Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 02:07 PM EDT

PDB ID	:	3VS9
Title	:	Crystal structure of type III PKS ArsC mutant
Authors	:	Satou, R.; Miyanaga, A.; Ozawa, H.; Funa, N.; Miyazono, K.; Tanokura, M.; Ohnishi, Y.; Horinouchi, S.
Deposited on	:	2012-04-23
Resolution	:	1.99 Å(reported)

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

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

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

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

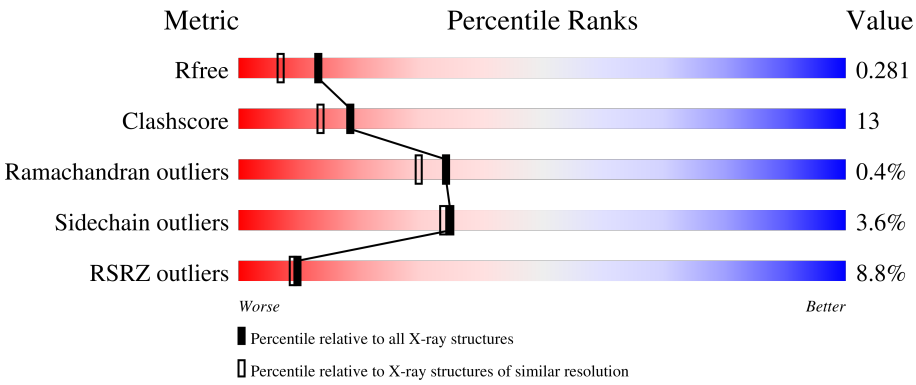
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	410	3% 80% 16% • •
1	B	410	9% 74% 21% • •
1	C	410	7% 81% 14% • •
1	D	410	8% 82% 14% • •
1	E	410	3% 82% 14% • •

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Mol	Chain	Length	Quality of chain
1	F	410	14% 69% 27%
1	G	410	11% 72% 22%
1	H	410	12% 63% 27% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27142 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3117	1985	540	577	15	0	0	0
1	B	397	3086	1966	536	569	15	0	0	0
1	C	396	3072	1956	532	569	15	0	0	0
1	D	401	3110	1978	540	577	15	0	0	0
1	E	400	3106	1976	539	576	15	0	0	0
1	F	401	3117	1985	540	577	15	0	0	0
1	G	397	3076	1961	536	564	15	0	0	0
1	H	383	2977	1899	519	544	15	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

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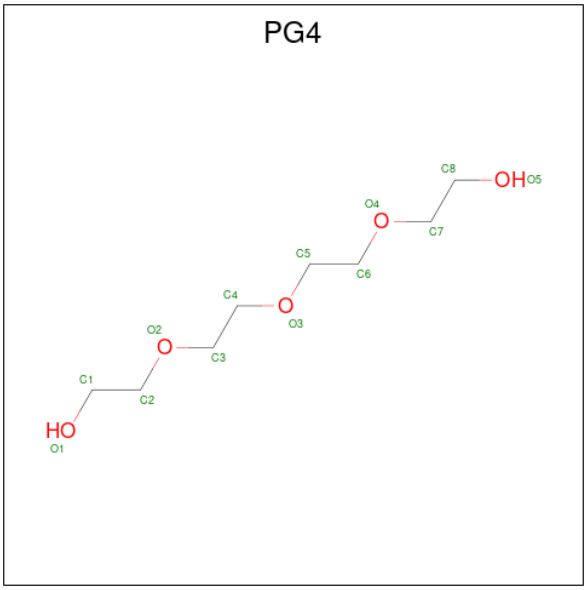
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0
3	G	1	Total C O 13 8 5	0	0
3	H	1	Total C O 13 8 5	0	0

- Molecule 4 is water.

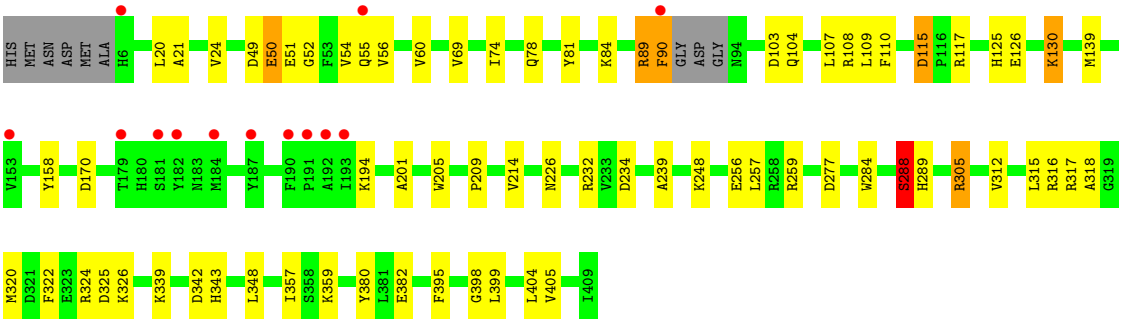
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	372	372	372	0	0
			Total	O		
4	B	243	243	243	0	0
			Total	O		
4	C	338	338	338	0	0
			Total	O		
4	D	343	343	343	0	0
			Total	O		
4	E	368	368	368	0	0
			Total	O		
4	F	270	270	270	0	0
			Total	O		
4	G	235	235	235	0	0
			Total	O		
4	H	200	200	200	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.

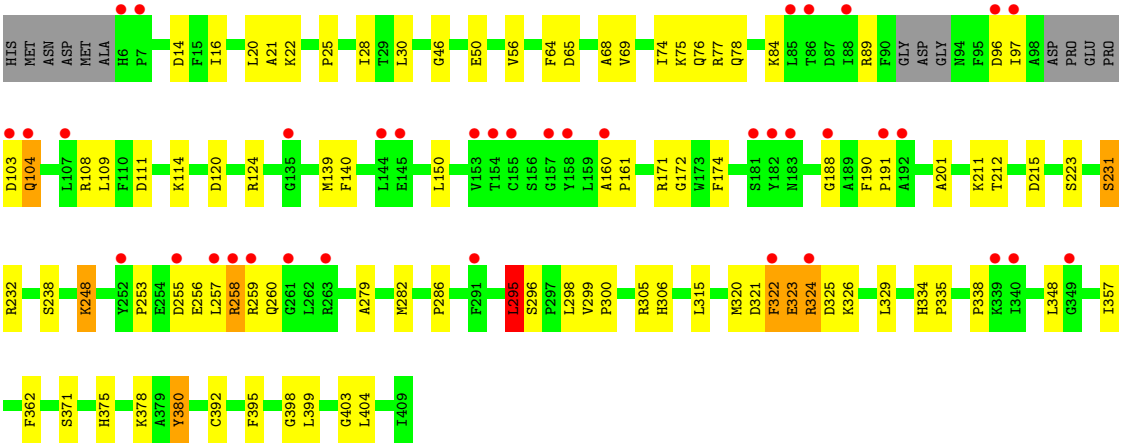
- Molecule 1: Type III polyketide synthase

Chain A:



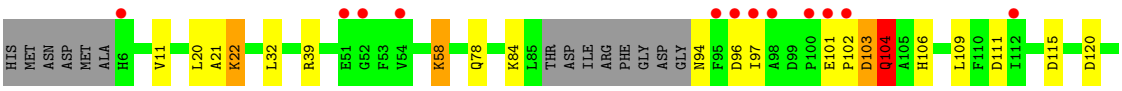
- Molecule 1: Type III polyketide synthase

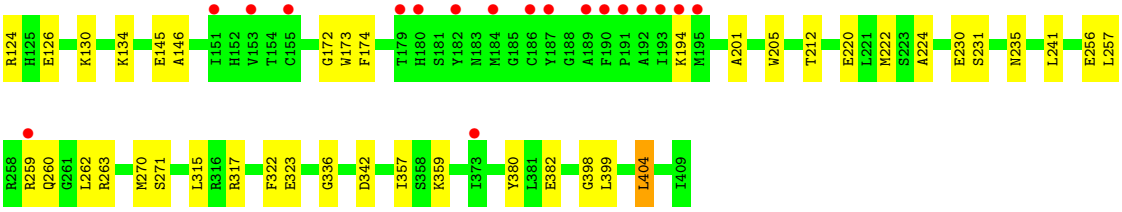
Chain B:



- Molecule 1: Type III polyketide synthase

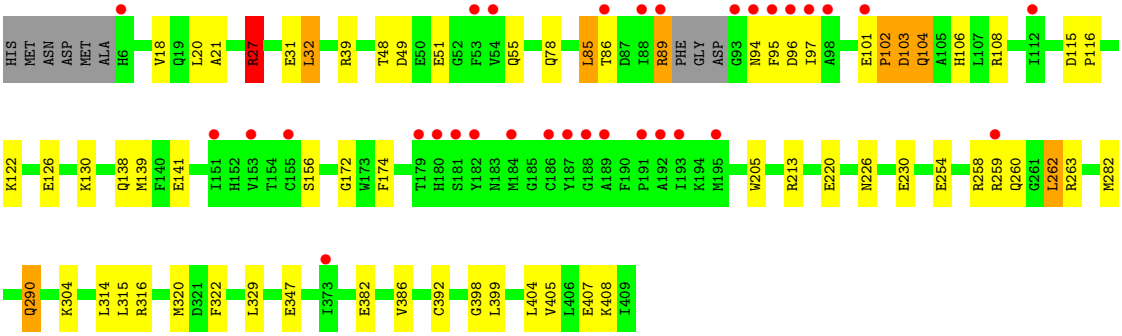
Chain C:





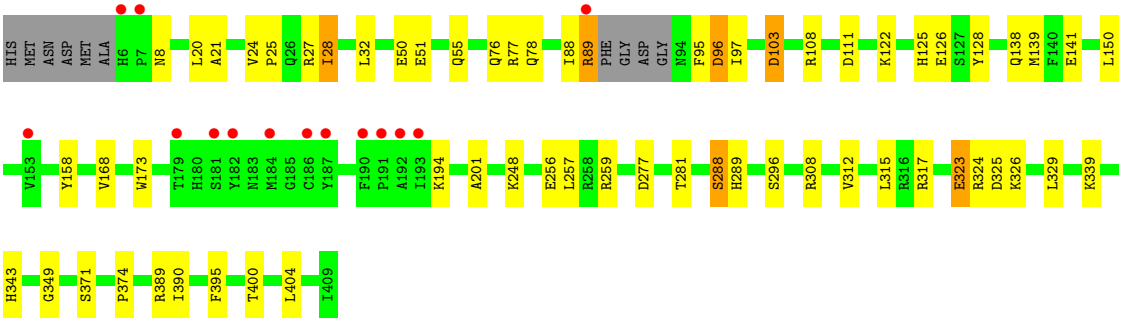
- Molecule 1: Type III polyketide synthase

Chain D:



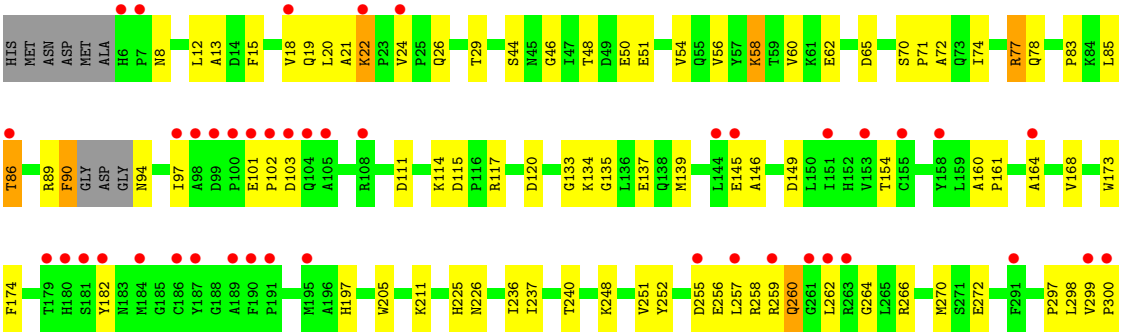
- Molecule 1: Type III polyketide synthase

