total	C	N	O	S	0	0	0
			998	623	173	199	3			
2	I	130	Total	C	N	O	S	0	0	0
			976	610	167	196	3			
2	J	131	Total	C	N	O	S	0	0	0
			1007	628	175	201	3			

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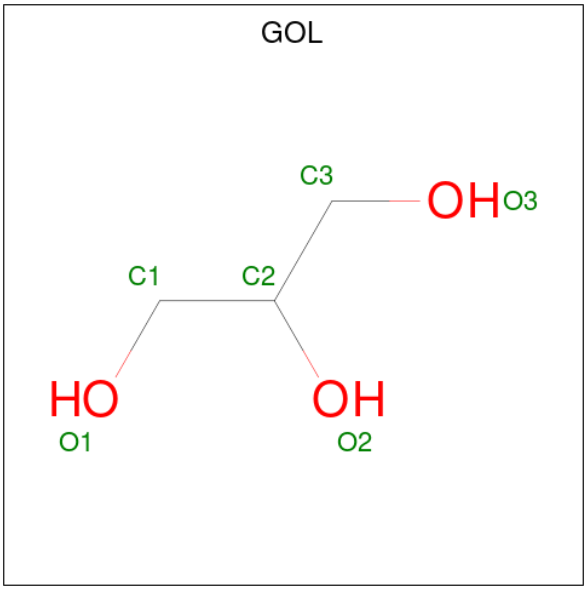
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	130	Total	C	N	O	S	0	0	0
			967	603	165	196	3			
2	L	130	Total	C	N	O	S	0	0	0
			942	585	160	194	3			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

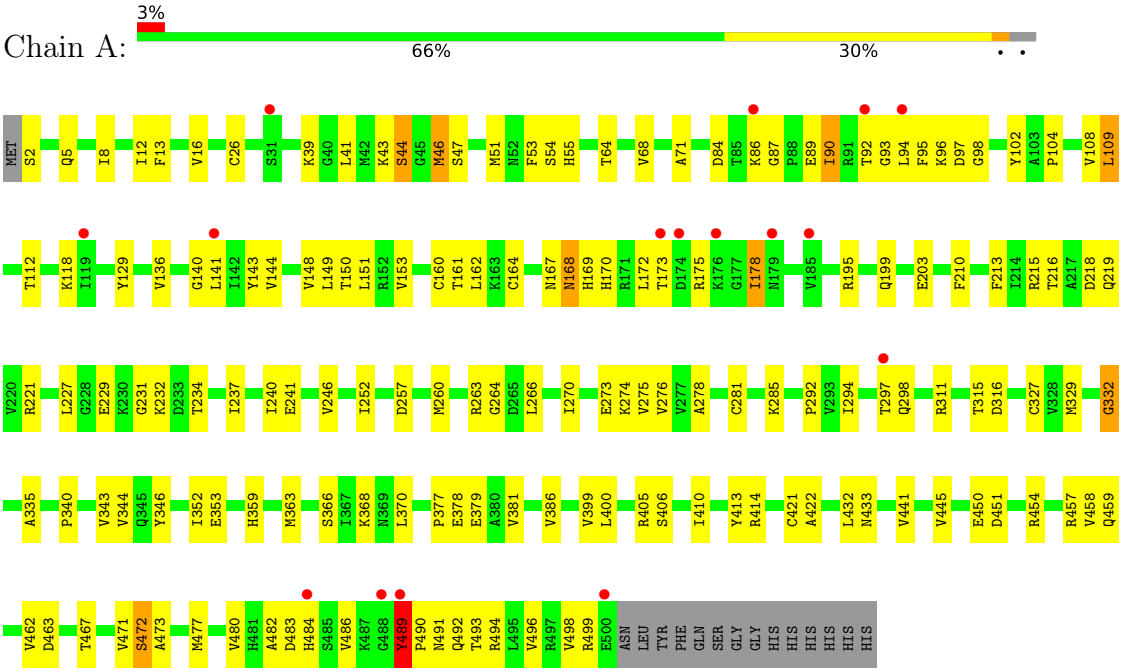
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	7	Total O 7 7	0	0
4	C	25	Total O 25 25	0	0
4	D	13	Total O 13 13	0	0
4	E	5	Total O 5 5	0	0
4	F	5	Total O 5 5	0	0
4	G	2	Total O 2 2	0	0
4	H	5	Total O 5 5	0	0
4	I	1	Total O 1 1	0	0
4	J	4	Total O 4 4	0	0
4	L	1	Total O 1 1	0	0

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.

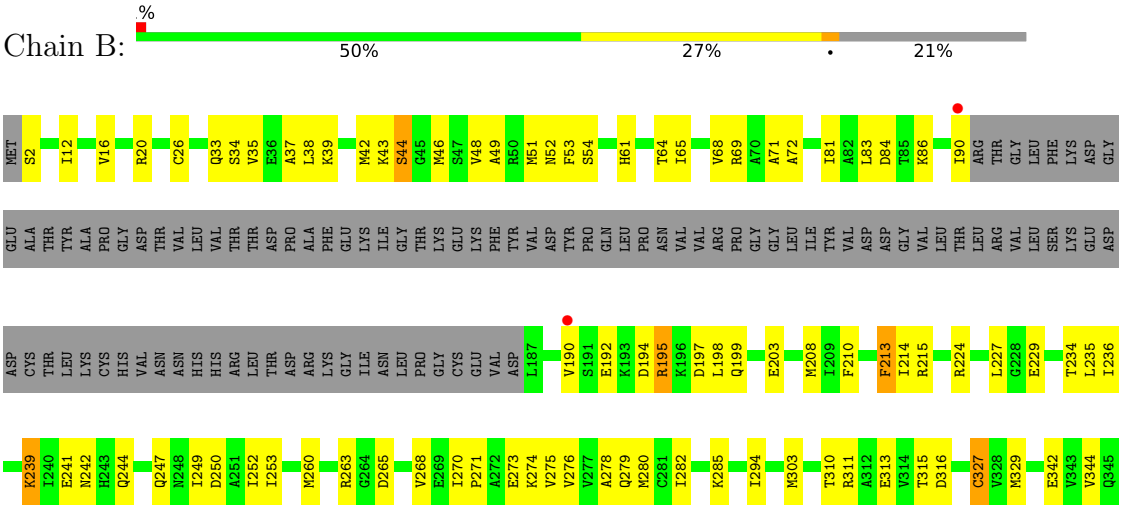
• Molecule 1: Pyruvate kinase

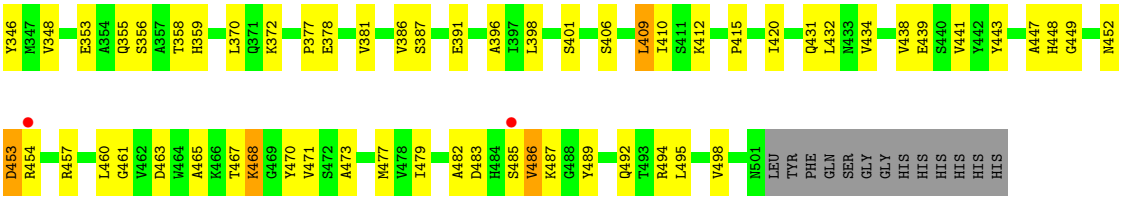
Chain A:



• Molecule 1: Pyruvate kinase

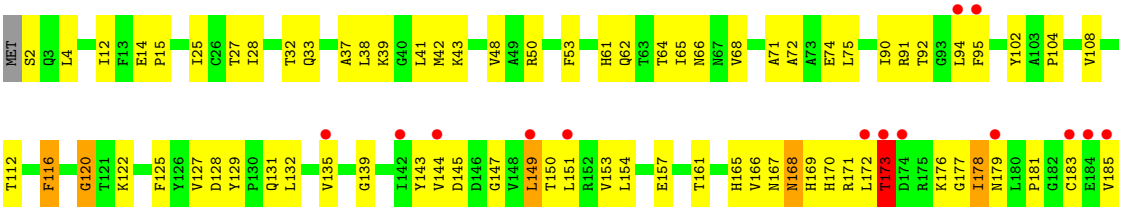
Chain B:

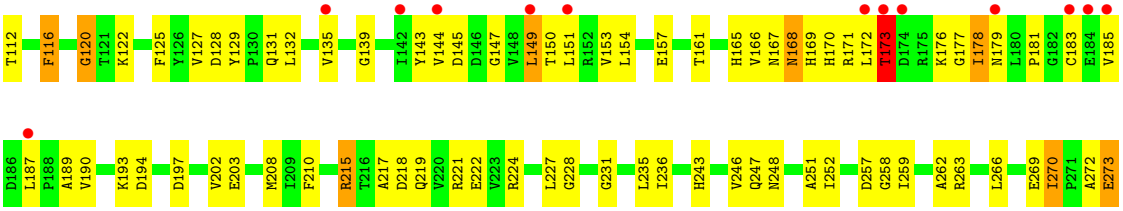


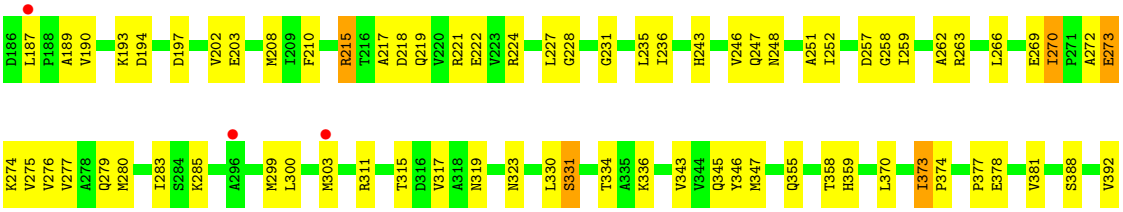


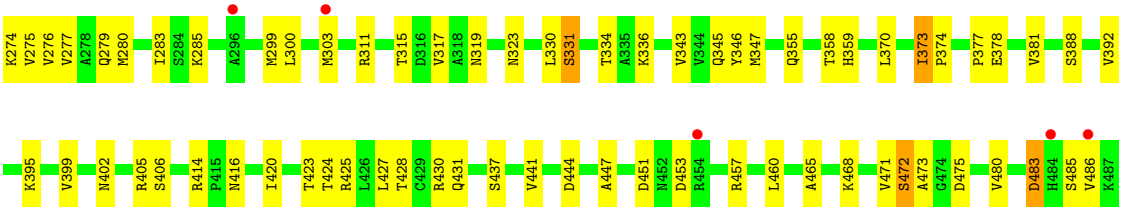
• Molecule 1: Pyruvate kinase

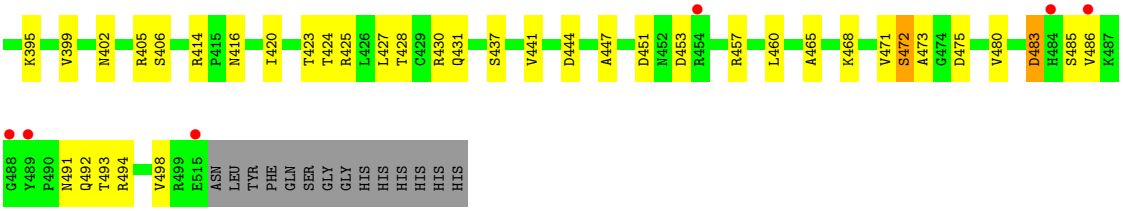
Chain C:





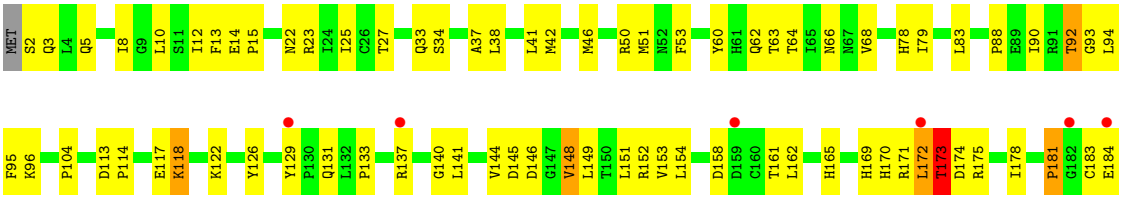


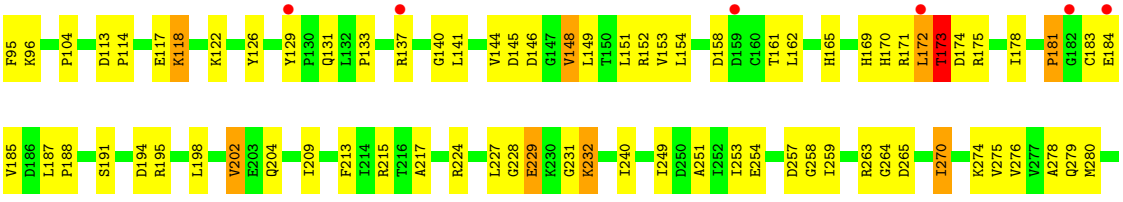


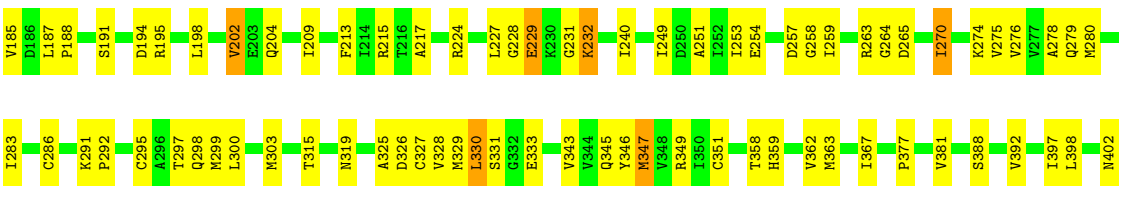


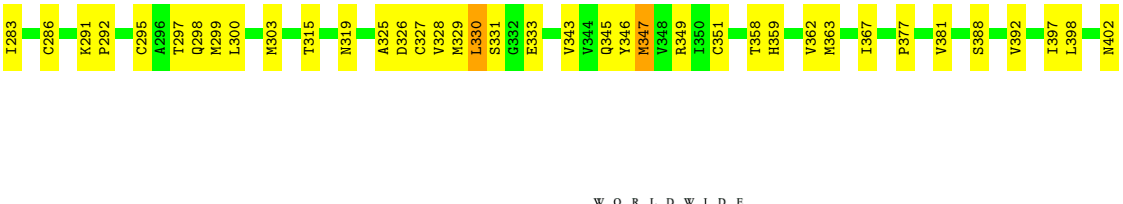
• Molecule 1: Pyruvate kinase

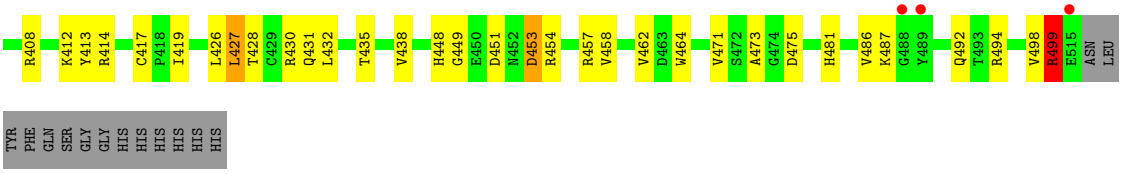
Chain D:



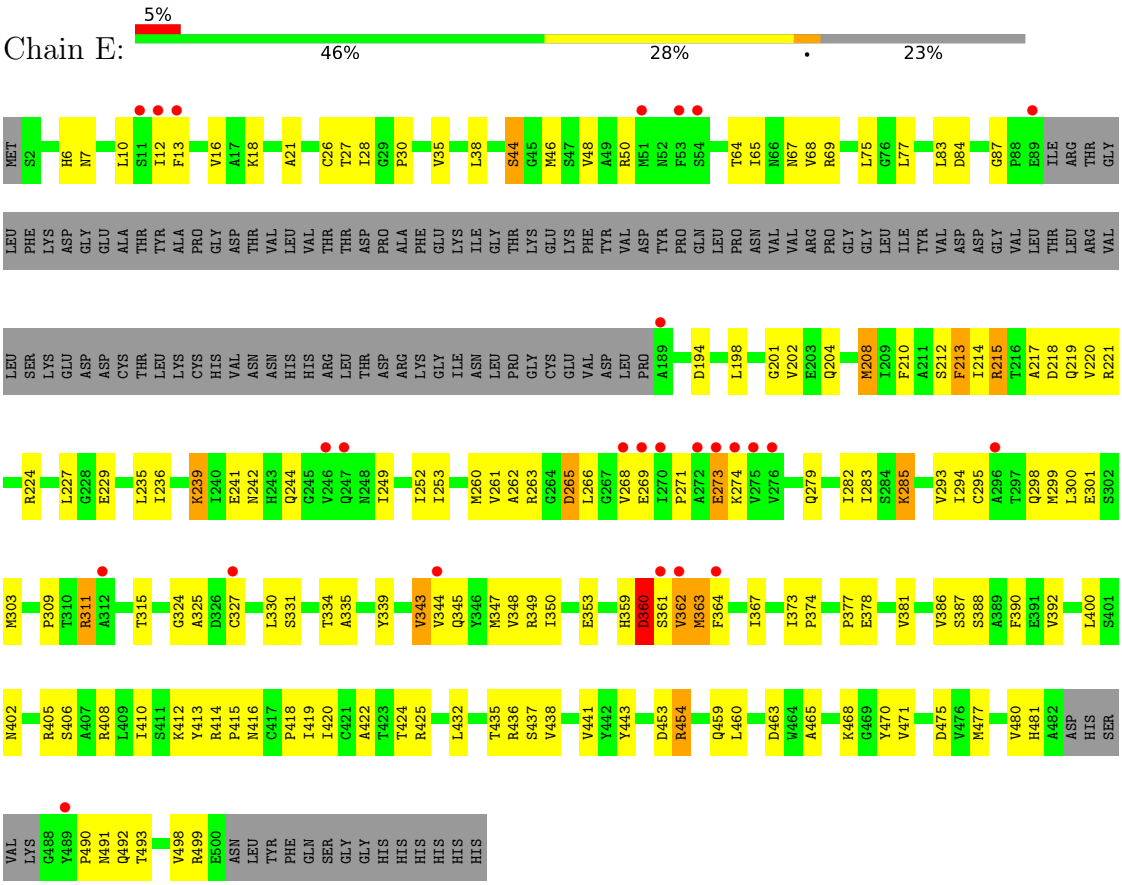




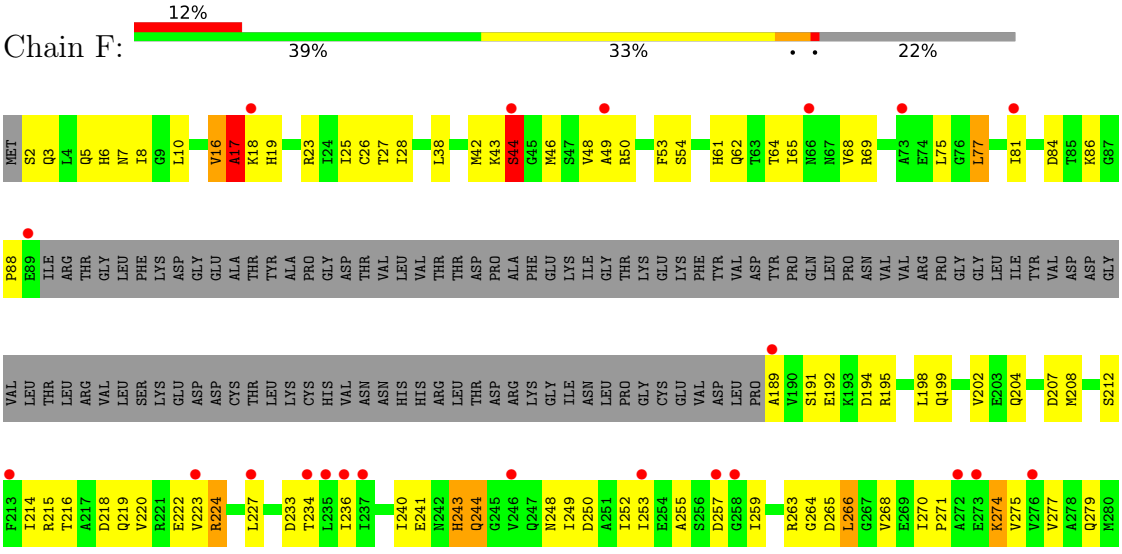


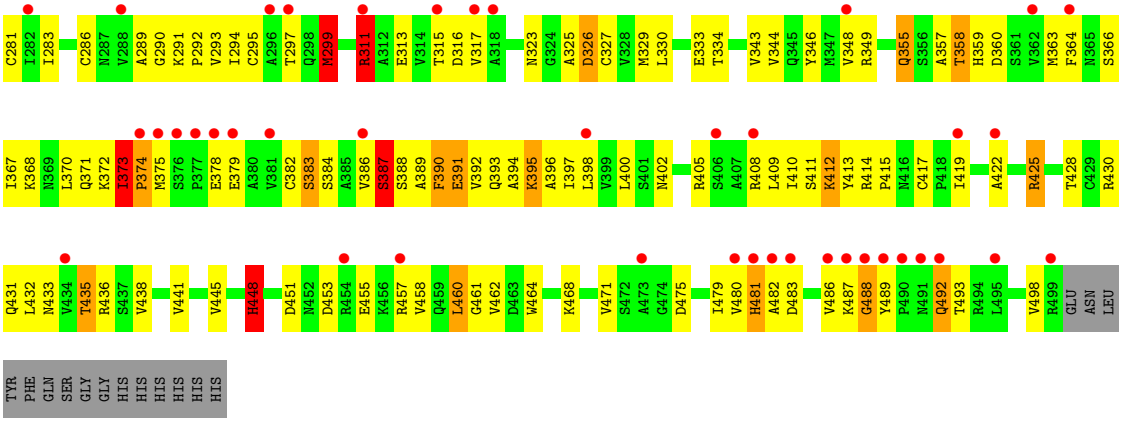


• Molecule 1: Pyruvate kinase



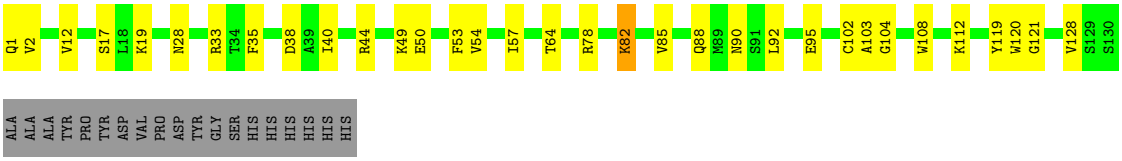
• Molecule 1: Pyruvate kinase





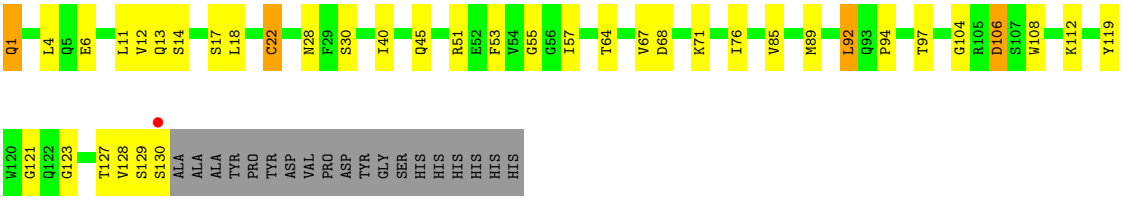
• Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain G:



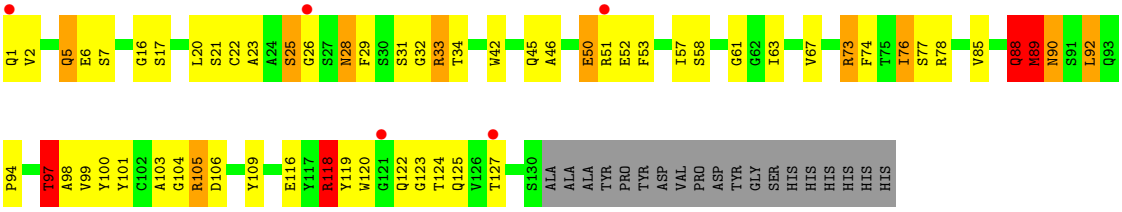
• Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain H:



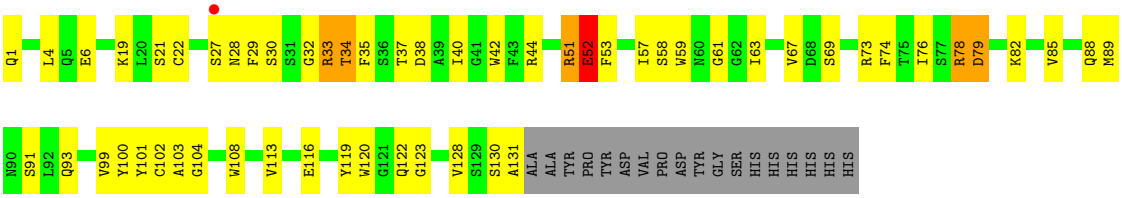
• Molecule 2: Camelid single-domain antibody 42 (sdAb42)

Chain I:

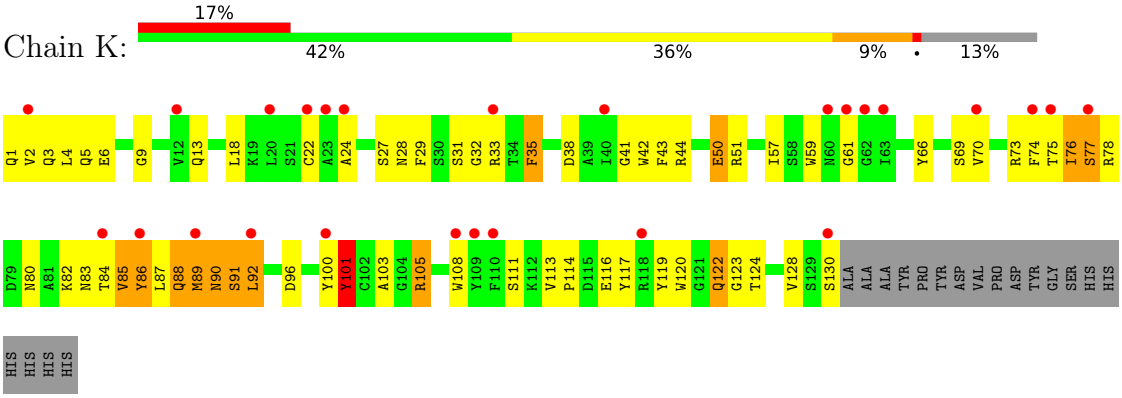


• Molecule 2: Camelid single-domain antibody 42 (sdAb42)

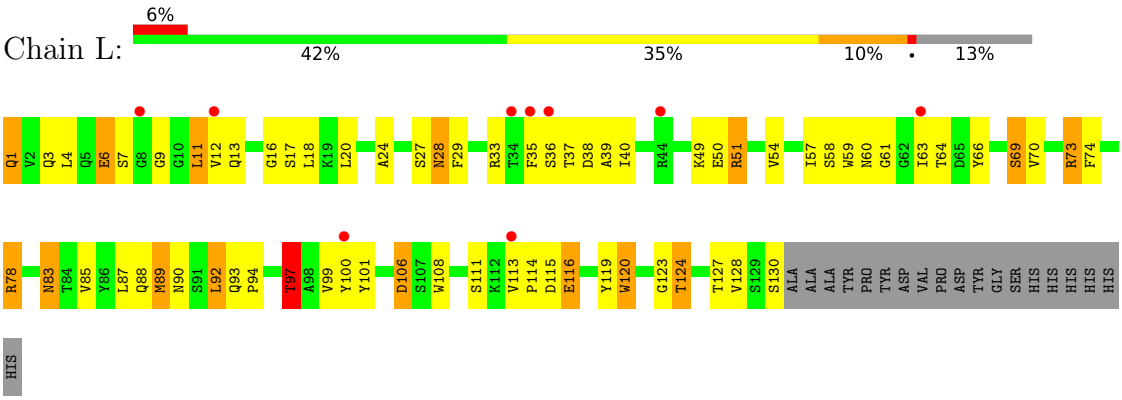
Chain J:



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



• Molecule 2: Camelid single-domain antibody 42 (sdAb42)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.52Å 170.81Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.80 48.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-2.80) 99.8 (48.35-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.228 , 0.272 0.236 , 0.274	Depositor DCC
R_{free} test set	6274 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	84.9	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25898	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL

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	A	0.70	1/3744 (0.0%)	0.89	5/5098 (0.1%)
1	B	0.72	3/3037 (0.1%)	0.91	6/4124 (0.1%)
1	C	0.70	1/3733 (0.0%)	0.96	20/5084 (0.4%)
1	D	0.65	3/3751 (0.1%)	0.94	15/5107 (0.3%)
1	E	0.65	1/2958 (0.0%)	1.03	13/4015 (0.3%)
1	F	0.75	5/2940 (0.2%)	1.24	32/4002 (0.8%)
2	G	0.86	3/1018 (0.3%)	0.99	5/1377 (0.4%)
2	H	0.69	0/1021	0.96	3/1381 (0.2%)
2	I	0.75	2/999 (0.2%)	1.19	15/1356 (1.1%)
2	J	0.67	0/1030	1.03	7/1393 (0.5%)
2	K	0.82	3/989 (0.3%)	1.39	16/1343 (1.2%)
2	L	0.74	2/964 (0.2%)	1.30	16/1314 (1.2%)
All	All	0.71	24/26184 (0.1%)	1.03	153/35594 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	4
1	D	0	3
1	E	0	1
1	F	0	8
2	G	0	1
2	I	0	5
2	J	0	2
2	K	0	5
2	L	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	35

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	91	SER	CB-OG	-14.07	1.24	1.42
1	F	374	PRO	N-CD	10.76	1.62	1.47
1	D	295	CYS	CB-SG	-9.04	1.66	1.82
1	F	391	GLU	C-O	8.36	1.39	1.23
2	I	88	GLN	CG-CD	-8.00	1.32	1.51
2	G	82	LYS	CE-NZ	7.57	1.68	1.49
1	B	327	CYS	CB-SG	-7.52	1.69	1.82
2	L	51	ARG	CG-CD	7.40	1.70	1.51
2	G	82	LYS	CD-CE	6.44	1.67	1.51
1	D	229	GLU	CG-CD	5.96	1.60	1.51
2	G	50	GLU	CD-OE1	5.92	1.32	1.25
2	L	51	ARG	CB-CG	5.89	1.68	1.52
1	A	441	VAL	CB-CG1	-5.83	1.40	1.52
1	F	387	SER	CB-OG	5.82	1.49	1.42
1	C	430	ARG	CG-CD	-5.75	1.37	1.51
2	K	101	TYR	CG-CD1	-5.72	1.31	1.39
1	F	390	PHE	CD2-CE2	-5.62	1.28	1.39
1	B	239	LYS	CE-NZ	5.54	1.62	1.49
1	B	273	GLU	CG-CD	5.46	1.60	1.51
2	I	97	THR	CB-CG2	5.45	1.70	1.52
1	E	239	LYS	CD-CE	-5.32	1.38	1.51
1	F	241	GLU	CG-CD	5.25	1.59	1.51
2	K	50	GLU	CB-CG	5.24	1.62	1.52
1	D	286	CYS	CB-SG	-5.20	1.73	1.81

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	391	GLU	OE1-CD-OE2	-19.83	99.51	123.30
1	F	460	LEU	CB-CG-CD2	-17.60	81.09	111.00
2	L	51	ARG	CG-CD-NE	15.62	144.61	111.80
1	E	361	SER	N-CA-C	15.55	152.99	111.00
2	K	50	GLU	CB-CA-C	-15.33	79.74	110.40
1	F	374	PRO	N-CA-C	-15.16	72.67	112.10
2	K	90	ASN	N-CA-C	14.47	150.06	111.00
1	C	120	GLY	N-CA-C	14.22	148.64	113.10
2	K	91	SER	N-CA-CB	13.74	131.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	50	GLU	CA-CB-CG	13.02	142.04	113.40
1	F	360	ASP	CB-CA-C	-12.94	84.53	110.40
1	E	361	SER	N-CA-CB	-12.93	91.11	110.50
1	E	361	SER	CB-CA-C	-12.78	85.82	110.10
2	J	35	PHE	N-CA-CB	-12.55	88.02	110.60
1	F	391	GLU	CA-CB-CG	12.52	140.94	113.40
1	F	375	MET	N-CA-CB	-12.23	88.58	110.60
1	F	372	LYS	CB-CA-C	-12.10	86.20	110.40
1	D	202	VAL	CG1-CB-CG2	-12.00	91.70	110.90
1	A	44	SER	CB-CA-C	-11.83	87.62	110.10
2	J	34	THR	N-CA-C	-11.61	79.67	111.00
1	C	178	ILE	CA-CB-CG1	11.16	132.20	111.00
1	F	391	GLU	CG-CD-OE2	11.10	140.49	118.30
2	L	92	LEU	CB-CG-CD2	-11.08	92.16	111.00
1	B	44	SER	CB-CA-C	-10.89	89.42	110.10
1	E	44	SER	CB-CA-C	-10.80	89.58	110.10
1	D	453	ASP	CB-CA-C	10.58	131.56	110.40
2	K	50	GLU	C-N-CA	10.38	147.64	121.70
2	K	90	ASN	CB-CA-C	-10.37	89.65	110.40
1	D	270	ILE	CG1-CB-CG2	-10.09	89.21	111.40
1	F	44	SER	CB-CA-C	-10.02	91.06	110.10
2	K	89	MET	CB-CA-C	-9.80	90.81	110.40
2	L	11	LEU	CB-CA-C	-9.76	91.65	110.20
1	B	468	LYS	CB-CA-C	9.50	129.41	110.40
2	K	77	SER	CB-CA-C	-9.28	92.47	110.10
1	D	453	ASP	N-CA-C	-9.24	86.04	111.00
1	A	472	SER	CB-CA-C	9.06	127.32	110.10
2	I	105	ARG	CB-CA-C	8.98	128.35	110.40
1	E	360	ASP	N-CA-C	8.94	135.14	111.00
2	I	46	ALA	CB-CA-C	8.68	123.12	110.10
1	F	227	LEU	CB-CA-C	8.65	126.64	110.20
1	E	468	LYS	CB-CA-C	8.57	127.53	110.40
1	D	92	THR	CB-CA-C	-8.40	88.91	111.60
1	B	485	SER	N-CA-C	8.40	133.69	111.00
1	F	311	ARG	CB-CG-CD	-8.36	89.86	111.60
1	F	227	LEU	N-CA-C	-8.36	88.44	111.00
1	B	485	SER	CB-CA-C	-8.28	94.37	110.10
1	F	17	ALA	N-CA-C	8.11	132.90	111.00
1	A	484	HIS	CB-CA-C	8.11	126.61	110.40
2	L	50	GLU	N-CA-CB	-7.98	96.24	110.60
2	I	97	THR	CA-CB-CG2	-7.91	101.33	112.40
2	J	52	GLU	CG-CD-OE2	-7.90	102.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	50	GLU	CA-CB-CG	7.88	130.75	113.40
2	I	25	SER	N-CA-C	7.76	131.94	111.00
2	L	13	GLN	CA-CB-CG	-7.73	96.40	113.40
1	C	173	THR	N-CA-C	-7.72	90.15	111.00
2	G	121	GLY	C-N-CA	-7.67	102.51	121.70
2	H	1	GLN	CB-CA-C	7.58	125.56	110.40
2	I	76	ILE	CG1-CB-CG2	-7.34	95.24	111.40
1	D	173	THR	CB-CA-C	-7.26	92.01	111.60
2	L	13	GLN	N-CA-CB	-7.26	97.54	110.60
1	E	360	ASP	C-N-CA	7.14	139.56	121.70
1	C	331	SER	N-CA-C	7.05	130.04	111.00
2	G	50	GLU	CB-CA-C	-7.03	96.35	110.40
1	C	183	CYS	CB-CA-C	-6.94	96.52	110.40
2	K	77	SER	N-CA-CB	6.83	120.74	110.50
2	L	116	GLU	N-CA-CB	-6.82	98.33	110.60
1	E	18	LYS	N-CA-C	-6.80	92.64	111.00
2	K	101	TYR	CB-CG-CD1	-6.75	116.95	121.00
2	H	92	LEU	CB-CG-CD1	-6.73	99.55	111.00
1	F	448	HIS	CB-CA-C	-6.70	97.00	110.40
2	L	51	ARG	CD-NE-CZ	6.70	132.97	123.60
2	I	25	SER	CB-CA-C	-6.64	97.49	110.10
2	I	92	LEU	CA-CB-CG	6.60	130.49	115.30
1	C	453	ASP	CB-CA-C	6.59	123.58	110.40
1	F	375	MET	CB-CA-C	-6.54	97.31	110.40
1	D	92	THR	N-CA-C	6.47	128.47	111.00
2	G	50	GLU	N-CA-CB	6.46	122.23	110.60
1	B	453	ASP	CB-CA-C	6.41	123.22	110.40
2	K	85	VAL	CG1-CB-CG2	-6.40	100.67	110.90
1	D	173	THR	N-CA-C	-6.39	93.75	111.00
2	L	11	LEU	CA-CB-CG	6.30	129.80	115.30
1	F	488	GLY	N-CA-C	6.29	128.81	113.10
1	C	149	LEU	CA-CB-CG	-6.25	100.93	115.30
2	G	82	LYS	CA-CB-CG	-6.21	99.73	113.40
2	J	52	GLU	CG-CD-OE1	6.20	130.69	118.30
1	F	391	GLU	CB-CG-CD	6.06	130.56	114.20
1	E	362	VAL	CB-CA-C	-6.05	99.90	111.40
1	F	448	HIS	N-CA-C	-6.04	94.68	111.00
1	C	173	THR	CB-CA-C	-6.03	95.31	111.60
1	F	481	HIS	N-CA-C	-6.03	94.71	111.00
1	F	19	HIS	N-CA-C	6.02	127.26	111.00
2	K	91	SER	CB-CA-C	-6.02	98.66	110.10
2	L	97	THR	CA-CB-CG2	-6.02	103.98	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	472	SER	CB-CA-C	6.01	121.53	110.10
1	A	489	TYR	CB-CA-C	5.98	122.36	110.40
2	I	90	ASN	CA-C-N	-5.95	104.12	117.20
1	C	120	GLY	C-N-CA	5.93	136.53	121.70
1	F	395	LYS	CD-CE-NZ	5.88	125.23	111.70
2	K	92	LEU	CB-CG-CD2	-5.85	101.05	111.00
1	F	311	ARG	CD-NE-CZ	-5.83	115.43	123.60
2	I	89	MET	C-N-CA	-5.80	107.20	121.70
1	F	468	LYS	CB-CA-C	5.72	121.83	110.40
1	C	373	ILE	C-N-CD	-5.69	108.07	120.60
1	E	229	GLU	CA-CB-CG	-5.69	100.88	113.40
1	D	172	LEU	CA-CB-CG	5.68	128.36	115.30
1	E	18	LYS	CB-CA-C	5.67	121.74	110.40
1	C	373	ILE	N-CA-C	-5.66	95.71	111.00
2	J	52	GLU	CA-CB-CG	5.65	125.83	113.40
2	I	90	ASN	CB-CA-C	5.64	121.69	110.40
2	J	79	ASP	CB-CG-OD1	5.64	123.38	118.30
2	K	88	GLN	CA-CB-CG	5.64	125.82	113.40
1	D	181	PRO	CB-CA-C	-5.64	97.91	112.00
1	F	448	HIS	C-N-CA	5.63	134.12	122.30
1	F	487	LYS	CB-CA-C	-5.63	99.14	110.40
2	L	49	LYS	C-N-CA	5.63	135.76	121.70
2	H	18	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	77	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	122	LYS	CB-CA-C	5.58	121.57	110.40
2	I	97	THR	OG1-CB-CG2	-5.57	97.18	110.00
1	E	21	ALA	N-CA-CB	-5.56	102.31	110.10
1	D	330	LEU	CB-CA-C	5.56	120.77	110.20
1	C	149	LEU	CB-CG-CD2	5.55	120.44	111.00
2	I	118	ARG	CG-CD-NE	-5.54	100.17	111.80
1	F	408	ARG	CB-CG-CD	5.51	125.93	111.60
1	E	208	MET	CB-CG-SD	-5.50	95.90	112.40
2	L	115	ASP	C-N-CA	5.48	135.40	121.70
1	F	299	MET	CA-CB-CG	-5.38	104.16	113.30
1	C	41	LEU	CB-CG-CD2	-5.36	101.89	111.00
2	J	34	THR	CB-CA-C	5.35	126.06	111.60
1	A	109	LEU	CA-CB-CG	5.34	127.59	115.30
1	C	280	MET	CG-SD-CE	-5.34	91.66	100.20
2	I	105	ARG	C-N-CA	5.31	134.97	121.70
1	D	347	MET	CA-CB-CG	-5.30	104.29	113.30
1	F	460	LEU	CB-CG-CD1	5.29	120.00	111.00
2	I	90	ASN	C-N-CA	5.27	134.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	468	LYS	CB-CA-C	5.26	120.92	110.40
1	D	95	PHE	CB-CA-C	5.25	120.90	110.40
1	F	266	LEU	CA-CB-CG	5.23	127.32	115.30
2	K	90	ASN	N-CA-CB	-5.21	101.21	110.60
2	L	89	MET	N-CA-CB	-5.20	101.25	110.60
1	C	437	SER	CB-CA-C	-5.19	100.24	110.10
1	D	427	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	17	ALA	CB-CA-C	-5.17	102.34	110.10
1	B	486	VAL	CB-CA-C	-5.13	101.65	111.40
2	I	76	ILE	CA-CB-CG1	5.12	120.73	111.00
1	C	203	GLU	CA-CB-CG	5.12	124.66	113.40
2	K	101	TYR	N-CA-CB	5.12	119.81	110.60
2	L	50	GLU	CB-CA-C	-5.09	100.21	110.40
2	L	50	GLU	CB-CG-CD	-5.07	100.50	114.20
1	F	360	ASP	N-CA-C	5.07	124.69	111.00
2	L	28	ASN	CB-CA-C	5.03	120.45	110.40
1	C	331	SER	CB-CA-C	-5.02	100.56	110.10
1	C	151	LEU	CB-CG-CD2	-5.01	102.49	111.00