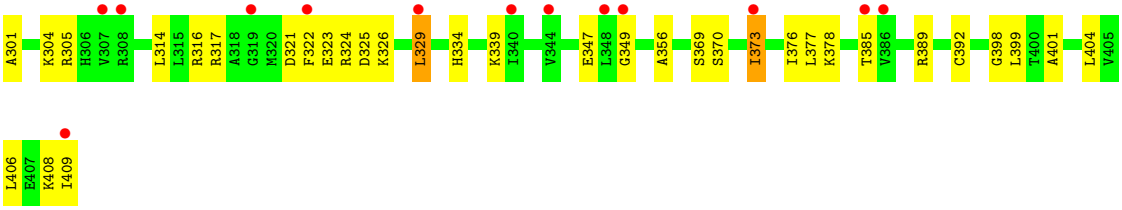
Chain E:



- Molecule 1: Type III polyketide synthase

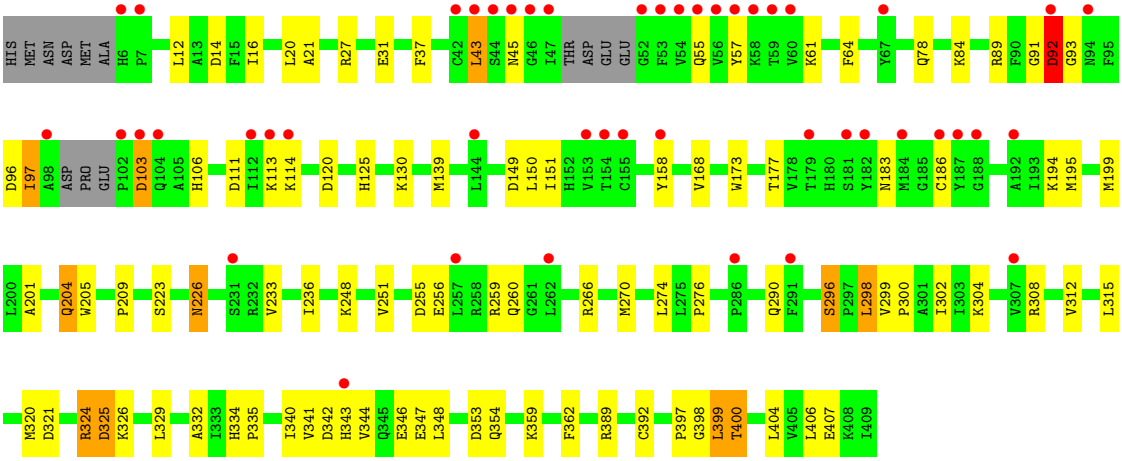
Chain F:





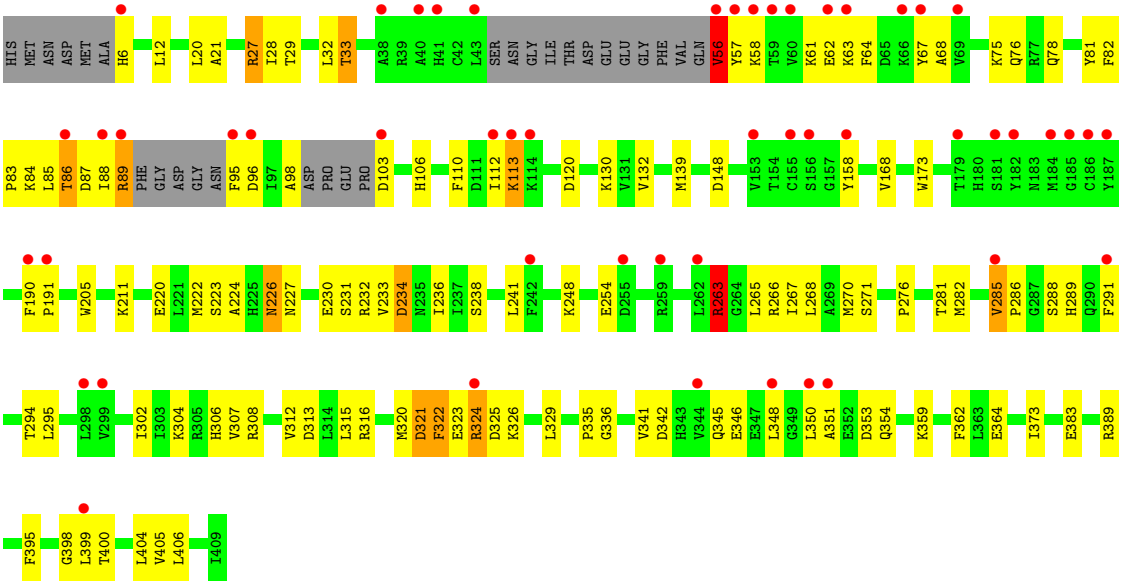
• Molecule 1: Type III polyketide synthase

Chain G:



• Molecule 1: Type III polyketide synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.92Å 142.72Å 129.87Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	37.78 – 1.99 37.78 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (37.78-1.99) 96.9 (37.78-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.273 0.218 , 0.281	Depositor DCC
R_{free} test set	11676 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27142	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2928e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, NA

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	1.04	4/3189 (0.1%)	0.94	6/4325 (0.1%)
1	B	1.05	2/3155 (0.1%)	0.92	3/4275 (0.1%)
1	C	1.01	0/3143	0.91	3/4263 (0.1%)
1	D	1.02	0/3181	0.92	5/4314 (0.1%)
1	E	1.03	2/3177 (0.1%)	0.92	5/4309 (0.1%)
1	F	1.04	0/3189	0.96	5/4325 (0.1%)
1	G	0.98	0/3146	0.89	1/4262 (0.0%)
1	H	0.98	3/3043 (0.1%)	0.88	2/4122 (0.0%)
All	All	1.02	11/25223 (0.0%)	0.92	30/34195 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	56	VAL	CB-CG2	8.56	1.70	1.52
1	H	56	VAL	CB-CG1	7.65	1.69	1.52
1	E	323	GLU	CG-CD	6.18	1.61	1.51
1	B	380	TYR	CD2-CE2	5.63	1.47	1.39
1	E	128	TYR	CD1-CE1	5.44	1.47	1.39
1	B	211	LYS	CE-NZ	5.31	1.62	1.49
1	A	126	GLU	CB-CG	5.30	1.62	1.52
1	A	194	LYS	CE-NZ	5.26	1.62	1.49
1	A	214	VAL	CB-CG2	5.17	1.63	1.52
1	H	132	VAL	CB-CG2	5.11	1.63	1.52
1	A	312	VAL	CB-CG1	5.08	1.63	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	305	ARG	NE-CZ-NH2	-7.78	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	E	77	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	27	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	E	111	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	111	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	F	149	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	E	317	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	213	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	F	77	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	F	120	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	404	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	77	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	213	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	F	404	LEU	CA-CB-CG	5.55	128.06	115.30
1	C	317	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	378	LYS	CD-CE-NZ	-5.49	99.08	111.70
1	D	139	MET	CG-SD-CE	-5.42	91.53	100.20
1	B	295	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	120	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	115	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	317	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	H	404	LEU	CA-CB-CG	5.23	127.32	115.30
1	D	282	MET	CG-SD-CE	5.21	108.54	100.20
1	G	93	GLY	N-CA-C	-5.12	100.30	113.10
1	A	288	SER	CA-CB-OG	-5.10	97.42	111.20
1	H	263	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	E	404	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	271	SER	CB-CA-C	-5.06	100.48	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3117	0	3108	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3086	0	3083	99	0
1	C	3072	0	3064	60	0
1	D	3110	0	3102	72	1
1	E	3106	0	3099	59	0
1	F	3117	0	3108	112	0
1	G	3076	0	3078	97	0
1	H	2977	0	2990	119	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	18	1	0
3	B	13	0	18	2	0
3	C	13	0	18	1	0
3	D	13	0	18	2	0
3	E	13	0	18	0	0
3	F	13	0	18	1	0
3	G	13	0	18	1	0
3	H	13	0	18	2	0
4	A	372	0	0	15	0
4	B	243	0	0	11	0
4	C	338	0	0	4	0
4	D	343	0	0	7	0
4	E	368	0	0	9	1
4	F	270	0	0	26	0
4	G	235	0	0	12	0
4	H	200	0	0	8	0
All	All	27142	0	24776	660	2

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 13.

All (660) 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)
1:H:263:ARG:HH11	1:H:263:ARG:CG	1.43	1.31
1:G:298:LEU:HD12	4:G:801:HOH:O	1.08	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:226:ASN:HD22	1:H:226:ASN:C	1.40	1.21
1:E:89:ARG:HG2	1:E:89:ARG:HH11	1.09	1.12
1:F:300:PRO:HG2	4:F:777:HOH:O	1.50	1.09
1:A:89:ARG:HH11	1:A:89:ARG:CG	1.65	1.09
1:C:101:GLU:HB2	1:C:103:ASP:HB3	1.35	1.07
1:H:263:ARG:NH1	1:H:263:ARG:HG2	1.30	1.07
1:B:22:LYS:H	1:B:84:LYS:NZ	1.55	1.05
1:H:226:ASN:ND2	1:H:226:ASN:O	1.89	1.04
1:C:101:GLU:CB	1:C:103:ASP:HB3	1.88	1.03
1:F:18:VAL:HG21	1:F:139:MET:HG2	1.42	1.02
1:G:324:ARG:HH11	1:G:324:ARG:HG2	0.86	0.99
1:F:323:GLU:HG2	4:F:842:HOH:O	1.62	0.98
1:E:89:ARG:HH11	1:E:89:ARG:CG	1.76	0.98
1:A:89:ARG:NH1	1:A:89:ARG:HG2	1.48	0.97
1:G:324:ARG:HH11	1:G:324:ARG:CG	1.75	0.97
1:B:139:MET:CE	1:B:248:LYS:HB2	1.93	0.97
1:E:108:ARG:NH2	4:E:962:HOH:O	1.98	0.96
1:G:324:ARG:HG2	1:G:324:ARG:NH1	1.69	0.95
1:H:226:ASN:C	1:H:226:ASN:ND2	2.16	0.95
1:H:33:THR:HG21	4:H:759:HOH:O	1.65	0.94
1:H:89:ARG:HD2	1:H:96:ASP:O	1.68	0.94
1:B:139:MET:HE1	1:B:248:LYS:HB2	1.46	0.94
1:C:101:GLU:HB3	1:C:103:ASP:CB	1.97	0.94
1:D:104:GLN:OE1	1:D:104:GLN:HA	1.67	0.94
1:B:223:SER:HA	3:B:502:PG4:H61	1.51	0.93
1:D:39:ARG:NH2	1:D:94:ASN:ND2	2.17	0.93
1:D:27:ARG:HG2	4:D:638:HOH:O	1.71	0.91
1:H:288:SER:OG	1:H:289:HIS:HD2	1.52	0.91
1:B:75:LYS:O	1:B:76:GLN:HG3	1.72	0.90
1:B:75:LYS:C	1:B:76:GLN:HG3	1.92	0.89
1:E:95:PHE:O	1:E:96:ASP:HB2	1.70	0.89
1:H:112:ILE:HG13	1:H:112:ILE:O	1.73	0.89
1:H:20:LEU:H	1:H:78:GLN:HE22	1.17	0.88
1:F:205:TRP:HE1	1:G:204:GLN:HG2	1.39	0.87
1:H:58:LYS:HD2	1:H:58:LYS:O	1.73	0.87
1:F:85:LEU:N	1:F:85:LEU:HD23	1.88	0.87
1:A:89:ARG:HH11	1:A:89:ARG:HG2	0.75	0.86
1:D:304:LYS:HZ3	1:D:347:GLU:HB2	1.39	0.86
1:H:220:GLU:HB3	1:H:222:MET:HE3	1.54	0.86
1:E:89:ARG:HG2	1:E:89:ARG:NH1	1.87	0.86
1:F:211:LYS:NZ	4:F:617:HOH:O	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:N	1:A:90:PHE:CD2	2.44	0.85
1:C:101:GLU:CB	1:C:103:ASP:CB	2.53	0.84
1:G:20:LEU:H	1:G:78:GLN:NE2	1.75	0.84
1:H:263:ARG:HH11	1:H:263:ARG:HG2	0.69	0.84
1:B:371:SER:O	1:B:375:HIS:HD2	1.60	0.84
1:F:20:LEU:H	1:F:78:GLN:NE2	1.76	0.84
1:D:39:ARG:NH2	1:D:94:ASN:HD22	1.75	0.83
1:B:76:GLN:NE2	4:B:730:HOH:O	2.08	0.83
1:C:101:GLU:HB3	1:C:103:ASP:HB2	1.58	0.83
1:E:277:ASP:OD2	4:E:745:HOH:O	1.96	0.83
1:G:20:LEU:H	1:G:78:GLN:HE22	1.26	0.83
1:H:110:PHE:HB3	1:H:226:ASN:OD1	1.79	0.83
1:F:18:VAL:CG2	1:F:139:MET:HG2	2.09	0.82
1:F:24:VAL:HG21	1:F:29:THR:HG22	1.61	0.82
1:B:139:MET:HE3	1:B:248:LYS:CB	2.09	0.82
1:E:126:GLU:OE2	4:E:724:HOH:O	1.97	0.82
1:B:14:ASP:O	1:B:16:ILE:HD12	1.80	0.81
1:H:139:MET:HE3	1:H:248:LYS:HB3	1.63	0.81
1:D:20:LEU:H	1:D:78:GLN:HE22	1.25	0.81
1:A:320:MET:CE	1:A:405:VAL:HG11	2.10	0.80
1:G:329:LEU:HD22	1:G:389:ARG:HB2	1.63	0.80
1:B:25:PRO:HG2	1:B:28:ILE:HD12	1.63	0.79
1:F:24:VAL:CG2	1:F:29:THR:CG2	2.59	0.79
1:H:112:ILE:O	1:H:113:LYS:HG3	1.82	0.79
1:H:263:ARG:CG	1:H:263:ARG:NH1	2.15	0.79
1:A:256:GLU:OE1	1:A:259:ARG:NH2	2.12	0.79
1:B:139:MET:CE	1:B:248:LYS:CB	2.60	0.79
1:A:20:LEU:H	1:A:78:GLN:NE2	1.81	0.79
1:F:18:VAL:HG21	1:F:139:MET:CG	2.13	0.79
1:C:220:GLU:HB3	1:C:222:MET:HE3	1.65	0.78
1:F:20:LEU:H	1:F:78:GLN:HE22	1.30	0.78
1:A:320:MET:HE1	1:A:405:VAL:HG11	1.65	0.78
1:D:101:GLU:O	1:D:104:GLN:N	2.17	0.78
1:E:125:HIS:CE1	1:E:158:TYR:H	2.00	0.78
1:C:220:GLU:HB3	1:C:222:MET:CE	2.13	0.78
1:G:341:VAL:HG23	4:G:647:HOH:O	1.83	0.78
1:F:300:PRO:CG	4:F:777:HOH:O	2.19	0.77
1:B:259:ARG:NH1	1:B:260:GLN:CG	2.48	0.77
1:B:22:LYS:H	1:B:84:LYS:HZ1	1.32	0.76
1:H:20:LEU:H	1:H:78:GLN:NE2	1.83	0.76
1:F:24:VAL:HG21	1:F:29:THR:CG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LEU:CD1	1:E:88:ILE:HD13	2.15	0.76
1:F:205:TRP:NE1	1:G:204:GLN:HG2	1.99	0.76
1:A:125:HIS:CE1	1:A:158:TYR:H	2.04	0.76
1:F:164:ALA:O	1:F:168:VAL:HG23	1.86	0.76
1:E:20:LEU:H	1:E:78:GLN:HE22	1.30	0.76
1:C:20:LEU:H	1:C:78:GLN:HE22	1.33	0.75
1:A:277:ASP:OD2	4:A:703:HOH:O	2.04	0.75
1:D:226:ASN:HB3	3:D:502:PG4:H51	1.69	0.75
1:H:351:ALA:H	1:H:354:GLN:HE21	1.32	0.75
1:G:299:VAL:HB	1:G:300:PRO:HD3	1.69	0.75
1:E:20:LEU:H	1:E:78:GLN:NE2	1.85	0.75
1:E:323:GLU:HB3	4:E:864:HOH:O	1.86	0.74
1:G:256:GLU:OE2	1:G:259:ARG:NH2	2.19	0.74
1:E:25:PRO:O	1:E:28:ILE:CG2	2.35	0.74
1:A:20:LEU:H	1:A:78:GLN:HE22	1.36	0.74
1:G:89:ARG:HG3	1:G:96:ASP:HB3	1.69	0.74
1:B:395:PHE:HD2	4:B:649:HOH:O	1.69	0.73
1:C:22:LYS:HB2	1:C:22:LYS:NZ	2.03	0.73
1:D:55:GLN:OE1	1:D:55:GLN:HA	1.88	0.73
1:H:383:GLU:OE2	4:H:652:HOH:O	2.07	0.73
1:A:239:ALA:HA	3:A:502:PG4:H72	1.70	0.73
1:G:97:ILE:N	1:G:97:ILE:CD1	2.52	0.73
1:H:308:ARG:O	1:H:312:VAL:HG23	1.88	0.73
1:E:32:LEU:HD11	1:E:88:ILE:HD13	1.71	0.73
1:D:101:GLU:O	1:D:103:ASP:N	2.23	0.72
1:A:90:PHE:N	1:A:90:PHE:HD2	1.84	0.72
1:D:21:ALA:H	1:D:78:GLN:HE21	1.38	0.72
1:E:323:GLU:CB	4:E:864:HOH:O	2.36	0.72
1:F:15:PHE:CB	1:F:378:LYS:HB2	2.20	0.71
1:G:407:GLU:OE1	4:G:830:HOH:O	2.08	0.71
1:A:339:LYS:O	1:A:343:HIS:HD2	1.74	0.71
1:C:101:GLU:C	1:C:103:ASP:N	2.40	0.71
1:B:21:ALA:HB1	1:B:84:LYS:HE3	1.72	0.70
1:B:76:GLN:HG2	4:B:744:HOH:O	1.91	0.70
1:B:223:SER:HA	3:B:502:PG4:C6	2.21	0.70
1:F:205:TRP:HE1	1:G:204:GLN:CG	2.03	0.70
1:H:29:THR:O	1:H:33:THR:HG23	1.91	0.70
1:A:288:SER:HB3	1:A:289:HIS:CD2	2.26	0.70
1:D:20:LEU:H	1:D:78:GLN:NE2	1.89	0.70
1:B:14:ASP:OD1	1:B:16:ILE:HD11	1.90	0.70
1:H:106:HIS:CE1	1:H:130:LYS:NZ	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:HE3	1:B:248:LYS:HB2	1.71	0.70
1:D:382:GLU:OE1	4:D:727:HOH:O	2.09	0.69
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.35	0.69
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.56	0.69
1:E:89:ARG:CG	1:E:89:ARG:NH1	2.49	0.69
1:B:22:LYS:H	1:B:84:LYS:CE	2.05	0.69
1:F:256:GLU:OE2	1:F:259:ARG:NH2	2.25	0.69
1:C:39:ARG:NH2	1:C:94:ASN:OD1	2.26	0.69
1:H:21:ALA:H	1:H:78:GLN:HE21	1.40	0.69
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.07	0.68
1:H:321:ASP:O	1:H:325:ASP:HB2	1.92	0.68
1:D:39:ARG:HH21	1:D:94:ASN:HD22	1.38	0.68
1:E:25:PRO:O	1:E:28:ILE:HG22	1.93	0.68
1:B:259:ARG:NH1	1:B:260:GLN:HG2	2.08	0.68
1:B:321:ASP:OD1	1:B:324:ARG:HB3	1.94	0.68
1:A:305:ARG:CD	4:A:747:HOH:O	2.42	0.68
1:F:65:ASP:HB2	4:F:785:HOH:O	1.94	0.68
1:B:139:MET:HE3	1:B:248:LYS:HB3	1.76	0.68
1:C:323:GLU:HB2	4:C:866:HOH:O	1.94	0.68
1:G:125:HIS:CE1	1:G:158:TYR:H	2.11	0.67
1:G:139:MET:HE3	1:G:248:LYS:HB3	1.76	0.67
1:C:323:GLU:OE1	4:C:866:HOH:O	2.12	0.67
1:G:14:ASP:OD2	4:G:760:HOH:O	2.12	0.67
1:H:106:HIS:CE1	1:H:130:LYS:HZ2	2.12	0.67
1:A:90:PHE:HD2	1:A:90:PHE:H	1.34	0.67
1:G:97:ILE:N	1:G:97:ILE:HD13	2.10	0.67
1:A:284:TRP:CD1	4:A:722:HOH:O	2.47	0.67
1:B:322:PHE:CE2	1:B:326:LYS:HD3	2.29	0.67
1:H:276:PRO:HD2	1:H:306:HIS:CE1	2.30	0.67
1:G:57:TYR:O	1:G:61:LYS:HG3	1.95	0.66
1:G:397:PRO:O	1:G:400:THR:HG23	1.94	0.66
1:C:126:GLU:OE1	4:C:811:HOH:O	2.13	0.66
1:B:258:ARG:CG	1:B:258:ARG:HH11	2.08	0.66
1:F:300:PRO:CD	4:F:777:HOH:O	2.41	0.66
1:G:92:ASP:OD1	1:G:92:ASP:N	2.24	0.66
1:D:89:ARG:HD3	1:D:96:ASP:O	1.95	0.66
1:E:339:LYS:HB3	1:E:343:HIS:NE2	2.10	0.66
1:B:103:ASP:N	1:B:103:ASP:OD1	2.26	0.66
1:F:329:LEU:HD11	1:F:389:ARG:HB2	1.78	0.66
1:H:220:GLU:HB3	1:H:222:MET:CE	2.24	0.66
1:H:288:SER:OG	1:H:289:HIS:CD2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:PRO:HD2	4:F:608:HOH:O	1.96	0.65
1:F:21:ALA:H	1:F:78:GLN:HE21	1.43	0.65
1:H:89:ARG:NH2	1:H:98:ALA:HB2	2.11	0.65
1:H:270:MET:HG2	4:H:668:HOH:O	1.96	0.65
1:H:89:ARG:HD3	1:H:96:ASP:HB3	1.79	0.65
1:A:289:HIS:HE1	4:A:907:HOH:O	1.79	0.65
1:C:230:GLU:O	1:C:235:ASN:ND2	2.29	0.65
1:D:101:GLU:HB3	1:D:103:ASP:OD2	1.97	0.65
1:H:324:ARG:HB3	1:H:324:ARG:NH1	2.11	0.65
1:B:139:MET:HE2	1:B:140:PHE:CE2	2.32	0.64
1:B:259:ARG:HH12	1:B:260:GLN:CG	2.10	0.64
1:C:58:LYS:HZ2	1:C:58:LYS:CB	2.08	0.64
1:H:353:ASP:HA	4:H:764:HOH:O	1.97	0.64
1:D:97:ILE:HG22	1:D:108:ARG:HH22	1.63	0.64
1:F:86:THR:O	1:F:89:ARG:NH1	2.29	0.64
1:G:347:GLU:OE2	4:G:751:HOH:O	2.15	0.64
1:B:321:ASP:O	1:B:325:ASP:HB2	1.96	0.64
1:H:32:LEU:HD12	1:H:95:PHE:CD2	2.33	0.64
1:F:304:LYS:HZ2	1:F:347:GLU:HB2	1.63	0.64
1:A:21:ALA:H	1:A:78:GLN:HE21	1.46	0.64
1:F:349:GLY:HA2	4:F:866:HOH:O	1.97	0.64
1:A:339:LYS:O	1:A:343:HIS:CD2	2.51	0.63
1:G:324:ARG:CG	1:G:324:ARG:NH1	2.46	0.63
1:D:263:ARG:HG3	1:F:46:GLY:HA3	1.78	0.63
1:B:258:ARG:HH11	1:B:258:ARG:HG3	1.63	0.63
1:H:75:LYS:HE2	1:H:364:GLU:OE2	1.99	0.63
1:H:351:ALA:H	1:H:354:GLN:NE2	1.96	0.63
1:A:339:LYS:CG	4:A:642:HOH:O	2.45	0.63
1:B:334:HIS:ND1	4:B:606:HOH:O	2.30	0.63
1:C:20:LEU:H	1:C:78:GLN:NE2	1.96	0.63
1:H:58:LYS:HD2	1:H:58:LYS:C	2.19	0.63
1:B:50:GLU:OE1	1:B:50:GLU:HA	1.98	0.62
1:F:300:PRO:HD2	4:F:777:HOH:O	1.98	0.62
1:B:305:ARG:NH2	1:F:103:ASP:HB2	2.13	0.62
1:F:154:THR:HG22	1:F:182:TYR:CE1	2.35	0.62
1:F:19:GLN:HE22	1:F:22:LYS:NZ	1.98	0.62
1:F:323:GLU:HB3	4:F:784:HOH:O	1.98	0.62
1:F:85:LEU:HD23	1:F:85:LEU:H	1.62	0.62
1:D:89:ARG:NE	1:D:96:ASP:HB3	2.15	0.62
1:D:104:GLN:OE1	1:D:104:GLN:CA	2.44	0.62
1:H:20:LEU:N	1:H:78:GLN:HE22	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLU:O	1:C:104:GLN:N	2.24	0.61
1:G:12:LEU:HD23	1:G:251:VAL:HG22	1.82	0.61
1:B:22:LYS:N	1:B:84:LYS:CE	2.64	0.61
1:E:25:PRO:O	1:E:28:ILE:HG23	1.99	0.61
1:B:89:ARG:HB2	1:B:96:ASP:HB2	1.82	0.61
1:D:304:LYS:NZ	1:D:347:GLU:OE1	2.34	0.61
1:H:263:ARG:HH11	1:H:263:ARG:CB	2.11	0.61
1:G:103:ASP:O	1:G:106:HIS:HD2	1.83	0.61
1:G:168:VAL:HG13	1:G:173:TRP:HB2	1.82	0.61
1:H:282:MET:HG3	1:H:295:LEU:CD1	2.30	0.61
1:F:329:LEU:CD1	1:F:389:ARG:HB2	2.31	0.61