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	GLY	Peptide
1	B	372	LYS	Peptide
1	C	120	GLY	Peptide
1	C	168	ASN	Peptide
1	C	173	THR	Peptide
1	C	373	ILE	Peptide
1	D	173	THR	Peptide
1	D	195	ARG	Sidechain
1	D	499	ARG	Sidechain
1	E	360	ASP	Peptide
1	F	17	ALA	Peptide
1	F	233	ASP	Peptide
1	F	311	ARG	Sidechain
1	F	373	ILE	Peptide
1	F	425	ARG	Sidechain
1	F	44	SER	Peptide
1	F	448	HIS	Peptide
1	F	492	GLN	Peptide
2	G	49	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	I	106	ASP	Peptide
2	I	118	ARG	Sidechain
2	I	5	GLN	Peptide
2	I	73	ARG	Sidechain
2	I	88	GLN	Sidechain
2	J	51	ARG	Peptide
2	J	52	GLU	Sidechain
2	K	101	TYR	Sidechain
2	K	50	GLU	Peptide,Mainchain
2	K	76	ILE	Peptide
2	K	90	ASN	Peptide
2	L	51	ARG	Sidechain
2	L	6	GLU	Peptide
2	L	73	ARG	Sidechain
2	L	78	ARG	Sidechain

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	A	3687	0	3598	165	0
1	B	2996	0	2955	131	0
1	C	3672	0	3562	187	0
1	D	3691	0	3610	167	0
1	E	2920	0	2857	143	1
1	F	2901	0	2817	176	7
2	G	995	0	932	30	1
2	H	998	0	934	33	0
2	I	976	0	891	72	0
2	J	1007	0	945	43	1
2	K	967	0	878	67	6
2	L	942	0	818	69	0
3	A	6	0	8	0	0
3	B	18	0	24	0	0
3	C	12	0	15	0	0
3	D	12	0	16	1	0
3	E	6	0	8	2	0
3	F	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	0	1	0
4	B	7	0	0	0	0
4	C	25	0	0	0	0
4	D	13	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	2	0	0	1	0
4	H	5	0	0	0	0
4	I	1	0	0	0	0
4	J	4	0	0	0	0
4	L	1	0	0	0	0
All	All	25898	0	24876	1216	8

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 24.