1:G:404:LEU:HD13	4:G:674:HOH:O	2.00	0.61
1:H:29:THR:O	1:H:33:THR:CG2	2.49	0.61
1:H:263:ARG:HH11	1:H:263:ARG:CA	2.13	0.61
1:G:89:ARG:HG2	4:G:809:HOH:O	2.00	0.61
1:B:256:GLU:OE2	1:B:260:GLN:OE1	2.18	0.60
1:E:21:ALA:H	1:E:78:GLN:HE21	1.48	0.60
1:F:356:ALA:O	4:F:662:HOH:O	2.16	0.60
1:D:101:GLU:C	1:D:103:ASP:N	2.55	0.60
1:B:20:LEU:H	1:B:78:GLN:HE22	1.48	0.60
1:E:339:LYS:O	1:E:343:HIS:CD2	2.55	0.60
1:E:324:ARG:NH1	1:E:325:ASP:OD1	2.34	0.60
1:A:305:ARG:HD3	4:A:747:HOH:O	2.00	0.60
1:C:22:LYS:HB2	1:C:22:LYS:HZ3	1.67	0.60
1:G:324:ARG:HB2	1:G:325:ASP:OD1	2.02	0.60
1:B:14:ASP:CG	1:B:16:ILE:HD11	2.22	0.59
1:F:205:TRP:CZ2	1:G:201:ALA:HA	2.37	0.59
1:C:22:LYS:NZ	1:C:22:LYS:CB	2.65	0.59
1:F:255:ASP:O	4:F:800:HOH:O	2.17	0.59
1:B:103:ASP:CG	1:B:104:GLN:H	2.04	0.59
1:E:288:SER:HB2	4:E:632:HOH:O	2.03	0.59
1:F:259:ARG:HG2	1:F:259:ARG:HH11	1.67	0.59
1:A:305:ARG:HD2	4:A:747:HOH:O	2.01	0.59
1:A:288:SER:HB3	1:A:289:HIS:HD2	1.65	0.58
1:B:259:ARG:HH12	1:B:260:GLN:HG2	1.67	0.58
1:G:325:ASP:OD1	1:G:325:ASP:N	2.36	0.58
1:A:339:LYS:HB2	4:A:642:HOH:O	2.02	0.58
1:F:70:SER:HB2	1:F:71:PRO:CD	2.34	0.58
1:G:321:ASP:CB	1:G:324:ARG:HD3	2.34	0.58
1:D:101:GLU:OE1	1:D:103:ASP:OD2	2.21	0.58
1:H:398:GLY:N	1:H:399:LEU:HA	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:PHE:CE2	1:G:236:ILE:HG23	2.39	0.58
1:A:342:ASP:OD1	1:A:359:LYS:HE2	2.03	0.58
1:E:32:LEU:HD12	1:E:88:ILE:HD13	1.84	0.57
1:B:22:LYS:O	1:B:84:LYS:HE2	2.04	0.57
1:C:21:ALA:H	1:C:78:GLN:HE21	1.52	0.57
1:E:103:ASP:OD2	1:E:103:ASP:N	2.33	0.57
1:D:97:ILE:CG2	1:D:108:ARG:NH2	2.68	0.57
1:H:89:ARG:HH22	1:H:98:ALA:HB2	1.69	0.57
1:D:382:GLU:HG2	4:F:776:HOH:O	2.05	0.56
1:A:56:VAL:O	1:A:60:VAL:HG23	2.05	0.56
1:B:259:ARG:NH1	1:B:260:GLN:HG3	2.20	0.56
1:H:227:ASN:ND2	1:H:230:GLU:HG3	2.20	0.56
1:E:24:VAL:HG12	1:E:28:ILE:HG23	1.87	0.56
1:G:300:PRO:HB3	1:G:343:HIS:CD2	2.40	0.56
1:F:205:TRP:CE2	1:G:204:GLN:HG2	2.40	0.56
1:E:89:ARG:HH11	1:E:89:ARG:N	2.04	0.56
1:A:201:ALA:HA	1:C:205:TRP:CZ2	2.41	0.56
1:A:382:GLU:OE2	4:A:801:HOH:O	2.18	0.56
1:E:339:LYS:HB3	1:E:343:HIS:CD2	2.40	0.56
1:F:392:CYS:SG	1:F:406:LEU:HD12	2.46	0.56
4:F:603:HOH:O	1:G:400:THR:HG21	2.05	0.56
1:F:133:GLY:O	1:F:137:GLU:HG3	2.06	0.55
1:B:22:LYS:N	1:B:84:LYS:HE2	2.21	0.55
1:B:46:GLY:HA3	1:C:263:ARG:HG3	1.88	0.55
1:G:340:ILE:O	1:G:344:VAL:HG23	2.06	0.55
1:D:260:GLN:HB2	1:D:262:LEU:HD13	1.88	0.55
1:G:274:LEU:HD23	1:G:400:THR:HG22	1.88	0.55
1:C:130:LYS:HZ2	1:C:134:LYS:HE3	1.71	0.55
1:D:49:ASP:OD2	1:D:51:GLU:HB3	2.06	0.55
1:D:138:GLN:O	1:D:141:GLU:HG2	2.07	0.55
1:G:300:PRO:HB3	1:G:343:HIS:HD2	1.72	0.55
1:C:212:THR:HB	1:C:256:GLU:HG2	1.87	0.55
1:G:346:GLU:O	1:G:346:GLU:HG3	2.03	0.55
1:H:32:LEU:HD12	1:H:95:PHE:CE2	2.42	0.55
1:B:150:LEU:HD12	1:B:215:ASP:O	2.07	0.55
1:B:299:VAL:HB	1:B:300:PRO:HD3	1.89	0.55
1:A:69:VAL:HG11	1:A:74:ILE:HD12	1.89	0.55
1:B:22:LYS:H	1:B:84:LYS:HZ3	1.52	0.55
1:B:56:VAL:HG23	4:B:702:HOH:O	2.06	0.55
1:F:24:VAL:HG23	1:F:29:THR:HG23	1.89	0.55
1:H:241:LEU:HD21	1:H:336:GLY:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LYS:CB	4:A:642:HOH:O	2.54	0.54
1:F:101:GLU:HB3	4:F:832:HOH:O	2.07	0.54
1:G:321:ASP:HB3	1:G:324:ARG:HD3	1.88	0.54
1:G:353:ASP:OD1	1:G:354:GLN:N	2.40	0.54
1:F:325:ASP:O	1:F:329:LEU:HD22	2.07	0.54
1:H:320:MET:HE1	1:H:329:LEU:HD21	1.88	0.54
1:D:260:GLN:CB	1:D:262:LEU:HD13	2.38	0.54
1:G:332:ALA:O	1:G:392:CYS:HA	2.08	0.54
1:C:104:GLN:HA	1:C:106:HIS:HD2	1.72	0.54
1:F:260:GLN:HB3	1:F:262:LEU:HG	1.88	0.54
1:G:150:LEU:C	1:G:150:LEU:HD23	2.28	0.54
1:E:32:LEU:HD12	1:E:88:ILE:CD1	2.37	0.54
1:A:50:GLU:O	1:A:54:VAL:HG23	2.07	0.54
1:B:201:ALA:HA	1:H:205:TRP:CZ2	2.42	0.54
1:D:263:ARG:HH11	1:D:263:ARG:CG	2.21	0.54
1:G:226:ASN:ND2	4:G:716:HOH:O	2.41	0.54
1:F:15:PHE:HB2	1:F:378:LYS:HB2	1.88	0.54
1:F:304:LYS:NZ	1:F:347:GLU:HB2	2.23	0.54
1:H:57:TYR:CE1	1:H:61:LYS:HD2	2.43	0.53
1:H:232:ARG:O	1:H:233:VAL:C	2.46	0.53
1:A:139:MET:HE3	1:A:248:LYS:HB3	1.90	0.53
1:G:195:MET:O	1:G:199:MET:HG3	2.09	0.53
1:F:301:ALA:O	4:F:860:HOH:O	2.19	0.53
1:G:398:GLY:N	1:G:399:LEU:HA	2.23	0.53
1:H:63:LYS:HD2	1:H:236:ILE:HD11	1.90	0.53
1:H:268:LEU:HD12	1:H:405:VAL:HG12	1.90	0.53
1:F:226:ASN:HB3	3:F:502:PG4:H52	1.89	0.53
1:F:146:ALA:HB2	1:F:173:TRP:CD1	2.44	0.53
1:H:85:LEU:O	1:H:87:ASP:N	2.42	0.53
1:C:256:GLU:OE1	1:C:259:ARG:NH2	2.38	0.53
1:F:205:TRP:CZ2	1:G:204:GLN:HG2	2.44	0.53
1:B:21:ALA:H	1:B:78:GLN:HE21	1.55	0.53
1:D:85:LEU:HD22	4:D:661:HOH:O	2.09	0.53
1:E:125:HIS:HE1	1:E:158:TYR:H	1.54	0.53
1:F:314:LEU:O	1:F:317:ARG:HB2	2.08	0.53
1:C:102:PRO:C	1:C:104:GLN:N	2.63	0.53
1:D:101:GLU:O	1:D:104:GLN:HB2	2.09	0.53
1:D:101:GLU:O	1:D:102:PRO:C	2.47	0.53
1:G:21:ALA:H	1:G:78:GLN:HE21	1.57	0.53
1:G:342:ASP:OD2	4:G:768:HOH:O	2.19	0.53
1:H:282:MET:HG3	1:H:295:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:TYR:HE2	1:G:183:ASN:HD22	1.58	0.52
1:H:63:LYS:HD2	1:H:236:ILE:CD1	2.39	0.52
1:B:253:PRO:HB2	1:B:255:ASP:OD1	2.10	0.52
1:D:32:LEU:HD22	1:D:95:PHE:CE1	2.45	0.52
1:H:190:PHE:HB2	1:H:191:PRO:CD	2.39	0.52
1:G:304:LYS:HD2	1:G:343:HIS:HB3	1.91	0.52
1:H:110:PHE:C	1:H:110:PHE:CD2	2.82	0.52
1:F:334:HIS:HB3	4:F:712:HOH:O	2.10	0.52
1:G:57:TYR:CE1	1:G:61:LYS:HD3	2.45	0.52
1:G:397:PRO:O	1:G:400:THR:CG2	2.57	0.52
1:H:227:ASN:HD21	1:H:230:GLU:HG3	1.74	0.52
1:C:222:MET:O	3:C:502:PG4:H81	2.10	0.52
1:G:20:LEU:N	1:G:78:GLN:NE2	2.53	0.52
1:G:150:LEU:HD23	1:G:151:ILE:N	2.26	0.52
1:B:259:ARG:HH11	1:B:260:GLN:HG3	1.74	0.51
1:F:373:ILE:HD13	1:F:376:ILE:HD12	1.92	0.51
1:E:288:SER:HB3	1:E:289:HIS:ND1	2.24	0.51
1:G:353:ASP:OD1	1:G:353:ASP:C	2.49	0.51
1:H:329:LEU:CD2	1:H:389:ARG:HB2	2.41	0.51
1:F:74:ILE:HG21	1:F:77:ARG:HG3	1.92	0.51
1:B:190:PHE:HB2	1:B:191:PRO:HD3	1.93	0.51
1:D:97:ILE:HG22	1:D:108:ARG:NH2	2.26	0.51
1:A:395:PHE:HD2	4:A:690:HOH:O	1.93	0.51
1:D:122:LYS:HE3	1:D:126:GLU:OE2	2.10	0.51
1:F:90:PHE:CD1	1:F:90:PHE:C	2.83	0.51
1:B:69:VAL:HG11	1:B:74:ILE:CD1	2.40	0.51
1:H:63:LYS:HG2	1:H:67:TYR:HD1	1.76	0.51
1:H:315:LEU:HD22	1:H:322:PHE:HA	1.92	0.51
1:H:342:ASP:OD1	1:H:359:LYS:HE2	2.10	0.51
1:E:27:ARG:NH2	4:E:681:HOH:O	2.44	0.51
1:E:324:ARG:CZ	1:E:325:ASP:OD1	2.59	0.51
1:G:43:LEU:HD11	1:G:113:LYS:C	2.31	0.51
1:C:241:LEU:HD21	1:C:336:GLY:O	2.11	0.51
1:D:18:VAL:HG23	4:D:913:HOH:O	2.11	0.51
1:D:51:GLU:OE1	1:D:51:GLU:HA	2.11	0.51
1:F:197:HIS:CB	1:F:270:MET:HE1	2.41	0.51
1:H:263:ARG:NH1	1:H:263:ARG:HA	2.24	0.51
1:A:315:LEU:CD2	1:A:322:PHE:HA	2.41	0.50
1:D:101:GLU:C	1:D:103:ASP:H	2.14	0.50
1:F:260:GLN:HG2	1:F:262:LEU:HD11	1.92	0.50
1:A:125:HIS:HE1	1:A:158:TYR:H	1.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:GLY:O	1:F:139:MET:HG3	2.11	0.50
1:F:298:LEU:C	1:F:300:PRO:HD2	2.30	0.50
1:H:324:ARG:HB3	1:H:324:ARG:CZ	2.40	0.50
1:A:104:GLN:NE2	1:A:107:LEU:CD1	2.75	0.50
1:G:270:MET:HG2	4:G:674:HOH:O	2.12	0.50
1:A:320:MET:HE1	1:A:405:VAL:CG1	2.37	0.50
1:F:12:LEU:HD23	1:F:251:VAL:HG22	1.93	0.50
1:F:24:VAL:HG23	1:F:29:THR:CG2	2.37	0.50
1:D:102:PRO:C	1:D:104:GLN:H	2.15	0.50
1:H:63:LYS:CD	1:H:236:ILE:CD1	2.89	0.50
1:C:130:LYS:HZ2	1:C:134:LYS:CE	2.24	0.50
1:H:64:PHE:O	1:H:68:ALA:HB3	2.11	0.50
1:B:20:LEU:H	1:B:78:GLN:NE2	2.09	0.50
1:B:255:ASP:OD1	1:B:255:ASP:N	2.44	0.50
1:E:371:SER:C	1:E:374:PRO:HD2	2.32	0.50
1:H:323:GLU:OE1	1:H:323:GLU:HA	2.12	0.50
1:B:392:CYS:HB2	1:B:404:LEU:HB3	1.94	0.49
1:C:11:VAL:HG11	1:C:257:LEU:HD22	1.94	0.49
1:F:266:ARG:HD3	4:F:753:HOH:O	2.12	0.49
1:B:338:PRO:HD2	4:B:601:HOH:O	2.11	0.49
1:C:101:GLU:O	1:C:102:PRO:C	2.47	0.49
1:H:20:LEU:N	1:H:78:GLN:NE2	2.55	0.49
1:H:64:PHE:O	1:H:68:ALA:CB	2.60	0.49
1:H:139:MET:CE	1:H:248:LYS:HB3	2.40	0.49
1:G:308:ARG:HA	1:G:348:LEU:HD21	1.95	0.49
1:G:315:LEU:HG	1:G:320:MET:HE3	1.95	0.49
1:H:263:ARG:NH1	1:H:263:ARG:CA	2.75	0.49
1:D:315:LEU:HD12	1:D:322:PHE:HA	1.95	0.49
1:A:49:ASP:OD2	1:A:52:GLY:N	2.46	0.49
1:B:120:ASP:C	1:B:120:ASP:OD1	2.50	0.49
1:G:223:SER:HA	3:G:502:PG4:H32	1.95	0.49
1:A:315:LEU:HD23	1:A:322:PHE:HA	1.95	0.49
1:B:282:MET:HG3	1:B:295:LEU:HD13	1.95	0.48
1:E:150:LEU:C	1:E:150:LEU:HD23	2.34	0.48
1:G:20:LEU:N	1:G:78:GLN:HE22	2.05	0.48
1:F:13:ALA:HB3	1:F:252:TYR:CE2	2.48	0.48
1:D:205:TRP:CZ2	1:E:201:ALA:HA	2.48	0.48
1:F:326:LYS:HG2	4:F:630:HOH:O	2.12	0.48
1:H:82:PHE:CG	1:H:83:PRO:HD2	2.48	0.48
1:H:304:LYS:O	1:H:307:VAL:HG12	2.14	0.48
1:A:104:GLN:NE2	1:A:107:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:N	1:D:78:GLN:HE22	2.04	0.48
1:A:205:TRP:CZ2	1:C:201:ALA:HA	2.49	0.48
1:G:103:ASP:O	1:G:106:HIS:CD2	2.66	0.48
1:A:108:ARG:NH2	4:A:846:HOH:O	1.98	0.47
1:D:39:ARG:HH22	1:D:94:ASN:ND2	2.08	0.47
1:F:317:ARG:HG2	1:G:209:PRO:HD3	1.96	0.47
1:F:323:GLU:CB	4:F:784:HOH:O	2.61	0.47
1:H:27:ARG:HG3	1:H:28:ILE:N	2.28	0.47
1:E:138:GLN:O	1:E:141:GLU:HG2	2.14	0.47
1:G:326:LYS:O	1:G:354:GLN:NE2	2.48	0.47
1:H:223:SER:HA	3:H:502:PG4:H32	1.96	0.47
1:G:233:VAL:HG23	4:G:657:HOH:O	2.14	0.47
1:H:83:PRO:HG2	1:H:88:ILE:HD11	1.96	0.47
1:A:357:ILE:HD12	1:A:380:TYR:CE1	2.50	0.47
1:E:168:VAL:HG13	1:E:173:TRP:HB2	1.96	0.47
1:E:395:PHE:HA	1:E:400:THR:O	2.14	0.47
1:B:84:LYS:HD2	4:B:788:HOH:O	2.14	0.47
4:B:624:HOH:O	1:F:134:LYS:HD2	2.14	0.47
1:A:115:ASP:OD2	1:A:117:ARG:NH2	2.32	0.47
1:A:130:LYS:HG2	4:A:811:HOH:O	2.14	0.47
1:B:315:LEU:HD12	1:B:315:LEU:N	2.28	0.47
1:B:322:PHE:O	1:B:323:GLU:C	2.52	0.47
1:D:304:LYS:NZ	1:D:347:GLU:HB2	2.19	0.47
1:B:14:ASP:O	1:B:16:ILE:CD1	2.58	0.47
1:B:69:VAL:HG11	1:B:74:ILE:HD12	1.97	0.47
1:G:27:ARG:HD2	1:G:31:GLU:OE2	2.15	0.47
1:B:371:SER:O	1:B:375:HIS:CD2	2.52	0.47
1:E:256:GLU:OE1	1:E:259:ARG:NH2	2.26	0.47
1:G:298:LEU:O	1:G:302:ILE:HG13	2.14	0.47
1:A:170:ASP:O	4:A:909:HOH:O	2.20	0.47
1:E:339:LYS:O	1:E:343:HIS:HD2	1.96	0.47
1:H:315:LEU:HD22	1:H:322:PHE:HD1	1.80	0.47
1:A:51:GLU:OE2	1:A:55:GLN:HG2	2.15	0.46
1:G:398:GLY:HA3	1:G:400:THR:HG22	1.97	0.46
1:G:335:PRO:HB2	1:G:362:PHE:CD1	2.51	0.46
1:D:320:MET:CE	1:D:329:LEU:HD21	2.45	0.46
1:E:89:ARG:HH11	1:E:89:ARG:CB	2.25	0.46
1:F:50:GLU:HA	1:F:50:GLU:OE1	2.16	0.46
1:F:174:PHE:CZ	1:G:276:PRO:HA	2.51	0.46
1:G:392:CYS:HB2	1:G:404:LEU:HB3	1.97	0.46
1:H:395:PHE:HA	1:H:400:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:MET:CE	1:B:329:LEU:HD11	2.45	0.46
1:D:20:LEU:N	1:D:78:GLN:NE2	2.62	0.46
1:F:373:ILE:HD13	1:F:373:ILE:HA	1.71	0.46
1:H:106:HIS:CE1	1:H:130:LYS:HZ1	2.30	0.46
1:H:320:MET:CE	1:H:329:LEU:HD21	2.46	0.46
1:A:232:ARG:NH1	1:A:234:ASP:OD1	2.42	0.46
1:D:226:ASN:CB	3:D:502:PG4:H51	2.42	0.46
1:C:256:GLU:O	1:C:260:GLN:HG3	2.15	0.46
1:F:272:GLU:HA	1:F:401:ALA:O	2.16	0.46
1:H:285:VAL:HA	1:H:286:PRO:HD3	1.80	0.46
1:E:339:LYS:CB	1:E:343:HIS:NE2	2.79	0.46
1:B:306:HIS:HB3	4:B:645:HOH:O	2.15	0.46
1:C:146:ALA:HB2	1:C:173:TRP:CD1	2.51	0.46
1:B:139:MET:HE2	1:B:140:PHE:HE2	1.79	0.45
1:B:335:PRO:HB2	1:B:362:PHE:CD1	2.50	0.45
1:F:299:VAL:N	1:F:300:PRO:CD	2.79	0.45
1:A:339:LYS:HB3	1:A:343:HIS:CD2	2.52	0.45
1:B:104:GLN:O	1:B:104:GLN:HG3	2.16	0.45
1:B:398:GLY:N	1:B:399:LEU:HA	2.31	0.45
1:C:102:PRO:C	1:C:104:GLN:H	2.19	0.45
1:F:83:PRO:HG3	1:F:97:ILE:HD12	1.98	0.45
1:H:190:PHE:HB2	1:H:191:PRO:HD2	1.98	0.45
1:H:315:LEU:HD21	1:H:329:LEU:CD1	2.46	0.45
1:B:97:ILE:HD13	1:B:108:ARG:HH12	1.81	0.45
1:B:326:LYS:HE3	1:B:326:LYS:HB3	1.79	0.45
1:F:225:HIS:O	1:F:226:ASN:C	2.54	0.45
1:H:266:ARG:O	1:H:406:LEU:HA	2.17	0.45
1:A:104:GLN:HE21	1:A:107:LEU:HD12	1.82	0.45
1:D:407:GLU:OE2	4:D:871:HOH:O	2.21	0.45
1:F:90:PHE:C	1:F:90:PHE:HD1	2.19	0.45
1:F:297:PRO:O	1:F:300:PRO:HD2	2.16	0.45
1:G:91:GLY:O	1:G:92:ASP:C	2.54	0.45
1:H:226:ASN:ND2	4:H:691:HOH:O	2.06	0.45
1:C:130:LYS:NZ	1:C:134:LYS:CE	2.80	0.45
1:H:329:LEU:HD23	1:H:389:ARG:HB2	1.99	0.45
1:C:382:GLU:OE1	4:C:809:HOH:O	2.21	0.45
1:B:305:ARG:HH22	1:F:103:ASP:HB2	1.78	0.45
1:C:220:GLU:HB3	1:C:222:MET:HE2	1.95	0.45
1:F:339:LYS:HD3	4:F:744:HOH:O	2.17	0.45
1:C:101:GLU:C	1:C:103:ASP:H	2.16	0.45
1:C:109:LEU:HD13	1:C:124:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:LYS:NZ	1:E:349:GLY:O	2.50	0.45
1:H:291:PHE:N	1:H:291:PHE:CD1	2.83	0.45
1:C:103:ASP:C	1:C:104:GLN:HG2	2.36	0.44
1:H:345:GLN:HG3	1:H:350:LEU:HB2	2.00	0.44
1:A:130:LYS:HB3	1:A:130:LYS:HE3	1.44	0.44
1:B:139:MET:HE3	1:B:248:LYS:HD3	1.99	0.44
1:E:32:LEU:HA	1:E:32:LEU:HD23	1.55	0.44
1:H:168:VAL:HG13	1:H:173:TRP:HB2	2.00	0.44
1:A:110:PHE:HB3	1:A:226:ASN:HD21	1.83	0.44
1:D:263:ARG:HA	1:D:263:ARG:HD3	1.90	0.44
1:D:398:GLY:N	1:D:399:LEU:HA	2.31	0.44
1:F:160:ALA:HA	1:F:161:PRO:C	2.38	0.44
1:B:298:LEU:CD2	1:F:102:PRO:HG2	2.48	0.44
4:B:659:HOH:O	1:C:382:GLU:HG2	2.17	0.44
1:B:160:ALA:HA	1:B:161:PRO:C	2.37	0.44
1:D:316:ARG:HD2	4:D:942:HOH:O	2.17	0.44
1:F:111:ASP:OD2	1:F:115:ASP:N	2.46	0.44
1:F:329:LEU:HD12	1:F:389:ARG:O	2.18	0.44
1:C:111:ASP:HB3	1:C:115:ASP:O	2.18	0.44
1:E:89:ARG:NH1	1:E:89:ARG:N	2.66	0.44
1:E:308:ARG:O	1:E:312:VAL:HG23	2.18	0.44
1:F:205:TRP:HZ2	1:G:204:GLN:HB3	1.82	0.44
1:B:322:PHE:CZ	1:B:326:LYS:HD3	2.52	0.44
1:D:103:ASP:O	1:D:104:GLN:OE1	2.36	0.44
1:F:24:VAL:CG2	1:F:24:VAL:O	2.63	0.44
1:D:258:ARG:O	1:D:259:ARG:C	2.56	0.44
1:F:145:GLU:OE2	1:F:145:GLU:HA	2.18	0.44
1:F:316:ARG:HD2	4:F:737:HOH:O	2.17	0.44
1:F:408:LYS:HG2	1:F:409:ILE:N	2.32	0.44
1:H:120:ASP:OD1	1:H:120:ASP:C	2.57	0.44
1:C:270:MET:HE2	1:C:270:MET:HB2	1.74	0.43
1:B:161:PRO:HD2	4:B:607:HOH:O	2.18	0.43
1:G:186:CYS:HB3	1:G:334:HIS:NE2	2.33	0.43
1:H:75:LYS:HE2	1:H:364:GLU:CD	2.38	0.43
1:D:382:GLU:HG2	1:F:48:THR:OG1	2.18	0.43
1:F:8:ASN:HA	1:G:205:TRP:CZ2	2.53	0.43
1:F:369:SER:OG	1:F:370:SER:N	2.52	0.43
1:C:101:GLU:O	1:C:103:ASP:N	2.52	0.43
1:E:139:MET:SD	1:E:248:LYS:HB3	2.58	0.43
1:E:315:LEU:HD21	1:E:329:LEU:HD11	2.01	0.43
1:F:322:PHE:O	1:F:326:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:HA	1:B:398:GLY:O	2.19	0.43
1:B:357:ILE:HD12	1:B:380:TYR:CE2	2.53	0.43
1:E:281:THR:HB	1:E:296:SER:HB3	2.00	0.43
1:G:149:ASP:OD1	1:G:177:THR:HB	2.18	0.43
1:H:148:ASP:HB3	1:H:211:LYS:HG2	2.00	0.43
1:H:322:PHE:O	1:H:326:LYS:HB3	2.18	0.43
1:F:70:SER:HB2	1:F:71:PRO:HD2	2.00	0.43
1:H:6:HIS:HB2	1:H:254:GLU:OE1	2.18	0.43
1:H:190:PHE:CB	1:H:191:PRO:CD	2.97	0.43
1:A:322:PHE:CZ	1:A:326:LYS:HD2	2.53	0.43
1:B:97:ILE:HD13	1:B:108:ARG:NH1	2.33	0.43
1:F:97:ILE:HB	4:F:798:HOH:O	2.18	0.43
1:H:321:ASP:O	1:H:323:GLU:N	2.51	0.43
1:B:111:ASP:OD2	1:B:114:LYS:HB2	2.19	0.43
1:B:172:GLY:HA2	1:B:174:PHE:CE2	2.54	0.43
1:F:398:GLY:N	1:F:399:LEU:HA	2.34	0.43
1:A:398:GLY:N	1:A:399:LEU:HA	2.33	0.43
1:D:156:SER:OG	1:D:220:GLU:HA	2.18	0.43
1:D:260:GLN:O	1:D:262:LEU:HD13	2.19	0.43
1:G:111:ASP:OD2	1:G:114:LYS:HG3	2.18	0.43
1:H:313:ASP:OD1	1:H:316:ARG:NH2	2.52	0.43
1:A:24:VAL:O	1:A:24:VAL:HG23	2.18	0.43
1:B:212:THR:O	1:B:253:PRO:HD2	2.19	0.43
1:C:315:LEU:HD12	1:C:322:PHE:HA	2.01	0.43
1:D:115:ASP:HA	1:D:116:PRO:HD2	1.83	0.43
1:F:26:GLN:HB2	1:F:74:ILE:O	2.18	0.43
1:H:81:TYR:CE1	1:H:224:ALA:HB2	2.54	0.43
1:H:324:ARG:HG2	1:H:324:ARG:O	2.19	0.43
1:E:8:ASN:N	1:E:8:ASN:HD22	2.17	0.42
1:G:106:HIS:NE2	1:G:130:LYS:HE3	2.34	0.42
1:D:254:GLU:O	1:D:258:ARG:HG2	2.19	0.42
1:E:339:LYS:HA	1:E:339:LYS:HD3	1.73	0.42
1:F:94:ASN:HB2	4:F:847:HOH:O	2.19	0.42
1:F:240:THR:HG22	4:F:681:HOH:O	2.18	0.42
1:G:341:VAL:HG11	1:G:359:LYS:HG3	2.01	0.42
1:H:112:ILE:O	1:H:112:ILE:CG1	2.43	0.42
1:H:234:ASP:OD2	1:H:294:THR:HA	2.19	0.42
1:D:386:VAL:HA	1:D:408:LYS:HG2	2.01	0.42
1:D:106:HIS:CE1	1:D:130:LYS:CE	3.02	0.42
1:G:37:PHE:O	4:G:767:HOH:O	2.21	0.42
1:G:120:ASP:C	1:G:120:ASP:OD1	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:HB1	1:A:320:MET:HE2	2.00	0.42
1:B:392:CYS:O	1:B:403:GLY:HA2	2.19	0.42
1:F:19:GLN:HE22	1:F:22:LYS:HZ3	1.68	0.42
1:H:58:LYS:NZ	1:H:62:GLU:OE2	2.49	0.42
1:H:353:ASP:CA	4:H:764:HOH:O	2.64	0.42
1:G:84:LYS:HB2	1:G:84:LYS:HE2	1.76	0.42
1:H:84:LYS:HB3	1:H:84:LYS:HE2	1.82	0.42
1:A:339:LYS:HG2	4:A:642:HOH:O	2.12	0.42
1:D:27:ARG:O	1:D:31:GLU:HG3	2.19	0.42
1:E:194:LYS:HE2	1:E:194:LYS:HB3	1.91	0.42
1:E:389:ARG:C	1:E:390:ILE:HG13	2.40	0.42
1:C:103:ASP:OD1	1:C:103:ASP:O	2.37	0.42
1:D:290:GLN:NE2	4:D:663:HOH:O	2.53	0.42
1:F:324:ARG:O	1:F:324:ARG:HG2	2.18	0.42
1:H:56:VAL:HB	1:H:57:TYR:H	1.56	0.42
1:H:76:GLN:HB3	4:H:773:HOH:O	2.20	0.42
1:B:171:ARG:HD2	1:B:171:ARG:HA	1.80	0.42
1:E:95:PHE:O	1:E:96:ASP:CB	2.51	0.42
1:F:56:VAL:O	1:F:60:VAL:HG23	2.19	0.42
1:B:188:GLY:O	1:B:191:PRO:HD2	2.19	0.42
1:D:172:GLY:HA2	1:D:174:PHE:CE2	2.55	0.42
1:F:72:ALA:N	4:F:608:HOH:O	2.49	0.42
1:G:266:ARG:O	1:G:406:LEU:HA	2.20	0.42
1:H:12:LEU:HB2	1:H:265:LEU:HB2	2.02	0.42
1:H:67:TYR:CD2	1:H:233:VAL:HG13	2.55	0.42
1:H:315:LEU:CD2	1:H:322:PHE:HA	2.50	0.42
1:F:15:PHE:CG	1:F:378:LYS:HB2	2.55	0.41
1:F:264:GLY:O	1:F:408:LYS:HA	2.20	0.41
1:B:64:PHE:O	1:B:68:ALA:CB	2.68	0.41
1:B:109:LEU:HD13	1:B:124:ARG:HG2	2.02	0.41
1:C:58:LYS:HZ3	1:C:58:LYS:HG2	1.61	0.41
1:H:335:PRO:HG3	1:H:362:PHE:HB2	2.03	0.41
1:A:324:ARG:NE	1:A:325:ASP:OD1	2.40	0.41
1:D:320:MET:HE2	1:D:329:LEU:HD21	2.02	0.41
1:E:97:ILE:HD12	1:E:97:ILE:N	2.34	0.41
1:G:64:PHE:CZ	1:G:236:ILE:HG23	2.56	0.41
1:H:226:ASN:HA	3:H:502:PG4:H31	2.01	0.41
1:H:267:ILE:HG21	1:H:270:MET:HE2	2.03	0.41
1:B:64:PHE:O	1:B:65:ASP:C	2.59	0.41
1:B:321:ASP:N	1:B:325:ASP:OD2	2.43	0.41
1:E:122:LYS:HE3	4:E:724:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ILE:HD12	1:G:248:LYS:NZ	2.36	0.41
1:B:296:SER:O	1:B:299:VAL:HG23	2.20	0.41
1:F:259:ARG:HG2	1:F:259:ARG:NH1	2.33	0.41
1:H:148:ASP:CB	1:H:211:LYS:HG2	2.51	0.41
1:H:233:VAL:HA	1:H:236:ILE:HD12	2.02	0.41
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.76	0.41
1:F:13:ALA:HB3	1:F:252:TYR:HE2	1.84	0.41
1:F:236:ILE:O	1:F:237:ILE:C	2.55	0.41
1:H:341:VAL:HG23	4:H:678:HOH:O	2.20	0.41
1:B:258:ARG:CG	1:B:258:ARG:NH1	2.76	0.41
1:D:89:ARG:NE	1:D:96:ASP:CB	2.83	0.41
1:D:314:LEU:HD11	1:D:405:VAL:HG23	2.01	0.41
1:F:58:LYS:HD3	1:F:62:GLU:OE2	2.20	0.41
1:G:97:ILE:N	1:G:97:ILE:HD12	2.33	0.41
1:B:111:ASP:OD1	1:B:111:ASP:C	2.59	0.41
1:C:102:PRO:O	1:C:104:GLN:N	2.53	0.41
1:G:103:ASP:OD1	1:G:103:ASP:N	2.50	0.41
1:H:281:THR:HG21	1:H:302:ILE:CD1	2.51	0.41
1:A:81:TYR:CE1	1:A:109:LEU:HD11	2.56	0.41
1:C:172:GLY:HA2	1:C:174:PHE:CE2	2.56	0.41
1:C:194:LYS:HE2	1:C:194:LYS:HB3	1.97	0.41
1:C:398:GLY:N	1:C:399:LEU:HA	2.34	0.41
1:F:373:ILE:O	1:F:377:LEU:HG	2.21	0.41
1:G:226:ASN:ND2	1:G:226:ASN:O	2.53	0.41
1:G:256:GLU:O	1:G:260:GLN:HG3	2.20	0.41
1:G:308:ARG:O	1:G:312:VAL:HG23	2.20	0.41
1:D:392:CYS:HB2	1:D:404:LEU:HB3	2.03	0.41
1:E:51:GLU:O	1:E:55:GLN:HG2	2.21	0.41
1:C:22:LYS:HB2	1:C:22:LYS:HZ2	1.85	0.40
1:C:342:ASP:OD1	1:C:359:LYS:HE2	2.21	0.40
1:C:357:ILE:HD12	1:C:380:TYR:CE2	2.57	0.40
1:B:231:SER:O	1:B:232:ARG:C	2.59	0.40
1:B:286:PRO:HD2	1:H:158:TYR:O	2.21	0.40
1:C:270:MET:HG2	1:C:404:LEU:HD23	2.02	0.40
1:E:323:GLU:HA	4:E:864:HOH:O	2.20	0.40
1:D:106:HIS:CE1	1:D:130:LYS:HE3	2.57	0.40
1:G:194:LYS:HA	1:G:270:MET:SD	2.61	0.40
1:A:320:MET:HE3	1:A:405:VAL:HG11	1.98	0.40
1:C:124:ARG:HD3	1:C:224:ALA:O	2.22	0.40
1:C:260:GLN:HB2	1:C:262:LEU:HG	2.02	0.40
1:G:296:SER:OG	1:G:298:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:HG21	1:D:108:ARG:CZ	2.51	0.40
1:G:321:ASP:OD2	1:G:324:ARG:CD	2.69	0.40