All (1216) 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:G:82:LYS:NZ	2:G:82:LYS:CE	1.68	1.56
1:D:185:VAL:HG12	1:D:187:LEU:CD2	1.53	1.35
1:F:441:VAL:CG1	1:F:460:LEU:HD21	1.54	1.35
1:F:441:VAL:HG11	1:F:460:LEU:CD2	1.60	1.31
1:A:143:TYR:CD1	1:A:150:THR:HG22	1.66	1.29
1:B:44:SER:O	1:B:344:VAL:HG12	1.35	1.25
2:I:16:GLY:O	2:I:92:LEU:HD12	1.27	1.25
1:A:472:SER:O	1:A:498:VAL:HG21	1.33	1.23
1:D:172:LEU:HD23	1:D:173:THR:O	1.34	1.21
1:C:27:THR:HG22	1:C:50:ARG:HD3	1.19	1.19
1:C:149:LEU:HD21	1:C:170:HIS:HB3	1.24	1.19
1:A:472:SER:O	1:A:498:VAL:CG2	1.92	1.17
1:D:185:VAL:CG1	1:D:187:LEU:CD2	2.26	1.14
2:L:11:LEU:HD23	2:L:127:THR:OG1	1.48	1.12
1:C:149:LEU:HD21	1:C:170:HIS:CB	1.80	1.11
1:C:27:THR:CG2	1:C:50:ARG:HD3	1.79	1.11
1:D:185:VAL:CG1	1:D:187:LEU:HD21	1.78	1.11
1:C:185:VAL:HG12	1:C:187:LEU:HD13	1.18	1.09
1:C:276:VAL:CG2	1:D:315:THR:HG22	1.81	1.09
2:G:1:GLN:HG2	2:G:2:VAL:H	1.02	1.09
1:A:54:SER:HA	1:A:86:LYS:HG2	1.17	1.08
1:C:149:LEU:HD21	1:C:170:HIS:CG	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LEU:CD2	1:D:173:THR:O	2.02	1.07
2:L:18:LEU:O	2:L:89:MET:HB2	1.53	1.07
1:B:44:SER:O	1:B:344:VAL:CG1	2.02	1.07
1:D:92:THR:O	1:D:126:TYR:O	1.70	1.07
1:C:27:THR:HG21	1:C:50:ARG:HH11	0.90	1.06
2:I:16:GLY:O	2:I:92:LEU:CD1	2.04	1.05
2:G:1:GLN:HG3	2:G:28:ASN:HB2	1.38	1.04
1:C:149:LEU:CD2	1:C:170:HIS:HB3	1.87	1.04
2:H:97:THR:HG22	2:H:128:VAL:H	1.18	1.04
1:C:276:VAL:HG22	1:D:315:THR:CG2	1.89	1.03
1:C:27:THR:HG21	1:C:50:ARG:NH1	1.73	1.03
1:D:292:PRO:HA	1:D:326:ASP:OD2	1.59	1.02
1:A:143:TYR:CE1	1:A:150:THR:HG22	1.95	1.02
1:A:44:SER:O	1:A:344:VAL:CG1	2.08	1.01
1:C:27:THR:CG2	1:C:50:ARG:HH11	1.74	1.01
2:I:1:GLN:HG2	2:I:2:VAL:H	1.24	1.01
1:A:44:SER:O	1:A:344:VAL:HG12	1.57	1.01
1:C:185:VAL:CG1	1:C:187:LEU:HD13	1.90	1.01
1:F:207:ASP:OD2	1:F:430:ARG:HB3	1.61	1.00
1:C:276:VAL:HG22	1:D:315:THR:HG22	1.01	1.00
1:A:143:TYR:CE1	1:A:150:THR:CG2	2.44	1.00
1:F:441:VAL:HG12	1:F:460:LEU:HD21	1.35	1.00
1:C:149:LEU:HD11	1:C:170:HIS:ND1	1.77	1.00
1:C:179:ASN:OD1	1:C:179:ASN:O	1.79	0.99
2:G:1:GLN:HG2	2:G:2:VAL:N	1.74	0.99
1:F:441:VAL:CG1	1:F:460:LEU:CD2	2.28	0.99
2:H:13:GLN:HG3	2:H:14:SER:N	1.76	0.98
2:K:70:VAL:HB	2:K:74:PHE:CD2	1.99	0.98
1:C:303:MET:SD	1:C:343:VAL:HB	2.02	0.98
2:G:33:ARG:NH1	2:G:38:ASP:OD1	1.97	0.98
1:D:451:ASP:O	1:D:457:ARG:NH2	1.96	0.96
1:F:18:LYS:O	1:F:355:GLN:NE2	1.97	0.96
1:E:27:THR:HG21	1:E:50:ARG:HH11	1.23	0.96
1:D:185:VAL:HG12	1:D:187:LEU:HD23	1.48	0.95
2:I:94:PRO:O	2:I:97:THR:OG1	1.84	0.95
1:A:90:ILE:HG23	1:A:129:TYR:HB2	1.48	0.95
1:C:185:VAL:CG1	1:C:187:LEU:CD1	2.44	0.95
2:J:79:ASP:OD2	2:J:82:LYS:NZ	1.99	0.94
1:F:289:ALA:HB1	1:F:291:LYS:HE3	1.46	0.94
2:K:70:VAL:HB	2:K:74:PHE:HD2	1.26	0.94
1:D:249:ILE:O	1:D:253:ILE:HD12	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:GLN:OE1	2:K:28:ASN:CG	2.08	0.92
1:A:143:TYR:HD1	1:A:150:THR:HG22	1.14	0.92
1:C:185:VAL:HG11	1:C:187:LEU:HD11	1.49	0.92
2:I:1:GLN:HG2	2:I:2:VAL:N	1.82	0.92
1:A:102:TYR:CE1	1:A:172:LEU:HD12	2.05	0.92
1:C:27:THR:HG22	1:C:50:ARG:CD	2.00	0.91
1:F:270:ILE:HD11	1:F:274:LYS:HB2	1.51	0.90
1:F:386:VAL:HG13	1:F:415:PRO:HB3	1.54	0.90
1:C:185:VAL:HG12	1:C:187:LEU:CD1	2.01	0.89
1:A:215:ARG:HH21	1:A:219:GLN:HE22	1.17	0.89
1:A:492:GLN:HG2	1:C:494:ARG:HB3	1.54	0.89
1:E:44:SER:O	1:E:344:VAL:HG12	1.72	0.89
1:B:270:ILE:HG22	2:G:108:TRP:CH2	2.08	0.89
2:L:94:PRO:O	2:L:97:THR:OG1	1.91	0.88
1:B:239:LYS:NZ	1:B:260:MET:SD	2.45	0.88
1:D:185:VAL:HG11	1:D:187:LEU:HD21	1.53	0.88
1:C:149:LEU:HD21	1:C:170:HIS:ND1	1.88	0.88
1:D:27:THR:HG22	1:D:50:ARG:HD3	1.53	0.88
2:K:89:MET:HB3	2:K:92:LEU:HD21	1.54	0.88
2:K:82:LYS:O	2:K:84:THR:HG23	1.74	0.87
1:E:339:TYR:O	1:E:343:VAL:HG12	1.75	0.87
2:K:101:TYR:CD1	2:K:123:GLY:HA3	2.10	0.87
2:G:1:GLN:CG	2:G:2:VAL:H	1.88	0.86
1:B:270:ILE:HG22	2:G:108:TRP:CZ3	2.10	0.86
1:C:243:HIS:CE1	2:I:63:ILE:HD11	2.09	0.86
1:A:41:LEU:HB3	1:A:46:MET:HE2	1.58	0.86
1:F:349:ARG:NH1	2:L:37:THR:HG21	1.90	0.86
1:A:143:TYR:HE1	1:A:150:THR:HG21	1.40	0.86
2:I:125:GLN:OE1	2:I:127:THR:HG23	1.75	0.86
1:C:480:VAL:HG22	1:C:493:THR:HG22	1.59	0.85
1:A:143:TYR:HE1	1:A:150:THR:CG2	1.88	0.84
2:K:69:SER:O	2:K:73:ARG:NH2	2.10	0.84
2:K:101:TYR:HD1	2:K:123:GLY:HA3	1.43	0.84
1:B:54:SER:HA	1:B:86:LYS:HG3	1.59	0.84
2:L:111:SER:OG	2:L:116:GLU:OE1	1.94	0.84
1:B:401:SER:HB2	1:B:406:SER:OG	1.79	0.83
1:C:247:GLN:HG3	1:D:13:PHE:CE2	2.13	0.83
2:I:58:SER:HB3	2:I:63:ILE:CG2	2.08	0.83
2:I:17:SER:CB	2:I:90:ASN:HB3	2.08	0.83
2:J:51:ARG:HG2	2:J:51:ARG:HH11	1.43	0.82
2:H:11:LEU:HD12	2:H:127:THR:HB	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ILE:HG13	2:G:64:THR:HG22	1.61	0.82
2:L:57:ILE:HD11	2:L:61:GLY:HA2	1.60	0.82
2:K:84:THR:HG1	2:K:86:TYR:HH	1.02	0.82
1:F:387:SER:O	1:F:391:GLU:HG2	1.79	0.82
1:A:5:GLN:CG	1:B:370:LEU:HD11	2.09	0.82
1:A:93:GLY:HA3	1:A:175:ARG:H	1.44	0.82
1:C:299:MET:O	1:C:300:LEU:HD23	1.79	0.81
1:C:168:ASN:HD22	1:C:170:HIS:H	1.29	0.81
2:I:58:SER:OG	2:I:63:ILE:HG22	1.80	0.81
1:D:41:LEU:HB3	1:D:46:MET:HE2	1.59	0.81
2:I:28:ASN:HD22	2:I:33:ARG:H	1.27	0.81
1:A:143:TYR:CE1	1:A:150:THR:HG21	2.15	0.81
1:C:247:GLN:HG3	1:D:13:PHE:HE2	1.43	0.81
2:K:89:MET:O	2:K:92:LEU:HG	1.80	0.80
1:A:51:MET:HE3	1:A:53:PHE:HE1	1.46	0.80
1:C:185:VAL:HG11	1:C:187:LEU:CD1	2.08	0.80
1:A:170:HIS:CD2	1:A:172:LEU:HD23	2.16	0.80
1:C:423:THR:HG22	1:C:425:ARG:H	1.46	0.80
1:C:172:LEU:HG	1:C:173:THR:O	1.80	0.80
1:C:303:MET:SD	1:C:343:VAL:CB	2.69	0.80
1:F:441:VAL:HG22	1:F:464:TRP:CE3	2.17	0.80
2:L:6:GLU:O	2:L:7:SER:OG	1.99	0.80
1:E:378:GLU:OE2	1:E:405:ARG:NH1	2.14	0.80
1:D:185:VAL:HG12	1:D:187:LEU:HD22	1.60	0.80
2:K:35:PHE:HE2	2:K:85:VAL:HG23	1.46	0.79
1:B:260:MET:HG3	1:B:294:ILE:HB	1.65	0.79
1:F:441:VAL:HG11	1:F:460:LEU:CG	2.12	0.79
1:E:414:ARG:HG3	1:E:436:ARG:HH21	1.48	0.79
1:A:227:LEU:HD13	1:A:234:THR:CG2	2.13	0.78
1:F:411:SER:OG	1:F:436:ARG:O	2.01	0.78
2:K:57:ILE:HD12	2:K:77:SER:HA	1.63	0.78
1:D:27:THR:HG23	1:D:330:LEU:O	1.84	0.78
1:F:62:GLN:HE22	1:F:204:GLN:HG3	1.48	0.77
2:I:1:GLN:CG	2:I:2:VAL:H	1.96	0.77
1:B:486:VAL:HG22	1:B:487:LYS:H	1.49	0.77
2:L:58:SER:O	2:L:78:ARG:NH1	2.16	0.77
1:B:355:GLN:O	1:B:358:THR:HG22	1.84	0.77
1:D:249:ILE:HG13	1:D:253:ILE:HD11	1.65	0.77
1:A:5:GLN:HG2	1:B:370:LEU:HD11	1.65	0.77
1:E:27:THR:HG22	1:E:50:ARG:HB3	1.64	0.77
2:K:84:THR:OG1	2:K:86:TYR:OH	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:MET:O	1:F:367:ILE:HG13	1.85	0.76
1:A:143:TYR:CD1	1:A:150:THR:CG2	2.56	0.75
1:D:473:ALA:HA	1:D:498:VAL:HG23	1.68	0.75
1:F:395:LYS:HG3	1:F:475:ASP:HB3	1.66	0.75
1:E:480:VAL:HG22	1:E:493:THR:HG22	1.68	0.75
1:C:92:THR:HG22	1:C:178:ILE:HD12	1.66	0.75
1:E:7:ASN:HA	1:E:10:LEU:HG	1.68	0.75
1:D:377:PRO:O	1:D:381:VAL:HG23	1.87	0.75
1:F:383:SER:O	1:F:387:SER:OG	2.03	0.75
2:J:42:TRP:HD1	2:J:76:ILE:HD13	1.49	0.75
2:I:5:GLN:O	2:I:23:ALA:N	2.16	0.75
1:A:54:SER:CA	1:A:86:LYS:HG2	2.09	0.74
1:D:149:LEU:HD23	1:D:170:HIS:HB3	1.68	0.74
1:A:195:ARG:O	1:A:199:GLN:OE1	2.05	0.74
1:D:299:MET:O	1:D:300:LEU:HD23	1.88	0.74
1:F:3:GLN:O	1:F:7:ASN:ND2	2.20	0.74
1:F:397:ILE:HD12	1:F:417:CYS:SG	2.28	0.74
1:C:62:GLN:HG3	1:C:66:ASN:HD21	1.53	0.73
2:L:11:LEU:CD2	2:L:127:THR:OG1	2.31	0.73
2:L:27:SER:HB2	2:L:33:ARG:O	1.88	0.73
2:L:69:SER:O	2:L:73:ARG:NH2	2.21	0.73
1:C:104:PRO:HD3	1:C:169:HIS:CE1	2.23	0.73
2:H:97:THR:CG2	2:H:128:VAL:H	1.97	0.73
1:C:315:THR:HG22	1:D:276:VAL:HG22	1.70	0.73
1:A:227:LEU:HD13	1:A:234:THR:HG23	1.70	0.73
1:E:454:ARG:HD2	1:E:481:HIS:CD2	2.24	0.73
1:E:298:GLN:HA	1:E:301:GLU:HG3	1.70	0.72
1:A:170:HIS:CD2	1:A:172:LEU:CD2	2.72	0.72
1:F:279:GLN:OE1	1:F:323:ASN:ND2	2.22	0.72
1:C:243:HIS:CE1	2:I:63:ILE:CD1	2.71	0.72
1:D:38:LEU:O	1:D:42:MET:HG3	1.89	0.72
1:F:283:ILE:HA	1:F:293:VAL:HG21	1.71	0.72
1:F:441:VAL:HG11	1:F:460:LEU:HD23	1.67	0.72
1:B:401:SER:HB2	1:B:406:SER:HG	1.54	0.72
1:D:228:GLY:O	1:D:232:LYS:HG2	1.90	0.72
1:E:44:SER:O	1:E:344:VAL:CG1	2.38	0.72
1:B:38:LEU:O	1:B:42:MET:HG3	1.91	0.71
1:F:214:ILE:HG22	1:F:252:ILE:HD13	1.72	0.71
2:L:114:PRO:HB3	2:L:120:TRP:HH2	1.55	0.71
1:A:2:SER:N	1:A:359:HIS:NE2	2.39	0.71
1:B:198:LEU:HD12	1:B:227:LEU:HD21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLN:O	1:B:434:VAL:HG12	1.89	0.71
1:F:432:LEU:HD13	1:F:438:VAL:HG11	1.72	0.71
1:C:144:VAL:HG13	1:C:178:ILE:HG13	1.71	0.71
1:C:311:ARG:HH11	1:C:315:THR:HG21	1.54	0.71
1:E:27:THR:HG21	1:E:50:ARG:NH1	2.03	0.71
2:I:6:GLU:O	2:I:6:GLU:HG2	1.81	0.71
1:B:270:ILE:CG2	2:G:108:TRP:CH2	2.74	0.71
1:C:473:ALA:HA	1:C:498:VAL:HG12	1.71	0.71
2:I:28:ASN:HD21	2:I:31:SER:H	1.36	0.71
1:B:386:VAL:HG13	1:B:415:PRO:HB3	1.70	0.71
2:I:104:GLY:HA3	2:I:119:TYR:CE1	2.26	0.71
2:L:11:LEU:HD23	2:L:127:THR:HG1	1.55	0.71
1:B:192:GLU:HA	1:B:195:ARG:HG3	1.73	0.71
1:C:149:LEU:CD1	1:C:170:HIS:ND1	2.53	0.70
1:B:452:ASN:OD1	1:B:453:ASP:N	2.24	0.70
1:C:154:LEU:HD11	1:C:165:HIS:HB2	1.72	0.70
1:E:349:ARG:HD2	2:K:32:GLY:O	1.90	0.70
1:A:44:SER:O	1:A:344:VAL:HG11	1.91	0.70
1:B:242:ASN:ND2	1:B:244:GLN:OE1	2.24	0.70
1:E:406:SER:OG	1:E:490:PRO:CG	2.39	0.70
2:I:58:SER:CB	2:I:63:ILE:HG22	2.20	0.70
1:B:65:ILE:CG2	1:B:69:ARG:HH11	2.04	0.70
1:C:451:ASP:HB3	1:C:457:ARG:HH11	1.57	0.70
1:A:47:SER:HB3	1:A:433:ASN:HB3	1.73	0.70
1:D:51:MET:HE3	1:D:53:PHE:HE1	1.55	0.70
1:A:270:ILE:HG22	2:H:108:TRP:CH2	2.27	0.69
1:A:406:SER:OG	1:A:490:PRO:CG	2.40	0.69
1:A:480:VAL:HG22	1:A:493:THR:HG22	1.73	0.69
1:F:270:ILE:HG23	1:F:275:VAL:HG22	1.73	0.69
1:A:492:GLN:OE1	1:C:492:GLN:NE2	2.25	0.69
2:L:1:GLN:HG3	2:L:28:ASN:HD21	1.57	0.69
1:F:363:MET:CE	1:F:367:ILE:HD11	2.22	0.69
1:F:471:VAL:HG11	1:F:498:VAL:HG11	1.74	0.69
1:A:53:PHE:O	1:A:86:LYS:CE	2.41	0.69
1:A:170:HIS:HD2	1:A:172:LEU:CD2	2.04	0.69
1:F:53:PHE:HB2	1:F:84:ASP:O	1.92	0.69
2:L:33:ARG:HH12	2:L:106:ASP:HA	1.57	0.69
1:B:294:ILE:HG23	1:B:327:CYS:HB2	1.75	0.69
1:F:38:LEU:O	1:F:42:MET:HG3	1.93	0.69
2:I:17:SER:HB3	2:I:90:ASN:HB3	1.73	0.69
1:E:454:ARG:HD2	1:E:481:HIS:HD2	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ARG:HG2	1:F:236:ILE:HD11	1.75	0.68
2:H:97:THR:HG22	2:H:128:VAL:N	2.01	0.68
2:K:1:GLN:OE1	2:K:28:ASN:OD1	2.10	0.68
1:D:451:ASP:O	1:D:453:ASP:O	2.11	0.68
1:E:408:ARG:HG2	1:E:435:THR:HG21	1.75	0.68
1:F:290:GLY:HA2	1:F:412:LYS:HB2	1.76	0.68
1:C:247:GLN:CG	1:D:13:PHE:HE2	2.06	0.68
1:E:35:VAL:HG23	1:E:67:ASN:OD1	1.92	0.68
1:F:234:THR:HA	1:F:431:GLN:NE2	2.09	0.68
1:A:93:GLY:CA	1:A:175:ARG:H	2.06	0.68
1:A:94:LEU:HB3	1:A:118:LYS:HA	1.75	0.68
1:A:276:VAL:HG22	1:B:315:THR:HG22	1.76	0.68
1:F:44:SER:O	1:F:344:VAL:HG22	1.94	0.67
2:J:6:GLU:H	2:J:122:GLN:NE2	1.92	0.67
1:F:386:VAL:HG21	1:F:413:TYR:HB2	1.76	0.67
1:A:102:TYR:CE2	1:A:108:VAL:HG21	2.29	0.67
1:A:39:LYS:HG3	1:A:71:ALA:HB1	1.76	0.67
1:E:27:THR:HG23	1:E:330:LEU:O	1.95	0.67
1:C:102:TYR:O	1:C:168:ASN:ND2	2.24	0.66
1:E:271:PRO:HB2	1:E:273:GLU:HG3	1.76	0.66
1:E:87:GLY:N	1:E:194:ASP:OD1	2.23	0.66
2:L:113:VAL:HB	2:L:116:GLU:HG3	1.78	0.66
1:A:472:SER:C	1:A:498:VAL:HG21	2.13	0.66
1:E:283:ILE:HD13	1:E:325:ALA:HB2	1.77	0.66
1:E:300:LEU:HG	1:E:347:MET:HE2	1.78	0.66
2:K:59:TRP:CD1	2:K:108:TRP:HB2	2.31	0.66
2:J:6:GLU:OE2	2:J:101:TYR:HA	1.96	0.66
1:A:278:ALA:HB2	1:B:12:ILE:HD12	1.77	0.66
1:B:190:VAL:HG22	1:B:195:ARG:HG2	1.76	0.66
1:D:240:ILE:HD13	1:D:259:ILE:HG23	1.78	0.66
2:L:88:GLN:NE2	2:L:90:ASN:OD1	2.28	0.66
1:D:213:PHE:CE2	1:D:215:ARG:HD3	2.30	0.66
2:I:122:GLN:NE2	2:I:124:THR:OG1	2.26	0.66
2:K:13:GLN:NE2	2:K:130:SER:O	2.28	0.66
1:B:38:LEU:HD13	1:B:68:VAL:HG12	1.78	0.65
2:G:82:LYS:NZ	2:G:82:LYS:CD	2.58	0.65
1:F:387:SER:C	1:F:391:GLU:HG2	2.17	0.65
2:K:105:ARG:NH1	2:K:116:GLU:OE1	2.30	0.65
1:A:315:THR:HG22	1:B:276:VAL:HG22	1.76	0.65
1:B:377:PRO:O	1:B:381:VAL:HG23	1.96	0.65
1:C:42:MET:HE1	1:C:71:ALA:C	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:GLN:OE1	2:K:28:ASN:ND2	2.30	0.65
1:B:463:ASP:O	1:B:467:THR:HG23	1.97	0.65
2:I:58:SER:CB	2:I:63:ILE:CG2	2.75	0.65
1:E:26:CYS:SG	1:E:46:MET:HG3	2.36	0.65
1:D:402:ASN:O	1:D:428:THR:HG21	1.97	0.64
2:I:42:TRP:HD1	2:I:76:ILE:HD12	1.62	0.64
1:B:398:LEU:HB3	1:B:479:ILE:HD13	1.78	0.64
1:F:2:SER:OG	1:F:359:HIS:NE2	2.23	0.64
1:A:170:HIS:HD2	1:A:172:LEU:HD21	1.63	0.64
1:C:27:THR:O	1:C:334:THR:HG23	1.97	0.64
2:J:51:ARG:HG2	2:J:51:ARG:NH1	2.09	0.64
2:L:1:GLN:HG2	2:L:119:TYR:CD2	2.33	0.64
1:F:395:LYS:HE3	1:F:475:ASP:CG	2.17	0.64
1:A:102:TYR:O	1:A:169:HIS:HA	1.98	0.64
1:F:445:VAL:O	1:F:448:HIS:O	2.16	0.64
1:F:441:VAL:CG1	1:F:460:LEU:CG	2.73	0.64
1:E:471:VAL:HG11	1:E:498:VAL:HG11	1.80	0.64
2:J:40:ILE:HG21	2:J:85:VAL:HG11	1.80	0.64
1:B:192:GLU:H	1:B:192:GLU:CD	2.00	0.63
1:C:243:HIS:O	1:C:246:VAL:HG22	1.98	0.63
1:C:2:SER:N	1:C:359:HIS:NE2	2.45	0.63
1:C:143:TYR:O	1:C:178:ILE:HG23	1.98	0.63
2:H:40:ILE:HG21	2:H:85:VAL:HG11	1.79	0.63
2:J:42:TRP:CD1	2:J:76:ILE:HD13	2.31	0.63
2:K:42:TRP:CG	2:K:87:LEU:HD12	2.33	0.63
1:E:324:GLY:O	1:E:414:ARG:NH2	2.32	0.63
1:F:441:VAL:HG22	1:F:464:TRP:HE3	1.62	0.63
1:D:249:ILE:HG13	1:D:253:ILE:CD1	2.28	0.63
1:E:27:THR:CG2	1:E:50:ARG:HH11	2.04	0.63
1:A:94:LEU:HB3	1:A:118:LYS:HG3	1.79	0.63
1:C:299:MET:HE3	1:C:317:VAL:HG22	1.80	0.63
1:E:249:ILE:HG12	1:E:282:ILE:CD1	2.27	0.63
2:K:73:ARG:NH1	2:K:96:ASP:OD2	2.32	0.63
1:E:198:LEU:HD13	1:E:227:LEU:HD21	1.81	0.63
2:I:45:GLN:HB3	2:I:99:VAL:HG13	1.80	0.63
2:L:39:ALA:HA	2:L:78:ARG:HH12	1.64	0.63
2:L:113:VAL:O	2:L:116:GLU:HB2	1.97	0.63
1:E:214:ILE:HG22	1:E:252:ILE:HD13	1.80	0.63
1:E:345:GLN:HG3	2:K:32:GLY:HA2	1.80	0.62
1:F:330:LEU:HD21	1:F:343:VAL:HG22	1.80	0.62
1:B:378:GLU:HG3	1:B:489:TYR:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LEU:O	1:F:202:VAL:HG22	1.99	0.62
1:A:400:LEU:HD22	1:A:422:ALA:HB3	1.80	0.62
1:E:274:LYS:O	1:E:274:LYS:HG2	1.99	0.62
1:F:363:MET:HE3	1:F:367:ILE:HD11	1.81	0.62
1:D:217:ALA:HB2	1:D:251:ALA:HB1	1.81	0.62
1:A:263:ARG:NH2	1:A:316:ASP:OD1	2.33	0.62
1:C:144:VAL:HG12	1:C:145:ASP:H	1.65	0.62
2:L:28:ASN:O	2:L:29:PHE:CD2	2.53	0.62
2:K:74:PHE:CD1	2:K:89:MET:HA	2.34	0.62
1:A:471:VAL:HG21	1:A:477:MET:HE2	1.81	0.62
2:H:13:GLN:HE22	2:H:130:SER:HA	1.65	0.62
1:A:94:LEU:O	1:A:118:LYS:O	2.18	0.62
1:B:52:ASN:OD1	1:B:54:SER:OG	2.18	0.62
1:D:88:PRO:O	1:D:187:LEU:HD12	2.00	0.62
1:E:241:GLU:HB2	1:E:265:ASP:HB3	1.82	0.62
1:F:6:HIS:ND1	1:F:359:HIS:HA	2.15	0.62
2:L:57:ILE:HD13	2:L:64:THR:HG22	1.82	0.62
1:A:39:LYS:O	1:A:43:LYS:HG3	1.99	0.62
1:A:93:GLY:HA3	1:A:175:ARG:N	2.12	0.62
1:D:94:LEU:HB2	1:D:118:LYS:HA	1.82	0.61
1:F:189:ALA:HB2	1:F:219:GLN:HE21	1.64	0.61
2:L:28:ASN:O	2:L:29:PHE:HD2	1.83	0.61
1:D:471:VAL:HG23	1:D:475:ASP:HB2	1.82	0.61
1:F:384:SER:O	1:F:388:SER:OG	2.15	0.61
1:A:270:ILE:HG13	1:A:275:VAL:HG22	1.81	0.61
1:E:406:SER:OG	1:E:490:PRO:HG3	2.00	0.61
1:F:398:LEU:HD12	1:F:461:GLY:HA3	1.83	0.61
1:B:46:MET:HE3	1:B:49:ALA:HA	1.83	0.61
1:C:62:GLN:O	1:C:66:ASN:ND2	2.33	0.61
1:F:69:ARG:NH2	1:F:204:GLN:O	2.34	0.61
1:C:149:LEU:CD2	1:C:170:HIS:ND1	2.63	0.61
1:C:224:ARG:HE	1:C:236:ILE:HD12	1.65	0.61
1:B:441:VAL:HG11	1:B:460:LEU:HG	1.82	0.61
1:F:3:GLN:NE2	1:F:357:ALA:O	2.33	0.61
1:A:215:ARG:HH21	1:A:219:GLN:NE2	1.94	0.61
1:B:494:ARG:HG2	1:D:492:GLN:HB2	1.80	0.61
1:F:218:ASP:O	1:F:222:GLU:HG3	2.00	0.61
1:D:427:LEU:O	1:D:431:GLN:HG3	2.01	0.60
1:B:492:GLN:HE21	1:D:492:GLN:HE21	1.49	0.60
1:C:299:MET:CE	1:C:317:VAL:HG22	2.31	0.60
1:D:27:THR:CG2	1:D:50:ARG:HD3	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:38:ASP:HB2	2:K:105:ARG:O	2.01	0.60
1:A:90:ILE:HB	1:A:178:ILE:HB	1.82	0.60
1:B:265:ASP:O	1:B:268:VAL:HG22	2.01	0.60
1:D:202:VAL:HG11	1:D:231:GLY:HA3	1.82	0.60
2:G:1:GLN:HB2	2:G:28:ASN:HA	1.83	0.60
2:L:92:LEU:HB3	2:L:128:VAL:HG21	1.84	0.60
1:E:402:ASN:HB3	1:E:425:ARG:HE	1.67	0.60
1:F:43:LYS:O	2:L:29:PHE:HB3	2.00	0.60
2:L:39:ALA:HB2	2:L:108:TRP:O	2.02	0.60
1:A:112:THR:OG1	1:A:160:CYS:HB2	2.01	0.60
1:C:486:VAL:HG11	1:C:491:ASN:HD21	1.67	0.60
1:E:28:ILE:HG21	1:E:64:THR:HG23	1.84	0.60
1:F:7:ASN:HA	1:F:10:LEU:HG	1.83	0.60
2:L:73:ARG:NH1	2:L:93:GLN:HG3	2.17	0.60
1:C:27:THR:HG22	1:C:50:ARG:HB3	1.83	0.60
1:C:276:VAL:CG2	1:D:315:THR:CG2	2.66	0.60
1:C:28:ILE:HD12	1:C:38:LEU:HD21	1.83	0.60
1:D:83:LEU:HB3	1:D:209:ILE:HD13	1.83	0.60
1:D:279:GLN:O	1:D:283:ILE:HG13	2.02	0.60
1:F:25:ILE:HB	1:F:329:MET:HG3	1.84	0.60
2:K:6:GLU:CD	2:K:123:GLY:HA2	2.22	0.60
1:B:492:GLN:NE2	1:D:492:GLN:HE21	2.00	0.59
1:F:373:ILE:HG22	1:F:373:ILE:O	2.02	0.59
1:A:2:SER:N	1:A:359:HIS:HE2	2.00	0.59
1:A:41:LEU:HB3	1:A:46:MET:CE	2.30	0.59
1:F:349:ARG:HH12	2:L:37:THR:HG21	1.66	0.59
2:G:19:LYS:HD3	2:G:88:GLN:NE2	2.17	0.59
1:B:387:SER:O	1:B:391:GLU:HG3	2.02	0.59
1:D:114:PRO:O	1:D:117:GLU:HB2	2.03	0.59
2:J:44:ARG:NH2	2:J:52:GLU:OE2	2.34	0.59
1:C:388:SER:O	1:C:392:VAL:HG22	2.02	0.59
2:I:17:SER:HB2	2:I:90:ASN:HB3	1.82	0.59
2:K:42:TRP:HD1	2:K:76:ILE:HD13	1.66	0.59
1:A:87:GLY:O	1:A:89:GLU:HG2	2.03	0.59
1:A:311:ARG:HD2	1:B:275:VAL:HG11	1.83	0.59
2:J:1:GLN:HE21	2:J:28:ASN:HB2	1.67	0.59
1:A:340:PRO:O	1:A:343:VAL:HG12	2.02	0.59
1:B:33:GLN:HG3	1:B:64:THR:HG22	1.84	0.59
1:E:405:ARG:HG2	1:E:405:ARG:HH11	1.68	0.59
1:A:463:ASP:O	1:A:467:THR:HG23	2.02	0.59
1:F:458:VAL:O	1:F:462:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:LEU:HD22	2:L:128:VAL:HG21	1.83	0.59
1:F:65:ILE:O	1:F:69:ARG:HG3	2.03	0.59
2:K:27:SER:HB3	2:K:29:PHE:CE2	2.38	0.59
1:C:143:TYR:HB3	1:C:147:GLY:HA2	1.84	0.59
2:L:33:ARG:HB3	2:L:38:ASP:OD1	2.03	0.59
2:L:1:GLN:HG3	2:L:28:ASN:ND2	2.17	0.58
1:B:34:SER:OG	1:B:37:ALA:CB	2.50	0.58
1:A:12:ILE:HG13	1:B:274:LYS:HD3	1.83	0.58
1:F:386:VAL:HG21	1:F:413:TYR:CB	2.33	0.58
1:F:207:ASP:OD2	1:F:430:ARG:CB	2.45	0.58
2:I:28:ASN:ND2	2:I:33:ARG:H	1.99	0.58
1:A:270:ILE:HG22	2:H:108:TRP:CZ3	2.37	0.58