All (2) 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:H:324:ARG:NE	4:E:866:HOH:O[1_656]	2.09	0.11
1:D:230:GLU:OE2	1:H:321:ASP:OD2[1_454]	2.17	0.03

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	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
1	B	391/410 (95%)	371 (95%)	18 (5%)	2 (0%)	29	23
1	C	392/410 (96%)	380 (97%)	10 (3%)	2 (0%)	29	23
1	D	397/410 (97%)	385 (97%)	10 (2%)	2 (0%)	29	23
1	E	396/410 (97%)	381 (96%)	14 (4%)	1 (0%)	41	37
1	F	397/410 (97%)	379 (96%)	18 (4%)	0	100	100
1	G	391/410 (95%)	376 (96%)	13 (3%)	2 (0%)	29	23
1	H	375/410 (92%)	356 (95%)	15 (4%)	4 (1%)	14	8
All	All	3136/3280 (96%)	3013 (96%)	110 (4%)	13 (0%)	34	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PHE
1	B	323	GLU

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Mol	Chain	Res	Type
1	E	96	ASP
1	C	103	ASP
1	C	104	GLN
1	H	86	THR
1	G	45	ASN
1	G	92	ASP
1	H	113	LYS
1	H	322	PHE
1	D	86	THR
1	D	102	PRO
1	H	234	ASP