1:E:218:ASP:HA	1:E:221:ARG:HG2	1.84	0.58
1:E:454:ARG:CD	1:E:481:HIS:HD2	2.16	0.58
1:F:270:ILE:CD1	1:F:274:LYS:HB2	2.29	0.58
1:F:330:LEU:HD22	1:F:334:THR:HG23	1.84	0.58
1:F:194:ASP:O	1:F:198:LEU:HD12	2.03	0.58
2:I:20:LEU:HD21	2:I:100:TYR:HD2	1.67	0.58
2:K:91:SER:O	2:K:91:SER:OG	1.97	0.58
1:A:311:ARG:O	1:A:315:THR:HG23	2.04	0.58
1:E:84:ASP:HA	1:E:210:PHE:HB2	1.85	0.58
1:C:285:LYS:NZ	1:D:8:ILE:O	2.37	0.58
1:D:27:THR:HG21	1:D:50:ARG:HH11	1.69	0.58
1:D:299:MET:HE2	1:D:328:VAL:HG12	1.86	0.58
1:E:213:PHE:HD1	1:E:241:GLU:HG3	1.67	0.58
1:E:415:PRO:HG2	1:E:419:ILE:HD11	1.84	0.58
1:F:388:SER:HA	1:F:391:GLU:HG3	1.86	0.58
2:H:13:GLN:HE22	2:H:130:SER:C	2.05	0.58
1:D:146:ASP:H	1:D:148:VAL:HG23	1.68	0.58
1:F:248:ASN:O	1:F:252:ILE:HG13	2.04	0.58
1:F:482:ALA:HB2	1:F:489:TYR:O	2.03	0.58
1:F:62:GLN:NE2	1:F:62:GLN:HA	2.19	0.58
1:F:441:VAL:HG11	1:F:460:LEU:HD21	1.22	0.57
2:H:13:GLN:HE22	2:H:130:SER:CA	2.17	0.57
1:A:378:GLU:HG3	1:A:489:TYR:CD1	2.39	0.57
1:A:353:GLU:OE2	1:B:274:LYS:NZ	2.28	0.57
1:F:219:GLN:O	1:F:223:VAL:HG23	2.04	0.57
1:A:486:VAL:HG11	1:A:489:TYR:O	2.03	0.57
1:E:241:GLU:HB3	1:E:262:ALA:HB3	1.87	0.57
1:F:236:ILE:N	1:F:257:ASP:OD2	2.32	0.57
1:F:294:ILE:HG12	1:F:327:CYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:SER:HB3	2:J:63:ILE:HB	1.87	0.57
1:B:2:SER:N	1:B:359:HIS:HE2	2.02	0.57
1:C:218:ASP:O	1:C:222:GLU:HG3	2.04	0.57
1:D:25:ILE:HB	1:D:329:MET:HG3	1.87	0.57
1:B:64:THR:O	1:B:68:VAL:HG13	2.05	0.57
1:C:62:GLN:HG3	1:C:66:ASN:ND2	2.19	0.57
1:F:3:GLN:OE1	1:F:7:ASN:ND2	2.37	0.57
2:H:53:PHE:O	2:H:67:VAL:HG21	2.04	0.57
2:K:3:GLN:O	2:K:24:ALA:HA	2.05	0.57
1:C:14:GLU:HG3	1:C:15:PRO:HD2	1.87	0.57
1:F:400:LEU:HD12	1:F:422:ALA:HB3	1.86	0.57
1:D:458:VAL:O	1:D:462:VAL:HG23	2.05	0.56
1:D:359:HIS:HB3	1:D:362:VAL:HG23	1.86	0.56
1:A:93:GLY:O	1:A:94:LEU:HB2	2.05	0.56
1:A:102:TYR:HE2	1:A:108:VAL:HG21	1.67	0.56
1:C:2:SER:N	1:C:359:HIS:HE2	2.02	0.56
1:E:6:HIS:CD2	1:E:10:LEU:HD21	2.40	0.56
1:F:61:HIS:HA	1:F:64:THR:HG22	1.88	0.56
1:A:53:PHE:O	1:A:86:LYS:HE2	2.05	0.56
1:A:273:GLU:HG2	1:A:274:LYS:N	2.19	0.56
1:C:42:MET:CE	1:C:75:LEU:HD12	2.36	0.56
1:F:289:ALA:HB1	1:F:291:LYS:CE	2.29	0.56
1:F:289:ALA:CB	1:F:291:LYS:HE3	2.28	0.56
1:B:34:SER:OG	1:B:37:ALA:HB3	2.05	0.56
1:A:53:PHE:O	1:A:86:LYS:CG	2.53	0.56
1:A:148:VAL:O	1:A:168:ASN:ND2	2.34	0.56
1:F:388:SER:O	1:F:392:VAL:HG12	2.06	0.56
2:G:33:ARG:NH2	4:G:201:HOH:O	2.39	0.56
2:I:6:GLU:HG3	2:I:124:THR:OG1	2.05	0.56
2:L:89:MET:HE2	2:L:92:LEU:HD21	1.88	0.56
2:J:100:TYR:O	2:J:123:GLY:HA2	2.06	0.56
2:I:28:ASN:ND2	2:I:31:SER:H	2.04	0.56
1:D:188:PRO:O	1:D:215:ARG:NH2	2.37	0.55
1:E:69:ARG:NH2	1:E:204:GLN:O	2.38	0.55
2:H:13:GLN:HG3	2:H:14:SER:H	1.63	0.55
2:L:106:ASP:OD1	2:L:106:ASP:N	2.37	0.55
1:A:451:ASP:OD1	1:A:454:ARG:CA	2.54	0.55
1:C:303:MET:SD	1:C:343:VAL:HA	2.46	0.55
1:C:336:LYS:O	1:C:336:LYS:HG3	2.05	0.55
1:D:79:ILE:O	1:D:430:ARG:HG2	2.05	0.55
1:D:144:VAL:HG12	1:D:145:ASP:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:95:GLU:N	2:G:95:GLU:OE1	2.40	0.55
1:A:274:LYS:HD3	1:B:353:GLU:OE1	2.05	0.55
1:E:261:VAL:HG22	1:E:295:CYS:HA	1.89	0.55
2:L:89:MET:CE	2:L:92:LEU:HD21	2.36	0.55
1:C:64:THR:O	1:C:68:VAL:HG13	2.05	0.55
1:C:150:THR:HG23	1:C:167:ASN:HB2	1.89	0.55
1:D:158:ASP:HB2	1:D:161:THR:HG22	1.89	0.55
1:A:332:GLY:HA2	1:A:335:ALA:HB3	1.89	0.55
1:B:44:SER:O	1:B:344:VAL:HG11	2.00	0.55
1:B:214:ILE:HG22	1:B:252:ILE:HD13	1.89	0.55
1:C:451:ASP:OD2	1:C:457:ARG:HD3	2.07	0.55
2:I:7:SER:OG	2:I:21:SER:HB3	2.07	0.55
1:A:377:PRO:O	1:A:381:VAL:HG23	2.07	0.55
1:E:38:LEU:HD13	1:E:68:VAL:HG12	1.88	0.55
1:A:366:SER:O	1:A:370:LEU:HD22	2.05	0.55
1:B:447:ALA:C	1:B:448:HIS:HD1	2.10	0.55
1:D:34:SER:OG	1:D:37:ALA:CB	2.55	0.55
2:K:51:ARG:HE	2:K:114:PRO:HB2	1.72	0.55
1:C:270:ILE:HD12	1:D:12:ILE:HD12	1.88	0.54
1:C:451:ASP:O	1:C:457:ARG:NH1	2.41	0.54
1:E:198:LEU:O	1:E:202:VAL:HG13	2.07	0.54
1:A:311:ARG:HH22	1:B:316:ASP:CG	2.10	0.54
1:B:190:VAL:HG11	1:B:195:ARG:HH11	1.72	0.54
1:B:443:TYR:OH	1:B:449:GLY:O	2.24	0.54
2:I:74:PHE:N	2:I:74:PHE:HD1	2.05	0.54
2:K:1:GLN:HG2	2:K:28:ASN:HA	1.89	0.54
1:D:158:ASP:HB2	1:D:161:THR:CG2	2.36	0.54
1:D:388:SER:O	1:D:392:VAL:HG22	2.07	0.54
2:K:77:SER:O	2:K:86:TYR:HD1	1.90	0.54
1:A:5:GLN:HG3	1:B:370:LEU:HD11	1.86	0.54
1:B:54:SER:HA	1:B:86:LYS:CG	2.33	0.54
1:C:92:THR:HG23	1:C:176:LYS:O	2.07	0.54
1:C:27:THR:HG22	1:C:50:ARG:CG	2.38	0.54
1:C:444:ASP:HB3	1:C:447:ALA:HB3	1.90	0.54
2:H:104:GLY:HA3	2:H:119:TYR:CE2	2.42	0.54
1:A:229:GLU:O	1:A:232:LYS:HG2	2.08	0.54
1:B:342:GLU:OE1	1:B:342:GLU:N	2.36	0.54
1:C:420:ILE:CD1	1:C:465:ALA:HB2	2.38	0.54
1:E:454:ARG:CG	1:E:481:HIS:HD2	2.20	0.54
2:I:28:ASN:HD21	2:I:31:SER:N	2.02	0.54
1:B:48:VAL:HG11	1:B:208:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLN:O	1:B:203:GLU:HG3	2.07	0.54
1:C:423:THR:HG21	1:C:428:THR:HB	1.89	0.54
1:E:364:PHE:HZ	1:E:387:SER:OG	1.90	0.54
2:L:35:PHE:CD2	2:L:83:ASN:HA	2.42	0.54
1:B:471:VAL:HG12	1:B:498:VAL:HG21	1.90	0.54
1:C:311:ARG:NH1	1:C:315:THR:HG21	2.23	0.54
2:J:6:GLU:N	2:J:122:GLN:NE2	2.56	0.54
1:D:148:VAL:HB	1:D:170:HIS:CD2	2.43	0.54
1:E:364:PHE:HZ	1:E:387:SER:HG	1.52	0.54
1:A:26:CYS:HB2	1:A:46:MET:HG3	1.90	0.54
1:A:451:ASP:OD2	1:A:457:ARG:HB2	2.07	0.54
1:A:473:ALA:HA	1:A:498:VAL:HG23	1.90	0.54
1:B:39:LYS:O	1:B:43:LYS:HG3	2.08	0.54
2:K:18:LEU:O	2:K:89:MET:HG3	2.08	0.53
2:L:113:VAL:HB	2:L:116:GLU:CG	2.37	0.53
1:E:402:ASN:HB2	1:E:425:ARG:HH21	1.72	0.53
2:J:4:LEU:HD13	2:J:22:CYS:SG	2.48	0.53
1:B:213:PHE:HD1	1:B:241:GLU:HG3	1.73	0.53
1:B:406:SER:O	1:B:410:ILE:HG12	2.08	0.53
1:C:303:MET:SD	1:C:343:VAL:CA	2.96	0.53
2:J:34:THR:O	2:J:37:THR:OG1	2.20	0.53
1:A:246:VAL:HG11	1:B:12:ILE:HG21	1.91	0.53
1:E:217:ALA:O	1:E:220:VAL:HG12	2.08	0.53
1:E:416:ASN:O	1:E:416:ASN:ND2	2.41	0.53
2:I:89:MET:HE1	2:I:100:TYR:CE2	2.44	0.53
2:K:35:PHE:CE1	2:K:83:ASN:HA	2.44	0.53
2:L:70:VAL:HB	2:L:74:PHE:CD2	2.44	0.53
2:G:1:GLN:CG	2:G:28:ASN:HB2	2.27	0.53
1:A:266:LEU:O	1:A:270:ILE:HG12	2.09	0.53
1:C:228:GLY:O	1:C:231:GLY:N	2.36	0.53
1:C:423:THR:CG2	1:C:425:ARG:H	2.20	0.53
1:F:405:ARG:O	1:F:409:LEU:HD22	2.08	0.53
2:I:116:GLU:C	2:I:118:ARG:HH12	2.12	0.53
2:K:111:SER:O	2:K:117:TYR:OH	2.13	0.53
1:A:13:PHE:CZ	1:B:247:GLN:HG3	2.43	0.53
1:C:92:THR:HG22	1:C:178:ILE:CD1	2.38	0.53
1:D:454:ARG:HA	1:D:457:ARG:HH21	1.73	0.53
1:C:168:ASN:HD22	1:C:170:HIS:N	2.03	0.53
2:H:94:PRO:O	2:H:97:THR:HG23	2.09	0.53
1:B:48:VAL:HG11	1:B:208:MET:CE	2.39	0.53
1:B:208:MET:HB3	1:B:235:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:PRO:O	1:C:381:VAL:HG23	2.09	0.53
1:D:145:ASP:HB3	1:D:148:VAL:HG23	1.91	0.53
1:D:229:GLU:OE2	1:D:232:LYS:HB2	2.09	0.53
1:E:65:ILE:O	1:E:69:ARG:HG3	2.09	0.53
1:F:16:VAL:HG23	1:F:17:ALA:H	1.74	0.53
1:F:23:ARG:HG3	1:F:433:ASN:O	2.09	0.53
2:G:103:ALA:HB2	2:G:120:TRP:CE3	2.44	0.53
2:I:63:ILE:HD13	2:I:109:TYR:HE1	1.73	0.53
1:C:127:VAL:HG21	1:C:132:LEU:HD22	1.91	0.53
2:H:57:ILE:HG13	2:H:64:THR:HG22	1.91	0.53
2:I:73:ARG:C	2:I:74:PHE:HD1	2.12	0.53
2:J:44:ARG:NE	2:J:52:GLU:OE2	2.41	0.53
2:K:9:GLY:H	2:K:124:THR:HG21	1.73	0.53
1:C:53:PHE:HD2	1:C:197:ASP:OD2	1.92	0.52
1:A:8:ILE:O	1:B:285:LYS:NZ	2.42	0.52
1:D:283:ILE:HD13	1:D:325:ALA:HB2	1.91	0.52
2:I:74:PHE:N	2:I:74:PHE:CD1	2.75	0.52
2:I:50:GLU:O	2:I:51:ARG:C	2.47	0.52
2:J:6:GLU:N	2:J:122:GLN:HE22	2.06	0.52
2:I:101:TYR:HB3	2:I:120:TRP:CZ3	2.45	0.52
1:E:345:GLN:HG3	2:K:32:GLY:CA	2.39	0.52
1:A:102:TYR:HE1	1:A:172:LEU:HD12	1.70	0.52
1:A:311:ARG:HH21	1:A:315:THR:HG21	1.75	0.52
1:A:458:VAL:O	1:A:462:VAL:HG23	2.10	0.52
1:B:194:ASP:O	1:B:198:LEU:HD23	2.09	0.52
1:D:27:THR:CG2	1:D:50:ARG:HH11	2.22	0.52
1:D:34:SER:OG	1:D:37:ALA:HB2	2.10	0.52
1:D:94:LEU:HD12	1:D:118:LYS:HG3	1.92	0.52
1:D:471:VAL:HG21	1:D:498:VAL:HG11	1.92	0.52
1:F:483:ASP:N	1:F:483:ASP:OD1	2.42	0.52
2:K:57:ILE:HD11	2:K:61:GLY:HA2	1.91	0.52
1:D:131:GLN:O	1:D:131:GLN:HG2	2.10	0.52
2:K:92:LEU:HB3	2:K:128:VAL:HG21	1.92	0.52
1:A:264:GLY:N	1:A:297:THR:OG1	2.41	0.52
1:C:311:ARG:O	1:C:315:THR:HG23	2.10	0.52
1:F:3:GLN:HG2	1:F:359:HIS:HB2	1.91	0.52
2:L:1:GLN:HG2	2:L:119:TYR:HD2	1.75	0.52
1:C:143:TYR:HD1	1:C:181:PRO:HD3	1.73	0.52
1:D:185:VAL:CG1	1:D:187:LEU:HD23	2.18	0.52
1:E:27:THR:HG22	1:E:50:ARG:HD3	1.90	0.52
1:F:264:GLY:N	1:F:297:THR:OG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:101:TYR:CD1	2:L:123:GLY:HA3	2.45	0.52
1:A:210:PHE:CD2	1:A:260:MET:HE1	2.45	0.51
1:B:68:VAL:CG2	1:B:81:ILE:HD11	2.40	0.51
1:C:149:LEU:CD2	1:C:170:HIS:CB	2.61	0.51
2:I:42:TRP:CD1	2:I:76:ILE:HD12	2.45	0.51
1:A:94:LEU:CB	1:A:118:LYS:HA	2.39	0.51
1:A:406:SER:OG	1:A:490:PRO:HG2	2.09	0.51
1:C:399:VAL:HG21	1:C:406:SER:OG	2.10	0.51
1:D:62:GLN:HE22	1:D:204:GLN:HG3	1.75	0.51
1:E:16:VAL:HG21	1:E:353:GLU:OE2	2.10	0.51
1:F:3:GLN:HE21	1:F:358:THR:HA	1.74	0.51
2:L:54:VAL:HG13	2:L:70:VAL:HG11	1.91	0.51
1:D:432:LEU:HD13	1:D:438:VAL:HG11	1.92	0.51
1:F:6:HIS:HE1	1:F:358:THR:O	1.92	0.51
2:H:14:SER:HA	2:H:92:LEU:O	2.09	0.51
2:K:74:PHE:CE1	2:K:89:MET:HA	2.44	0.51
1:E:213:PHE:CD2	1:E:215:ARG:HD2	2.46	0.51
1:A:378:GLU:CD	1:A:378:GLU:H	2.14	0.51
1:A:459:GLN:HG3	1:A:463:ASP:OD1	2.11	0.51
1:D:240:ILE:HD11	1:D:259:ILE:HD12	1.93	0.51
1:E:239:LYS:HD2	1:E:260:MET:CE	2.41	0.51
2:G:1:GLN:HB2	2:G:28:ASN:CA	2.40	0.51
2:G:1:GLN:NE2	2:G:119:TYR:CD1	2.78	0.51
2:G:17:SER:HB3	2:G:90:ASN:HA	1.93	0.51
2:K:5:GLN:OE1	2:K:122:GLN:HG3	2.10	0.51
1:A:270:ILE:HG13	1:A:275:VAL:CG2	2.40	0.51
1:C:279:GLN:O	1:C:283:ILE:HG13	2.11	0.51
1:A:381:VAL:HG21	1:A:491:ASN:HA	1.93	0.51
1:B:61:HIS:O	1:B:65:ILE:HD12	2.11	0.51
1:D:38:LEU:HD13	1:D:68:VAL:HG12	1.92	0.51
1:A:16:VAL:HG21	1:A:352:ILE:HG22	1.93	0.51
1:D:263:ARG:HH11	1:D:279:GLN:HE22	1.59	0.51
1:E:416:ASN:O	1:E:416:ASN:CG	2.48	0.51
1:F:62:GLN:HA	1:F:62:GLN:HE21	1.76	0.51
2:I:103:ALA:HB2	2:I:120:TRP:CE3	2.45	0.51
1:B:398:LEU:HD11	1:B:461:GLY:HA3	1.93	0.51
1:F:214:ILE:CG2	1:F:252:ILE:HD13	2.39	0.51
1:F:398:LEU:CD1	1:F:461:GLY:HA3	2.40	0.51
2:J:74:PHE:CZ	2:J:89:MET:HG2	2.45	0.51
1:C:95:PHE:HZ	1:C:125:PHE:CD2	2.29	0.50
1:D:202:VAL:CG1	1:D:231:GLY:HA3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:ARG:CG	1:E:435:THR:HG21	2.41	0.50
1:F:293:VAL:O	1:F:326:ASP:HB2	2.11	0.50
1:B:473:ALA:HA	1:B:498:VAL:HG23	1.92	0.50
1:E:459:GLN:NE2	1:E:463:ASP:OD1	2.44	0.50
1:F:313:GLU:O	1:F:316:ASP:HB3	2.11	0.50
2:K:101:TYR:CE1	2:K:123:GLY:HA3	2.47	0.50
2:L:92:LEU:HD22	2:L:128:VAL:CG2	2.41	0.50
1:C:4:LEU:CD2	1:D:367:ILE:HD12	2.42	0.50
1:C:61:HIS:O	1:C:65:ILE:HG13	2.10	0.50
1:C:94:LEU:HD13	1:C:95:PHE:N	2.27	0.50
1:E:265:ASP:O	1:E:268:VAL:HG12	2.11	0.50
1:E:441:VAL:CG1	1:E:460:LEU:HG	2.41	0.50
1:F:28:ILE:HD11	1:F:46:MET:HE3	1.93	0.50
1:D:499:ARG:HH11	1:D:499:ARG:H	1.58	0.50
1:E:349:ARG:HG3	2:K:31:SER:O	2.12	0.50
1:A:53:PHE:O	1:A:86:LYS:HE3	2.10	0.50
1:E:13:PHE:O	2:K:105:ARG:NH2	2.45	0.50
1:E:300:LEU:HG	1:E:347:MET:CE	2.40	0.50
1:B:432:LEU:HD13	1:B:438:VAL:HG11	1.91	0.50
1:C:235:LEU:HD11	1:C:431:GLN:HB3	1.94	0.50
1:C:355:GLN:O	1:C:358:THR:HG22	2.11	0.50
1:A:494:ARG:HD2	1:A:496:VAL:HG12	1.93	0.50
1:B:311:ARG:HH21	1:B:315:THR:HG21	1.76	0.50
2:L:36:SER:C	2:L:38:ASP:H	2.15	0.50
1:E:441:VAL:HG11	1:E:460:LEU:HG	1.93	0.50
1:F:400:LEU:HD21	1:F:457:ARG:HB2	1.93	0.50
2:I:2:VAL:HG22	2:I:26:GLY:O	2.12	0.50
2:K:113:VAL:HB	2:K:116:GLU:HG3	1.94	0.50
1:E:294:ILE:HG23	1:E:327:CYS:HB2	1.94	0.50
1:F:259:ILE:HB	1:F:286:CYS:SG	2.51	0.50
2:G:40:ILE:HG21	2:G:85:VAL:HG21	1.94	0.50
2:J:27:SER:HB2	2:J:34:THR:HG22	1.94	0.50
1:C:258:GLY:O	1:C:259:ILE:HD13	2.12	0.49
1:D:154:LEU:HD11	1:D:165:HIS:HB2	1.94	0.49
2:H:6:GLU:CD	2:H:123:GLY:H	2.15	0.49
1:A:260:MET:SD	1:A:329:MET:HE1	2.51	0.49
1:A:406:SER:OG	1:A:490:PRO:CD	2.60	0.49
1:B:241:GLU:HB2	1:B:265:ASP:HB3	1.93	0.49
1:C:91:ARG:H	1:C:128:ASP:HB2	1.77	0.49
1:C:91:ARG:H	1:C:128:ASP:CB	2.24	0.49
1:E:261:VAL:O	1:E:263:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:PHE:CD1	2:G:112:LYS:HA	2.47	0.49
1:E:299:MET:O	1:E:300:LEU:HD23	2.12	0.49
1:F:453:ASP:O	1:F:455:GLU:N	2.46	0.49
2:K:35:PHE:HE1	2:K:80:ASN:HA	1.78	0.49
1:A:199:GLN:O	1:A:203:GLU:HB2	2.13	0.49
1:E:239:LYS:HD2	1:E:260:MET:HE2	1.94	0.49
1:F:263:ARG:HA	1:F:266:LEU:HB3	1.93	0.49
1:D:14:GLU:OE2	1:D:15:PRO:HD2	2.12	0.49
1:D:270:ILE:HD13	1:D:274:LYS:HB2	1.95	0.49
1:F:451:ASP:OD2	1:F:457:ARG:HD2	2.13	0.49
2:K:103:ALA:HB2	2:K:120:TRP:CD1	2.48	0.49
1:A:104:PRO:HB3	1:A:167:ASN:O	2.13	0.49
1:B:311:ARG:O	1:B:315:THR:HG23	2.13	0.49
1:B:439:GLU:OE1	1:B:470:TYR:OH	2.27	0.49
1:F:192:GLU:HA	1:F:195:ARG:HD3	1.95	0.49
2:I:45:GLN:HB3	2:I:99:VAL:CG1	2.42	0.49
1:B:486:VAL:HG22	1:B:487:LYS:N	2.24	0.49
1:C:247:GLN:HG3	1:D:13:PHE:CZ	2.46	0.49
1:D:2:SER:N	1:D:359:HIS:CE1	2.81	0.49
1:E:38:LEU:HD23	1:E:38:LEU:HA	1.49	0.49
1:E:242:ASN:HB2	1:E:269:GLU:OE1	2.13	0.49
2:I:6:GLU:OE2	2:I:122:GLN:NE2	2.46	0.49
1:A:294:ILE:HG12	1:A:327:CYS:HB2	1.95	0.49
1:B:198:LEU:HD12	1:B:227:LEU:CD2	2.38	0.49
1:B:271:PRO:HG2	1:B:274:LYS:HG3	1.94	0.49
1:C:330:LEU:HD11	1:C:347:MET:HG3	1.95	0.49
1:C:483:ASP:OD2	1:C:485:SER:HB2	2.13	0.49
1:D:270:ILE:HD11	1:D:275:VAL:CG2	2.43	0.49
1:E:28:ILE:HG21	1:E:64:THR:CG2	2.42	0.49
1:F:395:LYS:HE3	1:F:475:ASP:CB	2.42	0.49
1:F:460:LEU:HD23	1:F:460:LEU:C	2.33	0.49
1:F:488:GLY:O	1:F:489:TYR:HB3	2.12	0.49
2:G:57:ILE:HG13	2:G:64:THR:CG2	2.39	0.49
1:E:363:MET:HE2	1:E:367:ILE:HD11	1.95	0.49
1:F:64:THR:O	1:F:68:VAL:HG12	2.13	0.49
1:A:149:LEU:HB2	1:A:170:HIS:CD2	2.48	0.49
1:C:471:VAL:HG13	1:C:475:ASP:HB2	1.94	0.49
1:F:396:ALA:HA	1:F:417:CYS:HB2	1.94	0.49
1:F:398:LEU:CD2	1:F:479:ILE:HG23	2.43	0.49
2:G:1:GLN:NE2	2:G:119:TYR:HD1	2.11	0.49
2:H:45:GLN:HG3	2:H:51:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ASP:CG	1:B:311:ARG:HH22	2.15	0.48
1:C:247:GLN:CG	1:D:13:PHE:CE2	2.89	0.48
1:E:475:ASP:O	1:E:498:VAL:HG22	2.12	0.48
1:F:240:ILE:HD11	1:F:252:ILE:HG21	1.95	0.48
1:F:414:ARG:CZ	1:F:436:ARG:HD2	2.42	0.48
1:A:316:ASP:OD1	1:B:311:ARG:NH2	2.45	0.48
1:C:208:MET:HE2	1:C:210:PHE:HE1	1.78	0.48
1:E:215:ARG:NE	1:E:219:GLN:HE22	2.12	0.48
1:E:453:ASP:OD1	1:E:453:ASP:O	2.31	0.48
2:I:5:GLN:O	2:I:22:CYS:HA	2.12	0.48
2:J:113:VAL:HB	2:J:116:GLU:HG3	1.95	0.48
2:K:1:GLN:HB3	2:K:2:VAL:H	1.42	0.48
1:C:279:GLN:HE21	1:C:323:ASN:HD22	1.61	0.48
1:D:96:LYS:HD2	1:D:96:LYS:HA	1.75	0.48
1:D:117:GLU:HB3	1:D:118:LYS:NZ	2.27	0.48
1:D:133:PRO:HA	1:D:162:LEU:HD11	1.95	0.48
1:E:405:ARG:HH11	1:E:405:ARG:CG	2.26	0.48
2:K:6:GLU:HB3	2:K:22:CYS:HB2	1.96	0.48
1:A:257:ASP:O	1:A:292:PRO:HD2	2.14	0.48
1:B:84:ASP:HA	1:B:210:PHE:HB2	1.95	0.48
1:B:483:ASP:CB	1:D:494:ARG:NH1	2.77	0.48
1:C:104:PRO:HG3	1:C:168:ASN:O	2.13	0.48
1:C:208:MET:HE2	1:C:210:PHE:CE1	2.48	0.48
1:E:271:PRO:C	1:E:273:GLU:N	2.66	0.48
1:E:418:PRO:HG2	1:E:470:TYR:CD2	2.49	0.48
1:A:451:ASP:OD1	1:A:454:ARG:HA	2.13	0.48
1:C:345:GLN:NE2	2:J:32:GLY:HA2	2.28	0.48
1:E:283:ILE:HA	1:E:293:VAL:HG11	1.96	0.48
1:A:153:VAL:HA	1:A:164:CYS:SG	2.54	0.48
1:C:420:ILE:HD11	1:C:465:ALA:HB2	1.95	0.48
1:E:279:GLN:O	1:E:283:ILE:HG13	2.14	0.48
1:F:54:SER:HA	1:F:86:LYS:HG3	1.95	0.48
1:F:367:ILE:HA	1:F:370:LEU:HB2	1.96	0.48
2:J:130:SER:O	2:J:131:ALA:HB3	2.13	0.48
1:C:263:ARG:HD2	1:C:279:GLN:OE1	2.14	0.48
1:E:27:THR:O	1:E:334:THR:OG1	2.31	0.48
1:E:249:ILE:HG12	1:E:282:ILE:HD13	1.96	0.48
1:E:419:ILE:O	1:E:438:VAL:HA	2.14	0.48
1:F:330:LEU:HB3	1:F:333:GLU:HB2	1.96	0.48
1:F:374:PRO:CD	1:F:374:PRO:O	2.51	0.48
2:H:53:PHE:CD2	2:H:112:LYS:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:53:PHE:O	2:I:67:VAL:HG21	2.12	0.48
2:I:58:SER:HG	2:I:63:ILE:HG22	1.78	0.48
1:F:366:SER:O	1:F:370:LEU:HD13	2.13	0.48
1:F:216:THR:N	1:F:219:GLN:OE1	2.39	0.48
1:E:271:PRO:O	1:E:273:GLU:N	2.47	0.47
1:F:27:THR:C	1:F:28:ILE:HD13	2.35	0.47
1:F:479:ILE:O	1:F:493:THR:HA	2.13	0.47
1:E:386:VAL:HG21	1:E:413:TYR:HB2	1.96	0.47
1:F:6:HIS:CD2	1:F:10:LEU:HD21	2.49	0.47
1:F:250:ASP:O	1:F:253:ILE:HG22	2.14	0.47
1:B:192:GLU:CD	1:B:192:GLU:N	2.67	0.47
1:D:213:PHE:O	1:D:215:ARG:HG3	2.14	0.47
1:A:12:ILE:HG22	1:A:13:PHE:CE2	2.49	0.47
1:A:227:LEU:CD1	1:A:234:THR:HG23	2.42	0.47
1:B:250:ASP:OD1	1:B:285:LYS:HE3	2.14	0.47
1:C:112:THR:HG22	1:C:127:VAL:HG23	1.96	0.47
1:D:412:LYS:HD3	1:D:413:TYR:CE2	2.50	0.47
1:E:27:THR:OG1	1:E:331:SER:O	2.31	0.47
1:E:208:MET:HB3	1:E:235:LEU:HB2	1.95	0.47
1:F:46:MET:HE2	1:F:49:ALA:HA	1.96	0.47
2:L:101:TYR:HD1	2:L:123:GLY:HA3	1.80	0.47
1:A:94:LEU:HB3	1:A:118:LYS:CA	2.44	0.47
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.79	0.47
1:D:198:LEU:O	1:D:202:VAL:HG22	2.14	0.47
1:C:311:ARG:HH21	1:D:298:GLN:HB2	1.80	0.47
2:G:1:GLN:CG	2:G:2:VAL:N	2.53	0.47
2:J:22:CYS:HB3	2:J:85:VAL:HG13	1.96	0.47
2:J:104:GLY:HA3	2:J:119:TYR:CZ	2.49	0.47
1:B:51:MET:HE3	1:B:53:PHE:CE1	2.50	0.47
1:B:482:ALA:HB1	1:B:486:VAL:HG11	1.97	0.47
1:C:42:MET:HE2	1:C:75:LEU:HD12	1.97	0.47
1:D:258:GLY:O	1:D:259:ILE:HD13	2.13	0.47
1:D:264:GLY:H	1:D:297:THR:CB	2.28	0.47
1:D:451:ASP:C	1:D:453:ASP:O	2.53	0.47
1:E:75:LEU:CB	1:E:77:LEU:HD22	2.44	0.47
1:C:427:LEU:O	1:C:431:GLN:HG3	2.14	0.47
1:D:104:PRO:HD3	1:D:169:HIS:HB2	1.97	0.47
1:D:397:ILE:HD12	1:D:417:CYS:SG	2.54	0.47
1:E:83:LEU:HD13	1:E:201:GLY:HA3	1.97	0.47
1:E:432:LEU:HD13	1:E:438:VAL:HG11	1.96	0.47
2:K:89:MET:O	2:K:92:LEU:CG	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ILE:HD12	1:C:129:TYR:HB2	1.96	0.47
1:D:345:GLN:HG2	2:I:32:GLY:HA2	1.97	0.47
1:E:27:THR:HG22	1:E:50:ARG:CB	2.39	0.47
1:E:406:SER:O	1:E:410:ILE:HG12	2.15	0.47
2:G:44:ARG:HG2	2:G:54:VAL:CG2	2.45	0.47
1:D:270:ILE:CD1	1:D:275:VAL:HG23	2.45	0.47
1:B:495:LEU:HD22	1:D:381:VAL:HG22	1.97	0.46
1:C:43:LYS:O	2:J:29:PHE:HB3	2.15	0.46
1:C:202:VAL:CG2	1:C:227:LEU:HD23	2.44	0.46
1:E:239:LYS:NZ	3:E:601:GOL:H11	2.30	0.46
1:E:271:PRO:O	1:E:274:LYS:N	2.49	0.46
1:F:88:PRO:HD3	1:F:189:ALA:O	2.15	0.46
2:H:6:GLU:OE2	2:H:121:GLY:HA3	2.14	0.46
2:I:88:GLN:HG3	2:I:89:MET:N	2.31	0.46
2:J:103:ALA:HB2	2:J:120:TRP:CE3	2.50	0.46
2:L:20:LEU:HD12	2:L:87:LEU:HD23	1.97	0.46
1:F:364:PHE:CD2	1:F:390:PHE:HE2	2.33	0.46
1:F:402:ASN:OD1	1:F:457:ARG:NH2	2.48	0.46
1:C:4:LEU:HD21	1:D:367:ILE:HD12	1.98	0.46
1:C:402:ASN:HA	1:C:423:THR:HG23	1.96	0.46
1:E:364:PHE:CZ	1:E:387:SER:OG	2.66	0.46
1:E:477:MET:CE	1:E:498:VAL:CG1	2.93	0.46
2:L:100:TYR:O	2:L:123:GLY:HA2	2.15	0.46
1:C:27:THR:HG22	1:C:50:ARG:CB	2.46	0.46
1:C:131:GLN:O	1:C:135:VAL:HG12	2.16	0.46
1:F:6:HIS:CE1	1:F:358:THR:O	2.69	0.46
2:H:1:GLN:OE1	2:H:28:ASN:CG	2.54	0.46
1:B:278:ALA:O	1:B:282:ILE:HG13	2.16	0.46
1:C:311:ARG:HH11	1:C:315:THR:CG2	2.27	0.46
1:D:27:THR:HG21	1:D:50:ARG:NH1	2.31	0.46
1:E:274:LYS:O	1:E:274:LYS:CG	2.62	0.46
2:I:22:CYS:HB3	2:I:85:VAL:HG13	1.97	0.46
1:A:54:SER:O	1:A:55:HIS:ND1	2.42	0.46
1:C:32:THR:HA	1:C:37:ALA:HB1	1.97	0.46
1:C:215:ARG:HB2	1:C:219:GLN:OE1	2.16	0.46
1:D:41:LEU:HB3	1:D:46:MET:CE	2.37	0.46
2:L:40:ILE:HG21	2:L:85:VAL:HG11	1.97	0.46
1:A:281:CYS:SG	1:A:285:LYS:HE2	2.56	0.46
1:B:38:LEU:CD1	1:B:68:VAL:HG12	2.43	0.46
2:L:1:GLN:HE21	2:L:28:ASN:HD21	1.64	0.46
1:B:249:ILE:O	1:B:253:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ILE:CD1	1:B:465:ALA:HB2	2.46	0.46
1:C:486:VAL:CG1	1:C:491:ASN:HD21	2.27	0.46
1:D:172:LEU:HD23	1:D:173:THR:N	2.31	0.46
2:I:77:SER:O	2:I:85:VAL:HG23	2.16	0.46
2:L:58:SER:HB3	2:L:63:ILE:HG23	1.97	0.46
1:D:5:GLN:O	1:D:8:ILE:HG13	2.15	0.46
1:F:5:GLN:O	1:F:8:ILE:HG13	2.16	0.46
1:F:61:HIS:O	1:F:65:ILE:HD12	2.16	0.46
1:F:333:GLU:OE1	1:F:333:GLU:N	2.40	0.46
1:F:410:ILE:HD11	1:F:480:VAL:HG11	1.98	0.46
2:J:6:GLU:HA	2:J:21:SER:O	2.16	0.46
2:K:6:GLU:CG	2:K:123:GLY:HA2	2.46	0.46
1:A:213:PHE:N	1:A:241:GLU:OE2	2.49	0.46
1:D:141:LEU:O	1:D:181:PRO:HD2	2.15	0.46
1:D:144:VAL:HG13	1:D:178:ILE:CD1	2.46	0.46
1:D:151:LEU:N	1:D:151:LEU:HD22	2.31	0.46
1:E:224:ARG:CZ	1:E:236:ILE:HG13	2.46	0.46
1:F:389:ALA:HB2	1:F:397:ILE:HD11	1.98	0.46
1:A:53:PHE:O	1:A:86:LYS:HG2	2.16	0.45
1:C:471:VAL:HG11	1:C:498:VAL:HG21	1.97	0.45
1:E:388:SER:O	1:E:392:VAL:HG22	2.16	0.45
1:E:436:ARG:O	1:E:437:SER:HB2	2.16	0.45
1:F:290:GLY:CA	1:F:412:LYS:HB2	2.44	0.45
2:K:44:ARG:CB	2:K:100:TYR:HA	2.46	0.45
1:A:95:PHE:O	1:A:98:GLY:N	2.41	0.45
1:A:472:SER:O	1:A:498:VAL:HG23	2.05	0.45
1:B:65:ILE:HG21	1:B:69:ARG:HH11	1.78	0.45
1:B:224:ARG:HE	1:B:236:ILE:HG13	1.82	0.45
1:F:292:PRO:HG3	1:F:435:THR:HG22	1.99	0.45
2:H:1:GLN:OE1	2:H:28:ASN:CB	2.65	0.45
2:H:55:GLY:HA3	2:H:76:ILE:HD11	1.99	0.45
2:J:53:PHE:HD2	2:J:67:VAL:HG13	1.81	0.45
1:A:102:TYR:CD2	1:A:108:VAL:HG21	2.50	0.45
1:C:319:ASN:OD1	1:D:319:ASN:ND2	2.44	0.45
1:D:78:HIS:N	1:D:78:HIS:CD2	2.85	0.45
1:D:270:ILE:C	1:D:270:ILE:HD12	2.37	0.45
1:D:300:LEU:HG	1:D:347:MET:CE	2.46	0.45
2:G:1:GLN:OE1	2:G:1:GLN:N	2.45	0.45
2:J:93:GLN:C	2:J:128:VAL:HG11	2.36	0.45
1:C:116:PHE:CD1	1:C:116:PHE:N	2.85	0.45
1:C:235:LEU:HA	1:C:257:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ASN:HB2	1:D:351:CYS:SG	2.56	0.45
1:D:270:ILE:HG22	2:J:108:TRP:CH2	2.51	0.45
1:D:331:SER:N	1:D:333:GLU:OE1	2.49	0.45
1:E:261:VAL:O	1:E:261:VAL:HG23	2.17	0.45
1:E:491:ASN:CG	1:E:491:ASN:O	2.54	0.45
1:F:270:ILE:HD11	1:F:274:LYS:CB	2.34	0.45
2:I:7:SER:N	2:I:21:SER:O	2.50	0.45
1:D:140:GLY:O	1:D:153:VAL:HG22	2.16	0.45
1:D:253:ILE:O	1:D:291:LYS:NZ	2.49	0.45
1:E:420:ILE:HD12	1:E:465:ALA:HB2	1.98	0.45
1:F:26:CYS:SG	1:F:46:MET:HG3	2.56	0.45
1:F:75:LEU:HB2	1:F:77:LEU:HD12	1.99	0.45
1:F:191:SER:O	1:F:195:ARG:HD2	2.16	0.45
1:F:234:THR:HA	1:F:431:GLN:HE22	1.81	0.45
1:F:373:ILE:HA	1:F:374:PRO:C	2.37	0.45
2:L:4:LEU:HD12	2:L:120:TRP:HA	1.98	0.45
1:A:281:CYS:O	1:A:285:LYS:HG3	2.16	0.45
1:B:26:CYS:HB2	1:B:46:MET:SD	2.57	0.45
1:B:53:PHE:HD2	1:B:197:ASP:OD2	1.99	0.45
1:C:149:LEU:HD11	1:C:170:HIS:CE1	2.48	0.45
1:D:270:ILE:HD11	1:D:275:VAL:HG23	1.98	0.45
1:D:426:LEU:HA	1:D:426:LEU:HD23	1.63	0.45
1:E:345:GLN:O	1:E:349:ARG:HD3	2.17	0.45
1:A:140:GLY:O	1:A:153:VAL:HG23	2.16	0.45
1:B:263:ARG:HD2	1:B:279:GLN:OE1	2.17	0.45
1:C:42:MET:HE1	1:C:72:ALA:N	2.32	0.45
1:C:273:GLU:H	1:C:273:GLU:HG3	1.41	0.45
2:H:106:ASP:OD1	2:H:106:ASP:N	2.46	0.45
1:D:50:ARG:HD2	1:D:329:MET:SD	2.56	0.45
1:F:62:GLN:NE2	1:F:204:GLN:HG3	2.23	0.45
1:F:234:THR:HA	1:F:431:GLN:HE21	1.82	0.45
1:F:311:ARG:O	1:F:315:THR:HG23	2.17	0.45
2:H:28:ASN:OD1	2:H:30:SER:OG	2.34	0.45
2:J:19:LYS:HD3	2:J:88:GLN:HE22	1.82	0.45
2:K:35:PHE:CE1	2:K:80:ASN:HA	2.50	0.45
2:L:3:GLN:O	2:L:24:ALA:HA	2.17	0.45
1:A:379:GLU:OE2	1:A:413:TYR:OH	2.35	0.45
1:C:157:GLU:HB3	1:C:161:THR:O	2.16	0.45
1:D:133:PRO:CA	1:D:162:LEU:HD11	2.46	0.45
1:F:26:CYS:HB2	1:F:46:MET:HE3	1.97	0.45
1:F:68:VAL:CG1	1:F:81:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ILE:O	1:F:253:ILE:HB	2.17	0.45
1:F:293:VAL:HG13	1:F:325:ALA:HA	1.98	0.45
1:C:102:TYR:HE1	1:C:122:LYS:O	2.00	0.45
1:D:92:THR:OG1	1:D:93:GLY:N	2.47	0.45
2:J:59:TRP:CD1	2:J:108:TRP:HB2	2.52	0.45
2:L:99:VAL:HG22	2:L:101:TYR:CE1	2.52	0.45
1:A:483:ASP:CB	1:A:491:ASN:HD21	2.30	0.44
1:B:409:LEU:HD23	1:B:412:LYS:HD3	1.99	0.44
1:C:215:ARG:HH11	1:C:215:ARG:HG2	1.81	0.44
1:D:83:LEU:HB3	1:D:209:ILE:CD1	2.46	0.44
1:D:292:PRO:HG3	1:D:435:THR:HG22	1.99	0.44
1:D:299:MET:HE2	1:D:328:VAL:CG1	2.47	0.44
2:H:13:GLN:NE2	2:H:129:SER:O	2.50	0.44
2:I:50:GLU:O	2:I:52:GLU:HG2	2.17	0.44
1:A:136:VAL:HG12	1:A:153:VAL:HG21	1.98	0.44
1:A:141:LEU:HA	1:A:151:LEU:O	2.17	0.44
1:D:129:TYR:CZ	1:D:131:GLN:HB3	2.52	0.44
1:F:364:PHE:CZ	1:F:368:LYS:HD2	2.51	0.44
1:F:378:GLU:O	1:F:379:GLU:C	2.56	0.44
2:I:45:GLN:O	2:I:99:VAL:HG12	2.17	0.44
2:L:73:ARG:HH11	2:L:93:GLN:HG3	1.81	0.44
1:D:113:ASP:OD1	1:D:113:ASP:C	2.56	0.44
1:E:400:LEU:HD12	1:E:422:ALA:HB3	1.99	0.44
1:F:270:ILE:HG23	1:F:275:VAL:CG2	2.44	0.44
2:I:101:TYR:HB3	2:I:120:TRP:CE3	2.52	0.44
1:A:144:VAL:HG22	1:A:178:ILE:HD12	2.00	0.44
1:B:310:THR:HG23	1:B:313:GLU:OE1	2.17	0.44
1:E:266:LEU:HD12	1:E:266:LEU:HA	1.67	0.44
1:F:18:LYS:CB	1:F:355:GLN:HE21	2.30	0.44
2:K:43:PHE:HZ	2:K:117:TYR:CE1	2.35	0.44
2:L:9:GLY:H	2:L:124:THR:HG21	1.82	0.44
2:L:37:THR:H	2:L:59:TRP:HE3	1.65	0.44
1:B:61:HIS:C	1:B:65:ILE:HD12	2.38	0.44
1:D:454:ARG:HG3	1:D:457:ARG:NH2	2.32	0.44
1:F:382:CYS:HB2	1:F:413:TYR:HE2	1.83	0.44
1:A:218:ASP:OD1	1:A:221:ARG:NH1	2.51	0.44
1:B:195:ARG:HE	1:B:195:ARG:HB3	1.68	0.44
1:C:217:ALA:HB2	1:C:251:ALA:HB1	1.99	0.44
1:D:3:GLN:NE2	1:D:358:THR:HA	2.32	0.44
1:F:215:ARG:HD3	1:F:219:GLN:HE22	1.83	0.44
1:F:392:VAL:O	1:F:393:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:SER:HA	2:H:89:MET:O	2.17	0.44
2:K:122:GLN:OE1	2:K:123:GLY:N	2.51	0.44
2:K:9:GLY:HA3	2:K:124:THR:HG22	1.99	0.44
2:L:59:TRP:CD1	2:L:60:ASN:ND2	2.78	0.44
1:A:270:ILE:HD12	1:B:12:ILE:HD11	1.99	0.44
1:E:7:ASN:HA	1:E:10:LEU:CG	2.44	0.44
1:F:212:SER:OG	3:F:601:GOL:O2	2.35	0.44
1:F:265:ASP:O	1:F:268:VAL:HG12	2.18	0.44
2:H:12:VAL:HG22	2:H:13:GLN:H	1.83	0.44
1:A:216:THR:OG1	1:A:219:GLN:HG3	2.18	0.44
1:C:149:LEU:CD2	1:C:170:HIS:CG	2.78	0.44
2:J:101:TYR:CE1	2:J:123:GLY:HA3	2.53	0.44
1:E:253:ILE:HD12	1:E:285:LYS:HG2	1.98	0.43
1:F:271:PRO:HB2	1:F:274:LYS:HG3	2.00	0.43
2:I:101:TYR:CB	2:I:120:TRP:CZ3	3.01	0.43
1:B:227:LEU:HD13	1:B:234:THR:OG1	2.18	0.43
2:I:17:SER:HB3	2:I:90:ASN:CB	2.46	0.43
2:I:53:PHE:HD1	2:I:67:VAL:HG22	1.83	0.43
1:C:90:ILE:HB	1:C:178:ILE:O	2.19	0.43
1:C:414:ARG:HG3	1:C:414:ARG:HH11	1.83	0.43
1:F:344:VAL:O	1:F:348:VAL:HG23	2.18	0.43
2:H:12:VAL:O	2:H:128:VAL:HA	2.18	0.43
2:I:88:GLN:CG	2:I:89:MET:N	2.77	0.43
1:A:378:GLU:HG3	1:A:489:TYR:CG	2.54	0.43
1:B:20:ARG:CD	1:B:348:VAL:HG22	2.48	0.43
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.58	0.43
1:C:300:LEU:CD1	1:C:347:MET:HE3	2.48	0.43
1:F:27:THR:HA	1:F:50:ARG:HB3	2.01	0.43
1:A:64:THR:O	1:A:68:VAL:HG13	2.18	0.43
1:A:445:VAL:HG23	1:A:450:GLU:HA	2.00	0.43
1:C:94:LEU:HD13	1:C:95:PHE:H	1.83	0.43
1:C:104:PRO:HA	1:C:166:VAL:O	2.19	0.43
1:C:395:LYS:HG3	1:C:475:ASP:HB3	2.01	0.43
1:E:311:ARG:NH2	1:E:315:THR:HG21	2.33	0.43
1:E:348:VAL:HG12	2:K:31:SER:O	2.19	0.43
1:F:48:VAL:HG11	1:F:208:MET:HE3	2.00	0.43
1:F:481:HIS:H	1:F:492:GLN:HB3	1.83	0.43
2:I:28:ASN:O	2:I:29:PHE:HB2	2.17	0.43
1:A:26:CYS:SG	1:A:46:MET:HG3	2.58	0.43
1:A:274:LYS:HD2	1:A:274:LYS:HA	1.74	0.43
1:A:386:VAL:HG21	1:A:413:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ARG:HE	1:F:311:ARG:HB3	1.31	0.43
1:F:419:ILE:O	1:F:438:VAL:HA	2.18	0.43
2:I:1:GLN:OE1	2:I:1:GLN:N	2.43	0.43
1:C:102:TYR:CD1	1:C:108:VAL:HG21	2.54	0.43
1:C:127:VAL:HG21	1:C:132:LEU:CD2	2.49	0.43
1:E:359:HIS:HB3	1:E:362:VAL:HG23	2.01	0.43
1:F:236:ILE:HG21	1:F:236:ILE:HD13	1.77	0.43
2:K:103:ALA:HB1	2:K:117:TYR:HB3	2.01	0.43
1:B:35:VAL:HG13	1:B:71:ALA:HB2	2.00	0.43
1:C:102:TYR:C	1:C:168:ASN:HD21	2.15	0.43
1:C:149:LEU:CG	1:C:170:HIS:ND1	2.81	0.43
1:C:262:ALA:O	1:C:266:LEU:HB2	2.18	0.43
1:C:378:GLU:OE1	1:C:405:ARG:HD3	2.19	0.43
1:D:33:GLN:HG3	1:D:64:THR:HG22	2.01	0.43
1:E:7:ASN:CA	1:E:10:LEU:HG	2.44	0.43
1:E:373:ILE:HG22	1:E:374:PRO:HD3	2.00	0.43
1:F:243:HIS:CD2	1:F:244:GLN:OE1	2.72	0.43
2:I:5:GLN:N	2:I:23:ALA:O	2.50	0.43
2:L:33:ARG:HH12	2:L:106:ASP:CA	2.27	0.43
1:A:168:ASN:N	1:A:168:ASN:OD1	2.52	0.43
1:A:264:GLY:CA	1:A:298:GLN:HE21	2.32	0.43
1:A:399:VAL:O	1:A:421:CYS:HA	2.18	0.43
1:D:23:ARG:HB2	1:D:327:CYS:SG	2.58	0.43
1:D:62:GLN:O	1:D:66:ASN:ND2	2.50	0.43
2:I:57:ILE:HD11	2:I:61:GLY:HA2	2.00	0.43
2:L:12:VAL:O	2:L:128:VAL:HA	2.18	0.43
1:E:27:THR:CG2	1:E:50:ARG:HD3	2.49	0.43
1:E:367:ILE:HD13	1:E:412:LYS:O	2.19	0.43
2:J:99:VAL:HG12	2:J:101:TYR:CE2	2.53	0.43
1:C:277:VAL:HG12	1:D:12:ILE:HG22	2.00	0.42
1:E:13:PHE:CD1	1:E:13:PHE:N	2.87	0.42
1:E:420:ILE:CD1	1:E:465:ALA:HB2	2.48	0.42
1:F:274:LYS:HA	1:F:277:VAL:HG12	2.00	0.42
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.58	0.42
2:K:4:LEU:HD21	2:K:119:TYR:CE1	2.54	0.42
1:A:161:THR:C	1:A:162:LEU:HD12	2.39	0.42
1:A:482:ALA:HA	1:A:490:PRO:HA	2.01	0.42
1:B:65:ILE:CG2	1:B:69:ARG:NH1	2.78	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.66	0.42
1:D:198:LEU:HD22	1:D:227:LEU:HD21	2.00	0.42
1:F:283:ILE:HD13	1:F:325:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:ARG:NH1	2:J:38:ASP:OD1	2.51	0.42
2:L:78:ARG:HB2	2:L:85:VAL:HG23	2.01	0.42
1:C:42:MET:HE3	1:C:75:LEU:HD12	2.00	0.42
1:C:471:VAL:HG12	1:C:472:SER:N	2.35	0.42
1:B:2:SER:N	1:B:359:HIS:NE2	2.66	0.42
1:B:260:MET:HE3	1:B:294:ILE:HD12	2.00	0.42
1:C:266:LEU:O	1:C:270:ILE:HG23	2.19	0.42
1:C:300:LEU:HG	1:C:347:MET:CE	2.49	0.42
1:D:62:GLN:HG3	1:D:66:ASN:HD21	1.83	0.42
1:E:212:SER:HA	1:E:239:LYS:CE	2.49	0.42
1:F:389:ALA:HA	1:F:394:ALA:CB	2.49	0.42
2:I:1:GLN:HB2	2:I:28:ASN:HA	2.00	0.42
2:L:38:ASP:O	2:L:78:ARG:NH2	2.52	0.42
1:A:378:GLU:HG3	1:A:489:TYR:CE1	2.55	0.42
1:D:254:GLU:O	3:D:602:GOL:O2	2.29	0.42
1:E:330:LEU:N	1:E:330:LEU:HD12	2.34	0.42
1:F:460:LEU:HD23	1:F:461:GLY:N	2.34	0.42
2:I:105:ARG:HG3	2:I:116:GLU:O	2.20	0.42
2:L:33:ARG:HG3	2:L:33:ARG:HH11	1.85	0.42
1:A:13:PHE:CE2	1:B:247:GLN:HG3	2.55	0.42
1:A:363:MET:HE3	1:A:414:ARG:HG3	2.01	0.42
1:E:492:GLN:C	1:E:493:THR:HG23	2.40	0.42
1:F:283:ILE:HD12	1:F:323:ASN:HB2	2.01	0.42
1:C:27:THR:OG1	1:C:331:SER:O	2.38	0.42
1:C:27:THR:HA	1:C:50:ARG:HB3	2.01	0.42
1:C:190:VAL:HG13	1:C:194:ASP:HB3	2.02	0.42
1:D:224:ARG:NH2	1:D:257:ASP:OD2	2.53	0.42
1:D:408:ARG:HG2	1:D:435:THR:HG21	2.01	0.42
1:D:419:ILE:O	1:D:438:VAL:HA	2.20	0.42
1:F:299:MET:CE	1:F:317:VAL:HG22	2.50	0.42
1:F:389:ALA:HA	1:F:394:ALA:HB3	2.00	0.42
2:H:104:GLY:HA3	2:H:119:TYR:CZ	2.55	0.42
2:K:75:THR:HB	2:K:88:GLN:HB3	2.00	0.42
2:L:88:GLN:HA	2:L:88:GLN:OE1	2.20	0.42
1:A:136:VAL:CG1	1:A:153:VAL:HG21	2.49	0.42
1:B:16:VAL:HG21	1:B:356:SER:CB	2.50	0.42
1:E:350:ILE:HD13	1:E:350:ILE:HG21	1.85	0.42
1:C:272:ALA:O	1:C:273:GLU:C	2.57	0.42
1:D:114:PRO:O	1:D:117:GLU:CB	2.68	0.42
1:F:388:SER:HA	1:F:391:GLU:CG	2.48	0.42
2:I:63:ILE:CD1	2:I:109:TYR:HE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:VAL:HG13	2:L:101:TYR:OH	2.19	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.94	0.42
1:C:90:ILE:O	1:C:177:GLY:HA2	2.20	0.42
1:C:460:LEU:HD12	1:C:460:LEU:HA	1.84	0.42
1:D:471:VAL:HG23	1:D:475:ASP:CB	2.49	0.42
1:E:12:ILE:HA	1:E:12:ILE:HD13	1.78	0.42
1:E:239:LYS:HZ3	3:E:601:GOL:C1	2.33	0.42
2:I:97:THR:O	2:I:98:ALA:HB2	2.20	0.42
2:K:41:GLY:HA3	2:K:117:TYR:CE2	2.55	0.42
1:A:84:ASP:HA	1:A:210:PHE:HB2	2.01	0.41
1:A:494:ARG:HD2	1:A:496:VAL:CG1	2.50	0.41
1:B:276:VAL:O	1:B:280:MET:HG3	2.20	0.41
1:F:199:GLN:HA	1:F:199:GLN:OE1	2.20	0.41
2:J:38:ASP:O	2:J:78:ARG:NH2	2.40	0.41
2:J:51:ARG:NH1	2:J:101:TYR:CD2	2.84	0.41
1:B:441:VAL:CG1	1:B:460:LEU:HG	2.50	0.41
1:B:454:ARG:HA	1:B:457:ARG:HH21	1.86	0.41
1:D:162:LEU:HD12	1:D:162:LEU:N	2.36	0.41
1:E:402:ASN:CB	1:E:425:ARG:HH21	2.33	0.41
2:G:35:PHE:O	2:G:78:ARG:NH2	2.53	0.41
2:J:6:GLU:HG3	2:J:102:CYS:SG	2.61	0.41
2:L:17:SER:HA	2:L:89:MET:O	2.20	0.41
1:C:39:LYS:HD2	1:C:74:GLU:OE1	2.21	0.41
1:E:212:SER:OG	1:E:239:LYS:HE2	2.20	0.41
1:E:377:PRO:O	1:E:381:VAL:HG23	2.21	0.41
2:K:4:LEU:HD21	2:K:119:TYR:HE1	1.85	0.41
2:L:36:SER:C	2:L:38:ASP:N	2.73	0.41
1:A:264:GLY:HA2	1:A:298:GLN:HE21	1.86	0.41
1:B:90:ILE:HD13	1:B:90:ILE:HG21	1.84	0.41
1:B:467:THR:O	1:B:468:LYS:C	2.59	0.41
1:B:492:GLN:NE2	1:D:492:GLN:NE2	2.66	0.41
1:D:60:TYR:O	1:D:63:THR:HB	2.19	0.41
1:E:299:MET:HB3	1:E:347:MET:HE1	2.00	0.41
1:F:398:LEU:HD21	1:F:400:LEU:HD13	2.02	0.41
2:I:58:SER:HB3	2:I:63:ILE:HG23	1.97	0.41
2:I:100:TYR:O	2:I:123:GLY:HA2	2.20	0.41
2:L:120:TRP:N	2:L:120:TRP:CD1	2.88	0.41
1:A:240:ILE:HD11	1:A:252:ILE:HG21	2.01	0.41
1:B:396:ALA:HB3	1:B:477:MET:HG2	2.03	0.41
1:D:90:ILE:HD13	1:D:129:TYR:HB2	2.01	0.41
1:D:349:ARG:HD3	2:I:32:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:ASP:O	1:E:390:PHE:HZ	2.03	0.41
1:F:220:VAL:HG21	1:F:255:ALA:CB	2.50	0.41
1:F:398:LEU:HD22	1:F:479:ILE:HG23	2.02	0.41
1:F:409:LEU:HD13	1:F:409:LEU:HA	1.90	0.41
1:F:432:LEU:HD23	1:F:432:LEU:HA	1.64	0.41
2:G:104:GLY:HA3	2:G:119:TYR:CE2	2.56	0.41
2:L:66:TYR:HB3	2:L:70:VAL:HG23	2.02	0.41
1:A:237:ILE:HG23	1:A:237:ILE:HD12	1.80	0.41
1:A:311:ARG:HD2	1:B:275:VAL:CG1	2.47	0.41
1:C:143:TYR:HE1	1:C:181:PRO:HG3	1.86	0.41
1:C:423:THR:HG22	1:C:424:THR:N	2.36	0.41
1:D:486:VAL:HG12	1:D:487:LYS:N	2.35	0.41
1:F:88:PRO:HG3	1:F:189:ALA:HA	2.02	0.41
1:F:389:ALA:CB	1:F:397:ILE:HD11	2.51	0.41
2:I:103:ALA:HB2	2:I:120:TRP:CD2	2.56	0.41
2:L:16:GLY:C	2:L:92:LEU:HD12	2.41	0.41
1:C:303:MET:O	1:C:303:MET:HG2	2.21	0.41
1:D:62:GLN:HE22	1:D:204:GLN:CG	2.33	0.41
1:D:183:CYS:HB3	1:D:184:GLU:H	1.79	0.41
1:E:214:ILE:HD13	1:E:214:ILE:HA	1.91	0.41
1:E:424:THR:HG22	1:E:443:TYR:HB3	2.02	0.41
1:A:406:SER:O	1:A:410:ILE:HG13	2.21	0.41
1:B:263:ARG:H	1:B:263:ARG:HG3	1.59	0.41
1:E:75:LEU:HB2	1:E:77:LEU:HD22	2.02	0.41
2:J:44:ARG:HB3	2:J:100:TYR:CE2	2.56	0.41
2:K:51:ARG:HE	2:K:114:PRO:CB	2.33	0.41
2:L:36:SER:C	2:L:37:THR:HG23	2.41	0.41
1:A:89:GLU:HB3	4:A:706:HOH:O	2.21	0.41
1:A:329:MET:HB2	1:A:329:MET:HE3	1.82	0.41
1:B:42:MET:HE1	1:B:72:ALA:HB2	2.02	0.41
1:B:214:ILE:HD13	1:B:214:ILE:HA	1.89	0.41
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.20	0.41
1:C:12:ILE:HG12	1:D:278:ALA:HB2	2.02	0.41
1:C:139:GLY:N	1:C:153:VAL:O	2.33	0.41
1:C:272:ALA:O	1:C:275:VAL:N	2.54	0.41
1:C:416:ASN:C	1:C:416:ASN:OD1	2.59	0.41
1:D:451:ASP:OD2	1:D:457:ARG:HG3	2.21	0.41
1:E:236:ILE:HD13	1:E:236:ILE:HG21	1.64	0.41
1:E:242:ASN:OD1	1:E:244:GLN:NE2	2.50	0.41
1:E:260:MET:HG3	1:E:294:ILE:HB	2.01	0.41
2:J:57:ILE:HD11	2:J:61:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:77:SER:HB2	2:K:78:ARG:H	1.38	0.41
1:A:231:GLY:O	1:A:234:THR:HG22	2.21	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.91	0.41
1:D:454:ARG:HD3	1:D:481:HIS:ND1	2.36	0.41
1:F:425:ARG:O	1:F:428:THR:HB	2.21	0.41
2:J:33:ARG:HA	2:J:37:THR:OG1	2.21	0.41
2:L:9:GLY:HA3	2:L:124:THR:CG2	2.51	0.41
1:A:109:LEU:HD22	1:A:161:THR:HG21	2.03	0.40
1:B:12:ILE:HG21	1:B:12:ILE:HD13	1.84	0.40
1:B:260:MET:HE1	1:B:329:MET:SD	2.61	0.40
1:C:39:LYS:HG3	1:C:71:ALA:HB1	2.03	0.40
1:C:277:VAL:HG13	1:D:10:LEU:HD13	2.03	0.40
1:D:209:ILE:HD13	1:D:209:ILE:HA	1.94	0.40
1:D:213:PHE:CD2	1:D:215:ARG:NH1	2.88	0.40
1:D:240:ILE:CD1	1:D:259:ILE:HD12	2.51	0.40
1:E:30:PRO:HD2	1:E:335:ALA:O	2.21	0.40
2:G:12:VAL:HG21	2:G:92:LEU:HD13	2.03	0.40
2:I:1:GLN:HE21	2:I:119:TYR:HB3	1.86	0.40
1:A:96:LYS:O	1:A:97:ASP:HB2	2.21	0.40
1:B:83:LEU:O	1:B:83:LEU:HD23	2.21	0.40
1:C:25:ILE:HG23	1:C:48:VAL:HB	2.04	0.40
1:D:191:SER:O	1:D:194:ASP:HB2	2.21	0.40
1:E:27:THR:HA	1:E:50:ARG:HB3	2.03	0.40
2:I:118:ARG:HA	2:I:118:ARG:HD3	1.50	0.40
2:J:69:SER:O	2:J:73:ARG:NH1	2.49	0.40
1:C:193:LYS:O	1:C:197:ASP:OD1	2.38	0.40
1:C:218:ASP:OD1	1:C:221:ARG:NH1	2.54	0.40
1:D:129:TYR:OH	1:D:131:GLN:HB3	2.21	0.40
1:D:303:MET:HE1	1:D:343:VAL:HA	2.03	0.40
1:D:448:HIS:HB3	1:D:449:GLY:H	1.74	0.40
1:E:303:MET:SD	1:E:309:PRO:HD3	2.61	0.40
1:F:68:VAL:HG13	1:F:81:ILE:HD11	2.03	0.40
2:H:68:ASP:HA	2:H:71:LYS:HB2	2.03	0.40
1:C:33:GLN:HG3	1:C:64:THR:HG22	2.03	0.40
1:C:224:ARG:HE	1:C:236:ILE:CD1	2.30	0.40
2:J:22:CYS:HB3	2:J:85:VAL:CG1	2.50	0.40
2:K:28:ASN:O	2:K:29:PHE:HB2	2.20	0.40
1:C:189:ALA:HB3	1:C:222:GLU:OE1	2.22	0.40
1:C:248:ASN:O	1:C:252:ILE:HG13	2.22	0.40
1:C:266:LEU:HD12	1:C:266:LEU:HA	1.76	0.40
1:C:480:VAL:HG22	1:C:493:THR:CG2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:VAL:O	1:D:280:MET:HG3	2.22	0.40
1:E:48:VAL:HG11	1:E:208:MET:HE3	2.04	0.40
1:E:477:MET:HE2	1:E:477:MET:HB2	1.67	0.40
2:K:42:TRP:CD2	2:K:87:LEU:HD12	2.57	0.40
2:K:66:TYR:HE1	2:K:76:ILE:HG13	1.86	0.40