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	333/339 (98%)	323 (97%)	10 (3%)	41	41
1	B	329/339 (97%)	319 (97%)	10 (3%)	41	41
1	C	328/339 (97%)	318 (97%)	10 (3%)	41	41
1	D	332/339 (98%)	323 (97%)	9 (3%)	44	46
1	E	332/339 (98%)	325 (98%)	7 (2%)	53	57
1	F	333/339 (98%)	315 (95%)	18 (5%)	22	18
1	G	327/339 (96%)	312 (95%)	15 (5%)	27	23
1	H	317/339 (94%)	300 (95%)	17 (5%)	22	18
All	All	2631/2712 (97%)	2535 (96%)	96 (4%)	35	34

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	89	ARG
1	A	90	PHE
1	A	103	ASP

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Mol	Chain	Res	Type
1	A	130	LYS
1	A	209	PRO
1	A	257	LEU
1	A	288	SER
1	A	316	ARG
1	A	348	LEU
1	B	30	LEU
1	B	104	GLN
1	B	231	SER
1	B	238	SER
1	B	248	LYS
1	B	257	LEU
1	B	258	ARG
1	B	295	LEU
1	B	324	ARG
1	B	348	LEU
1	C	22	LYS
1	C	32	LEU
1	C	58	LYS
1	C	84	LYS
1	C	96	ASP
1	C	97	ILE
1	C	104	GLN
1	C	145	GLU
1	C	231	SER
1	C	404	LEU
1	D	27	ARG
1	D	32	LEU
1	D	48	THR
1	D	85	LEU
1	D	89	ARG
1	D	103	ASP
1	D	104	GLN
1	D	262	LEU
1	D	290	GLN
1	E	28	ILE
1	E	50	GLU
1	E	76	GLN
1	E	89	ARG
1	E	103	ASP
1	E	257	LEU
1	E	288	SER

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Mol	Chain	Res	Type
1	F	22	LYS
1	F	44	SER
1	F	51	GLU
1	F	54	VAL
1	F	58	LYS
1	F	86	THR
1	F	90	PHE
1	F	114	LYS
1	F	117	ARG
1	F	248	LYS
1	F	257	LEU
1	F	258	ARG
1	F	260	GLN
1	F	305	ARG
1	F	321	ASP
1	F	329	LEU
1	F	373	ILE
1	F	385	THR
1	G	43	LEU
1	G	55	GLN
1	G	92	ASP
1	G	97	ILE
1	G	103	ASP
1	G	204	GLN
1	G	226	ASN
1	G	255	ASP
1	G	290	GLN
1	G	296	SER
1	G	298	LEU
1	G	324	ARG
1	G	325	ASP
1	G	399	LEU
1	G	400	THR
1	H	27	ARG
1	H	33	THR
1	H	56	VAL
1	H	86	THR
1	H	89	ARG
1	H	103	ASP
1	H	226	ASN
1	H	231	SER
1	H	238	SER

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Mol	Chain	Res	Type
1	H	263	ARG
1	H	271	SER
1	H	285	VAL
1	H	321	ASP
1	H	324	ARG
1	H	346	GLU
1	H	348	LEU
1	H	373	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	104	GLN
1	A	125	HIS
1	A	226	ASN
1	A	289	HIS
1	A	290	GLN
1	A	343	HIS
1	B	6	HIS
1	B	55	GLN
1	B	78	GLN
1	B	226	ASN
1	B	260	GLN
1	B	289	HIS
1	B	290	GLN
1	B	375	HIS
1	C	78	GLN
1	C	104	GLN
1	C	106	HIS
1	C	226	ASN
1	C	290	GLN
1	D	6	HIS
1	D	78	GLN
1	D	94	ASN
1	D	226	ASN
1	D	290	GLN
1	D	343	HIS
1	E	8	ASN
1	E	76	GLN
1	E	78	GLN
1	E	104	GLN

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Mol	Chain	Res	Type
1	E	125	HIS
1	E	226	ASN
1	E	290	GLN
1	E	343	HIS
1	F	19	GLN
1	F	41	HIS
1	F	78	GLN
1	F	226	ASN
1	F	290	GLN
1	G	6	HIS
1	G	55	GLN
1	G	78	GLN
1	G	106	HIS
1	G	125	HIS
1	G	226	ASN
1	G	290	GLN
1	G	343	HIS
1	H	78	GLN
1	H	106	HIS
1	H	226	ASN
1	H	289	HIS
1	H	290	GLN
1	H	354	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PG4	C	502	-	12,12,12	0.58	0	11,11,11	0.62	0
3	PG4	F	502	-	12,12,12	0.60	0	11,11,11	0.31	0
3	PG4	D	502	-	12,12,12	0.61	0	11,11,11	0.52	0
3	PG4	A	502	-	12,12,12	0.55	0	11,11,11	0.67	0
3	PG4	H	502	-	12,12,12	0.51	0	11,11,11	0.35	0
3	PG4	E	502	-	12,12,12	0.43	0	11,11,11	0.85	0
3	PG4	B	502	-	12,12,12	0.64	0	11,11,11	0.51	0
3	PG4	G	502	-	12,12,12	0.55	0	11,11,11	0.38	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	PG4	C	502	-	-	5/10/10/10	-
3	PG4	F	502	-	-	3/10/10/10	-
3	PG4	D	502	-	-	4/10/10/10	-
3	PG4	A	502	-	-	8/10/10/10	-
3	PG4	H	502	-	-	7/10/10/10	-
3	PG4	E	502	-	-	5/10/10/10	-
3	PG4	B	502	-	-	6/10/10/10	-
3	PG4	G	502	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	502	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	E	502	PG4	O2-C3-C4-O3
3	C	502	PG4	O1-C1-C2-O2
3	H	502	PG4	O4-C7-C8-O5
3	B	502	PG4	O2-C3-C4-O3
3	C	502	PG4	O2-C3-C4-O3
3	A	502	PG4	O4-C7-C8-O5
3	B	502	PG4	O4-C7-C8-O5
3	D	502	PG4	O1-C1-C2-O2
3	G	502	PG4	O4-C7-C8-O5
3	H	502	PG4	O2-C3-C4-O3
3	A	502	PG4	O2-C3-C4-O3
3	G	502	PG4	O1-C1-C2-O2
3	H	502	PG4	O1-C1-C2-O2
3	E	502	PG4	C3-C4-O3-C5
3	E	502	PG4	O3-C5-C6-O4
3	C	502	PG4	C1-C2-O2-C3
3	F	502	PG4	C1-C2-O2-C3
3	B	502	PG4	C5-C6-O4-C7
3	G	502	PG4	C8-C7-O4-C6
3	C	502	PG4	C4-C3-O2-C2
3	G	502	PG4	C4-C3-O2-C2
3	E	502	PG4	C8-C7-O4-C6
3	H	502	PG4	C1-C2-O2-C3
3	C	502	PG4	O4-C7-C8-O5
3	A	502	PG4	C4-C3-O2-C2
3	A	502	PG4	O3-C5-C6-O4
3	B	502	PG4	C8-C7-O4-C6
3	A	502	PG4	C5-C6-O4-C7
3	D	502	PG4	O2-C3-C4-O3
3	A	502	PG4	C6-C5-O3-C4
3	A	502	PG4	C8-C7-O4-C6
3	H	502	PG4	C3-C4-O3-C5
3	G	502	PG4	O2-C3-C4-O3
3	H	502	PG4	O3-C5-C6-O4
3	A	502	PG4	C1-C2-O2-C3
3	H	502	PG4	C8-C7-O4-C6
3	E	502	PG4	O1-C1-C2-O2
3	D	502	PG4	O3-C5-C6-O4
3	D	502	PG4	C3-C4-O3-C5
3	G	502	PG4	O3-C5-C6-O4
3	B	502	PG4	C4-C3-O2-C2
3	F	502	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	B	502	PG4	O3-C5-C6-O4