All (8) 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:F:274:LYS:NZ	2:K:108:TRP:CD1[3_455]	1.04	1.16
1:F:274:LYS:NZ	2:K:108:TRP:NE1[3_455]	1.49	0.71
1:F:274:LYS:NZ	2:K:108:TRP:CG[3_455]	1.59	0.61
1:E:311:ARG:NH2	1:F:316:ASP:OD1[3_445]	1.77	0.43
2:G:128:VAL:O	2:J:91:SER:OG[4_454]	2.10	0.10
1:F:274:LYS:NZ	2:K:108:TRP:CE2[3_455]	2.12	0.08
1:F:274:LYS:NZ	2:K:108:TRP:CD2[3_455]	2.18	0.02
1:F:274:LYS:CE	2:K:108:TRP:CD1[3_455]	2.19	0.01

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	A	497/514 (97%)	461 (93%)	36 (7%)	0	100	100
1	B	400/514 (78%)	386 (96%)	14 (4%)	0	100	100
1	C	498/514 (97%)	474 (95%)	23 (5%)	1 (0%)	44	73
1	D	498/514 (97%)	473 (95%)	25 (5%)	0	100	100
1	E	389/514 (76%)	370 (95%)	19 (5%)	0	100	100
1	F	395/514 (77%)	370 (94%)	25 (6%)	0	100	100
2	G	128/149 (86%)	126 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	I	128/149 (86%)	121 (94%)	7 (6%)	0	100	100
2	J	129/149 (87%)	123 (95%)	6 (5%)	0	100	100
2	K	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
2	L	128/149 (86%)	122 (95%)	6 (5%)	0	100	100
All	All	3446/3978 (87%)	3270 (95%)	175 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	PRO

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	A	391/435 (90%)	380 (97%)	11 (3%)	38	72
1	B	320/435 (74%)	314 (98%)	6 (2%)	52	82
1	C	385/435 (88%)	375 (97%)	10 (3%)	41	75
1	D	392/435 (90%)	377 (96%)	15 (4%)	28	62
1	E	309/435 (71%)	299 (97%)	10 (3%)	34	68
1	F	303/435 (70%)	284 (94%)	19 (6%)	15	42
2	G	104/121 (86%)	103 (99%)	1 (1%)	73	91
2	H	105/121 (87%)	103 (98%)	2 (2%)	52	82
2	I	100/121 (83%)	92 (92%)	8 (8%)	10	30
2	J	106/121 (88%)	103 (97%)	3 (3%)	38	72
2	K	99/121 (82%)	94 (95%)	5 (5%)	20	51
2	L	92/121 (76%)	84 (91%)	8 (9%)	8	26
All	All	2706/3336 (81%)	2608 (96%)	98 (4%)	30	64

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	90	ILE
1	A	92	THR
1	A	168	ASN
1	A	173	THR
1	A	178	ILE
1	A	346	TYR
1	A	368	LYS
1	A	405	ARG
1	A	489	TYR
1	A	499	ARG
1	B	195	ARG
1	B	213	PHE
1	B	215	ARG
1	B	303	MET
1	B	346	TYR
1	B	409	LEU
1	C	116	PHE
1	C	171	ARG
1	C	215	ARG
1	C	269	GLU
1	C	270	ILE
1	C	273	GLU
1	C	274	LYS
1	C	346	TYR
1	C	441	VAL
1	C	483	ASP
1	D	118	LYS
1	D	137	ARG
1	D	148	VAL
1	D	152	ARG
1	D	171	ARG
1	D	174	ASP
1	D	175	ARG
1	D	232	LYS
1	D	265	ASP
1	D	346	TYR
1	D	363	MET
1	D	398	LEU
1	D	414	ARG
1	D	464	TRP
1	D	499	ARG

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Mol	Chain	Res	Type
1	E	213	PHE
1	E	215	ARG
1	E	265	ASP
1	E	273	GLU
1	E	285	LYS
1	E	311	ARG
1	E	343	VAL
1	E	363	MET
1	E	454	ARG
1	E	499	ARG
1	F	16	VAL
1	F	224	ARG
1	F	243	HIS
1	F	244	GLN
1	F	274	LYS
1	F	281	CYS
1	F	295	CYS
1	F	299	MET
1	F	326	ASP
1	F	346	TYR
1	F	355	GLN
1	F	358	THR
1	F	371	GLN
1	F	373	ILE
1	F	383	SER
1	F	387	SER
1	F	412	LYS
1	F	435	THR
1	F	486	VAL
2	G	102	CYS
2	H	22	CYS
2	H	106	ASP
2	I	25	SER
2	I	28	ASN
2	I	33	ARG
2	I	34	THR
2	I	50	GLU
2	I	78	ARG
2	I	89	MET
2	I	97	THR
2	J	30	SER
2	J	33	ARG

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Mol	Chain	Res	Type
2	J	78	ARG
2	K	33	ARG
2	K	35	PHE
2	K	86	TYR
2	K	105	ARG
2	K	122	GLN
2	L	1	GLN
2	L	69	SER
2	L	83	ASN
2	L	97	THR
2	L	106	ASP
2	L	120	TRP
2	L	124	THR
2	L	130	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	67	ASN
1	A	170	HIS
1	A	298	GLN
1	A	481	HIS
1	B	492	GLN
1	C	62	GLN
1	C	66	ASN
1	C	168	ASN
1	C	179	ASN
1	C	204	GLN
1	C	243	HIS
1	C	287	ASN
1	C	323	ASN
1	C	345	GLN
1	C	491	ASN
1	D	3	GLN
1	D	33	GLN
1	D	62	GLN
1	D	66	ASN
1	D	78	HIS
1	D	167	ASN
1	D	359	HIS
1	D	365	ASN

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Mol	Chain	Res	Type
1	E	61	HIS
1	E	219	GLN
1	E	369	ASN
1	E	481	HIS
1	F	6	HIS
1	F	7	ASN
1	F	62	GLN
1	F	355	GLN
2	G	88	GLN
2	H	13	GLN
2	I	28	ASN
2	I	88	GLN
2	J	1	GLN
2	J	5	GLN
2	J	28	ASN
2	J	88	GLN
2	J	122	GLN
2	L	28	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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	GOL	E	601	-	5,5,5	0.84	0	5,5,5	0.94	0
3	GOL	B	702	-	5,5,5	0.91	0	5,5,5	1.15	1 (20%)
3	GOL	B	701	-	5,5,5	1.47	2 (40%)	5,5,5	1.00	0
3	GOL	D	601	-	5,5,5	1.27	1 (20%)	5,5,5	0.95	0
3	GOL	C	602	-	5,5,5	1.44	2 (40%)	5,5,5	1.34	0
3	GOL	B	703	-	5,5,5	0.90	0	5,5,5	0.88	0
3	GOL	C	601	-	5,5,5	1.59	1 (20%)	5,5,5	1.44	1 (20%)
3	GOL	D	602	-	5,5,5	0.91	0	5,5,5	0.92	0
3	GOL	A	601	-	5,5,5	2.42	2 (40%)	5,5,5	0.95	0
3	GOL	F	601	-	5,5,5	1.26	1 (20%)	5,5,5	0.72	0

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	GOL	E	601	-	-	4/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-
3	GOL	B	701	-	-	4/4/4/4	-
3	GOL	D	601	-	-	0/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	B	703	-	-	1/4/4/4	-
3	GOL	C	601	-	-	1/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	4/4/4/4	-
3	GOL	F	601	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	GOL	C3-C2	4.40	1.69	1.51
3	C	601	GOL	C1-C2	3.04	1.64	1.51
3	C	602	GOL	C1-C2	2.28	1.61	1.51
3	B	701	GOL	C3-C2	2.24	1.60	1.51
3	D	601	GOL	C3-C2	2.20	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	GOL	C1-C2	2.19	1.60	1.51
3	C	602	GOL	C3-C2	2.08	1.60	1.51
3	F	601	GOL	C1-C2	2.04	1.60	1.51
3	B	701	GOL	C1-C2	2.03	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	GOL	O3-C3-C2	-2.37	98.82	110.20
3	B	702	GOL	C3-C2-C1	-2.04	103.77	111.70

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3
3	B	701	GOL	O1-C1-C2-C3
3	B	701	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-C3
3	C	602	GOL	C1-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3
3	B	702	GOL	C1-C2-C3-O3
3	D	602	GOL	O1-C1-C2-C3
3	E	601	GOL	O1-C1-C2-C3
3	E	601	GOL	C1-C2-C3-O3
3	F	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2
3	B	701	GOL	O1-C1-C2-O2
3	B	701	GOL	O2-C2-C3-O3
3	B	702	GOL	O2-C2-C3-O3
3	F	601	GOL	O2-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	E	601	GOL	O2-C2-C3-O3
3	E	601	GOL	O1-C1-C2-O2
3	C	601	GOL	C1-C2-C3-O3
3	B	703	GOL	O1-C1-C2-C3
3	D	602	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	GOL	2	0
3	D	602	GOL	1	0
3	F	601	GOL	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	A	499/514 (97%)	-0.05	16 (3%) 50 42	57, 71, 179, 197	0
1	B	404/514 (78%)	-0.16	4 (0%) 79 73	61, 83, 120, 173	0
1	C	499/514 (97%)	0.06	23 (4%) 38 30	51, 78, 173, 191	1 (0%)
1	D	499/514 (97%)	0.04	9 (1%) 67 60	64, 92, 140, 182	1 (0%)
1	E	395/514 (76%)	0.49	26 (6%) 26 19	73, 108, 130, 164	0
1	F	399/514 (77%)	1.13	63 (15%) 6 5	100, 124, 182, 219	0
2	G	130/149 (87%)	-0.18	0 100 100	64, 78, 100, 130	0
2	H	130/149 (87%)	-0.08	1 (0%) 82 77	75, 92, 127, 152	0
2	I	130/149 (87%)	0.60	5 (3%) 44 36	90, 131, 188, 206	0
2	J	131/149 (87%)	0.00	1 (0%) 82 77	69, 88, 112, 136	0
2	K	130/149 (87%)	1.34	26 (20%) 3 3	100, 170, 223, 236	0
2	L	130/149 (87%)	0.86	9 (6%) 24 18	115, 163, 211, 218	0
All	All	3476/3978 (87%)	0.27	183 (5%) 33 26	51, 96, 179, 236	2 (0%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	61	GLY	5.2
1	E	272	ALA	4.8
2	K	100	TYR	4.7
1	F	237	ILE	4.6
1	A	179	ASN	4.4
1	F	318	ALA	4.4
1	F	236	ILE	4.3
1	C	174	ASP	4.2
1	F	273	GLU	4.1
2	K	109	TYR	3.9
1	C	172	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	K	20	LEU	3.8
1	F	481	HIS	3.7
1	A	141	LEU	3.7
1	B	90	ILE	3.6
1	C	173	THR	3.6
1	F	376	SER	3.6
2	K	84	THR	3.6
1	F	257	ASP	3.6
1	E	189	ALA	3.6
1	E	270	ILE	3.5
1	F	406	SER	3.5
1	F	44	SER	3.5
1	F	272	ALA	3.4
1	F	66	ASN	3.4
1	C	515	GLU	3.4
1	F	422	ALA	3.3
1	E	247	GLN	3.3
1	D	515	GLU	3.3
1	F	315	THR	3.2
1	E	89	GLU	3.1
1	A	92	THR	3.1
2	L	35	PHE	3.1
1	F	234	THR	3.0
1	F	375	MET	3.0
1	F	486	VAL	3.0
2	K	22	CYS	3.0
1	B	485	SER	3.0
1	A	94	LEU	2.9
1	F	296	ALA	2.9
1	D	489	TYR	2.9
1	E	362	VAL	2.9
1	F	288	VAL	2.9
2	I	51	ARG	2.9
2	L	44	ARG	2.9
1	E	53	PHE	2.8
1	E	364	PHE	2.8
2	K	77	SER	2.8
2	K	75	THR	2.8
2	K	62	GLY	2.8
2	K	110	PHE	2.8
2	K	40	ILE	2.8
1	F	483	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	364	PHE	2.7
2	K	63	ILE	2.7
2	K	60	ASN	2.7
1	F	487	LYS	2.7
1	F	398	LEU	2.7
1	A	488	GLY	2.7
1	F	499	ARG	2.6
1	C	187	LEU	2.6
1	E	11	SER	2.6
2	K	118	ARG	2.6
2	K	24	ALA	2.6
1	F	419	ILE	2.6
1	C	303	MET	2.6
1	C	484	HIS	2.6
1	F	362	VAL	2.6
2	K	23	ALA	2.6
1	C	184	GLU	2.6
1	E	273	GLU	2.6
1	F	258	GLY	2.5
1	E	246	VAL	2.5
1	F	223	VAL	2.5
1	F	246	VAL	2.5
1	E	296	ALA	2.5
1	F	213	PHE	2.5
1	A	185	VAL	2.5
2	L	100	TYR	2.5
2	K	74	PHE	2.5
1	F	408	ARG	2.5
1	F	378	GLU	2.5
1	F	317	VAL	2.5
1	E	13	PHE	2.5
1	A	86	LYS	2.5
1	C	179	ASN	2.5
2	L	113	VAL	2.5
2	K	130	SER	2.4
1	B	454	ARG	2.4
1	D	137	ARG	2.4
1	C	185	VAL	2.4
1	F	492	GLN	2.4
1	C	488	GLY	2.4
1	C	183	CYS	2.4
1	E	327	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	189	ALA	2.4
1	F	89	GLU	2.4
2	K	12	VAL	2.4
1	F	297	THR	2.4
1	E	489	TYR	2.4
1	F	348	VAL	2.4
1	A	500	GLU	2.4
1	F	81	ILE	2.4
1	D	182	GLY	2.3
1	E	276	VAL	2.3
1	F	381	VAL	2.3
1	E	312	ALA	2.3
1	C	144	VAL	2.3
1	F	276	VAL	2.3
1	E	12	ILE	2.3
2	K	33	ARG	2.3
1	D	488	GLY	2.3
1	A	484	HIS	2.3
2	I	121	GLY	2.3
1	F	454	ARG	2.3
1	A	174	ASP	2.3
1	F	495	LEU	2.3
1	A	489	TYR	2.2
1	D	129	TYR	2.2
1	E	275	VAL	2.2
1	D	184	GLU	2.2
1	F	73	ALA	2.2
1	F	379	GLU	2.2
2	K	89	MET	2.2
1	C	151	LEU	2.2
1	F	374	PRO	2.2
1	F	490	PRO	2.2
2	I	26	GLY	2.2
2	K	70	VAL	2.2
2	J	27	SER	2.2
1	B	190	VAL	2.2
1	F	282	ILE	2.2
1	F	480	VAL	2.2
1	C	489	TYR	2.2
1	F	489	TYR	2.2
2	K	86	TYR	2.2
1	F	457	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	49	ALA	2.2
1	D	159	ASP	2.2
2	L	34	THR	2.2
2	L	63	ILE	2.2
2	I	1	GLN	2.2
1	D	172	LEU	2.2
1	E	269	GLU	2.1
1	F	377	PRO	2.1
1	C	142	ILE	2.1
1	C	486	VAL	2.1
1	A	31	SER	2.1
1	F	311	ARG	2.1
1	C	296	ALA	2.1
1	F	235	LEU	2.1
1	F	482	ALA	2.1
2	K	92	LEU	2.1
1	C	135	VAL	2.1
2	L	8	GLY	2.1
1	E	54	SER	2.1
1	E	361	SER	2.1
1	F	227	LEU	2.1
1	F	473	ALA	2.1
1	F	491	ASN	2.1
2	K	108	TRP	2.1
1	C	95	PHE	2.1
1	C	149	LEU	2.1
2	H	130	SER	2.1
2	K	2	VAL	2.1
2	L	12	VAL	2.1
1	E	274	LYS	2.1
1	A	173	THR	2.0
1	A	297	THR	2.0
1	A	119	ILE	2.0
1	C	454	ARG	2.0
1	E	268	VAL	2.0
1	E	344	VAL	2.0
1	A	176	LYS	2.0
1	F	488	GLY	2.0
1	C	94	LEU	2.0
2	I	127	THR	2.0
2	L	36	SER	2.0
1	F	253	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	51	MET	2.0
1	F	18	LYS	2.0
1	F	386	VAL	2.0
1	F	434	VAL	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, 95^{th} 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	GOL	C	602	6/6	0.58	0.22	89,93,95,98	0
3	GOL	C	601	6/6	0.65	0.16	84,87,94,108	0
3	GOL	A	601	6/6	0.66	0.21	78,85,85,86	0
3	GOL	F	601	6/6	0.74	0.14	104,110,112,112	0
3	GOL	B	702	6/6	0.79	0.12	92,94,95,101	0
3	GOL	E	601	6/6	0.81	0.10	112,115,116,118	0
3	GOL	D	602	6/6	0.82	0.13	90,92,94,94	0
3	GOL	B	703	6/6	0.87	0.11	95,100,100,103	0
3	GOL	B	701	6/6	0.87	0.17	82,84,85,87	0
3	GOL	D	601	6/6	0.90	0.12	85,89,92,98	0

6.5 Other polymers (i)

There are no such residues in this entry.