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	PG4	1	0
3	F	502	PG4	1	0
3	D	502	PG4	2	0
3	A	502	PG4	1	0
3	H	502	PG4	2	0
3	B	502	PG4	2	0
3	G	502	PG4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	401/410 (97%)	0.03	13 (3%)	47	46	19, 29, 50, 68	0
1	B	397/410 (96%)	0.51	38 (9%)	8	7	27, 38, 59, 84	0
1	C	396/410 (96%)	0.18	30 (7%)	13	13	18, 29, 55, 77	0
1	D	401/410 (97%)	0.24	32 (7%)	12	11	20, 30, 64, 80	0
1	E	400/410 (97%)	0.06	14 (3%)	44	43	20, 29, 52, 70	0
1	F	401/410 (97%)	0.78	56 (13%)	2	2	28, 41, 60, 71	0
1	G	397/410 (96%)	0.65	47 (11%)	4	4	25, 41, 69, 88	0
1	H	383/410 (93%)	0.69	51 (13%)	3	2	26, 41, 70, 89	0
All	All	3176/3280 (96%)	0.39	281 (8%)	10	9	18, 35, 63, 89	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	46	GLY	9.5
1	G	53	PHE	7.3
1	F	102	PRO	6.8
1	H	112	ILE	6.7
1	C	97	ILE	6.4
1	G	47	ILE	5.9
1	F	262	LEU	5.9
1	F	101	GLU	5.8
1	D	89	ARG	5.6
1	H	59	THR	5.3
1	H	114	LYS	5.2
1	G	114	LYS	5.2
1	D	93	GLY	5.0
1	F	300	PRO	5.0
1	G	43	LEU	4.9
1	B	85	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	97	ILE	4.7
1	G	55	GLN	4.5
1	H	67	TYR	4.5
1	G	42	CYS	4.4
1	D	88	ILE	4.4
1	A	90	PHE	4.4
1	B	257	LEU	4.3
1	F	322	PHE	4.3
1	G	60	VAL	4.3
1	F	153	VAL	4.2
1	B	104	GLN	4.2
1	G	44	SER	4.2
1	F	186	CYS	4.2
1	B	182	TYR	4.2
1	F	386	VAL	4.1
1	F	257	LEU	4.1
1	D	97	ILE	4.1
1	B	7	PRO	4.0
1	G	102	PRO	4.0
1	H	298	LEU	4.0
1	F	100	PRO	4.0
1	D	6	HIS	4.0
1	H	58	LYS	3.9
1	C	95	PHE	3.9
1	F	263	ARG	3.9
1	D	101	GLU	3.9
1	F	24	VAL	3.9
1	G	113	LYS	3.9
1	B	135	GLY	3.9
1	H	89	ARG	3.8
1	G	6	HIS	3.7
1	G	291	PHE	3.7
1	H	155	CYS	3.7
1	B	258	ARG	3.6
1	H	60	VAL	3.6
1	F	6	HIS	3.6
1	E	6	HIS	3.5
1	F	98	ALA	3.5
1	D	86	THR	3.5
1	G	155	CYS	3.5
1	F	348	LEU	3.5
1	B	261	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	112	ILE	3.5
1	F	182	TYR	3.4
1	B	188	GLY	3.4
1	F	340	ILE	3.4
1	G	112	ILE	3.4
1	C	6	HIS	3.4
1	G	182	TYR	3.4
1	C	192	ALA	3.4
1	H	43	LEU	3.4
1	H	57	TYR	3.4
1	F	308	ARG	3.3
1	F	187	TYR	3.3
1	H	348	LEU	3.3
1	F	255	ASP	3.3
1	H	6	HIS	3.3
1	F	181	SER	3.3
1	C	101	GLU	3.3
1	H	186	CYS	3.3
1	H	62	GLU	3.2
1	E	179	THR	3.2
1	H	103	ASP	3.2
1	D	95	PHE	3.2
1	B	324	ARG	3.2
1	G	67	TYR	3.2
1	G	92	ASP	3.2
1	E	187	TYR	3.1
1	H	182	TYR	3.1
1	B	153	VAL	3.1
1	B	349	GLY	3.1
1	G	58	LYS	3.1
1	A	187	TYR	3.1
1	H	113	LYS	3.1
1	G	45	ASN	3.1
1	G	181	SER	3.1
1	B	340	ILE	3.1
1	A	179	THR	3.0
1	G	307	VAL	3.0
1	C	112	ILE	3.0
1	D	192	ALA	3.0
1	F	158	TYR	3.0
1	G	57	TYR	3.0
1	D	54	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	329	LEU	3.0
1	H	185	GLY	3.0
1	F	259	ARG	3.0
1	F	349	GLY	3.0
1	B	6	HIS	3.0
1	B	96	ASP	3.0
1	F	319	GLY	3.0
1	B	158	TYR	3.0
1	B	192	ALA	3.0
1	C	182	TYR	2.9
1	E	182	TYR	2.9
1	H	66	LYS	2.9
1	F	7	PRO	2.9
1	H	40	ALA	2.9
1	H	344	VAL	2.9
1	H	38	ALA	2.9
1	F	18	VAL	2.9
1	G	94	ASN	2.9
1	A	184	MET	2.9
1	E	190	PHE	2.9
1	G	144	LEU	2.9
1	C	191	PRO	2.9
1	A	190	PHE	2.9
1	B	103	ASP	2.9
1	C	52	GLY	2.9
1	F	22	LYS	2.9
1	H	63	LYS	2.9
1	B	252	TYR	2.8
1	G	188	GLY	2.8
1	H	350	LEU	2.8
1	H	41	HIS	2.8
1	B	263	ARG	2.8
1	G	103	ASP	2.8
1	F	261	GLY	2.8
1	F	195	MET	2.8
1	D	191	PRO	2.8
1	C	98	ALA	2.8
1	E	89	ARG	2.8
1	F	105	ALA	2.7
1	G	257	LEU	2.7
1	H	86	THR	2.7
1	H	88	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	322	PHE	2.7
1	C	189	ALA	2.7
1	H	158	TYR	2.7
1	F	99	ASP	2.7
1	H	96	ASP	2.7
1	C	179	THR	2.7
1	E	184	MET	2.7
1	F	144	LEU	2.7
1	F	184	MET	2.7
1	A	6	HIS	2.7
1	C	96	ASP	2.7
1	D	182	TYR	2.7
1	G	184	MET	2.6
1	D	179	THR	2.6
1	B	88	ILE	2.6
1	D	94	ASN	2.6
1	D	195	MET	2.6
1	G	158	TYR	2.6
1	H	299	VAL	2.6
1	E	7	PRO	2.6
1	H	191	PRO	2.6
1	B	259	ARG	2.6
1	D	155	CYS	2.6
1	B	255	ASP	2.6
1	F	344	VAL	2.6
1	B	145	GLU	2.6
1	C	102	PRO	2.6
1	H	156	SER	2.6
1	C	195	MET	2.6
1	D	181	SER	2.6
1	C	186	CYS	2.6
1	C	51	GLU	2.6
1	H	153	VAL	2.6
1	D	187	TYR	2.5
1	G	192	ALA	2.5
1	D	184	MET	2.5
1	D	188	GLY	2.5
1	F	190	PHE	2.5
1	F	155	CYS	2.5
1	F	164	ALA	2.5
1	F	86	THR	2.5
1	C	373	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	373	ILE	2.5
1	C	153	VAL	2.5
1	E	153	VAL	2.5
1	H	56	VAL	2.5
1	C	187	TYR	2.5
1	G	262	LEU	2.5
1	C	155	CYS	2.5
1	E	192	ALA	2.4
1	F	180	HIS	2.4
1	H	324	ARG	2.4
1	C	190	PHE	2.4
1	A	191	PRO	2.4
1	D	96	ASP	2.4
1	H	181	SER	2.4
1	C	100	PRO	2.4
1	F	191	PRO	2.4
1	F	291	PHE	2.4
1	E	193	ILE	2.4
1	F	151	ILE	2.4
1	E	191	PRO	2.4
1	G	52	GLY	2.4
1	A	192	ALA	2.4
1	A	182	TYR	2.4
1	H	187	TYR	2.4
1	H	291	PHE	2.4
1	G	154	THR	2.4
1	B	339	LYS	2.4
1	B	191	PRO	2.4
1	F	373	ILE	2.4
1	G	286	PRO	2.3
1	H	255	ASP	2.3
1	C	259	ARG	2.3
1	D	153	VAL	2.3
1	F	145	GLU	2.3
1	B	144	LEU	2.3
1	H	179	THR	2.3
1	D	186	CYS	2.3
1	D	259	ARG	2.3
1	B	291	PHE	2.3
1	D	193	ILE	2.3
1	G	186	CYS	2.3
1	F	299	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	193	ILE	2.3
1	G	7	PRO	2.3
1	B	155	CYS	2.3
1	C	184	MET	2.2
1	A	181	SER	2.2
1	C	151	ILE	2.2
1	B	107	LEU	2.2
1	B	160	ALA	2.2
1	F	108	ARG	2.2
1	G	98	ALA	2.2
1	F	307	VAL	2.2
1	H	69	VAL	2.2
1	F	97	ILE	2.2
1	E	181	SER	2.2
1	C	193	ILE	2.2
1	H	259	ARG	2.2
1	G	231	SER	2.2
1	G	187	TYR	2.2
1	A	153	VAL	2.2
1	H	285	VAL	2.2
1	H	262	LEU	2.2
1	H	351	ALA	2.2
1	H	190	PHE	2.2
1	H	399	LEU	2.1
1	B	181	SER	2.1
1	E	186	CYS	2.1
1	G	179	THR	2.1
1	F	104	GLN	2.1
1	G	104	GLN	2.1
1	H	95	PHE	2.1
1	B	154	THR	2.1
1	G	59	THR	2.1
1	B	183	ASN	2.1
1	H	242	PHE	2.1
1	D	189	ALA	2.1
1	F	409	ILE	2.1
1	C	180	HIS	2.1
1	F	103	ASP	2.1
1	A	55	GLN	2.1
1	B	157	GLY	2.1
1	B	86	THR	2.1
1	G	54	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	56	VAL	2.1
1	G	153	VAL	2.1
1	D	180	HIS	2.1
1	D	151	ILE	2.1
1	C	194	LYS	2.1
1	D	53	PHE	2.0
1	F	179	THR	2.0
1	F	385	THR	2.0
1	C	54	VAL	2.0
1	D	98	ALA	2.0
1	F	189	ALA	2.0
1	G	343	HIS	2.0
1	H	184	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PG4	F	502	13/13	0.75	0.20	56,60,63,64	0
3	PG4	B	502	13/13	0.79	0.17	54,62,67,68	0
3	PG4	G	502	13/13	0.84	0.19	51,56,63,65	0
3	PG4	H	502	13/13	0.84	0.16	49,55,57,58	0
3	PG4	E	502	13/13	0.88	0.14	45,49,54,55	0
3	PG4	D	502	13/13	0.90	0.15	51,56,59,60	0
3	PG4	C	502	13/13	0.91	0.13	45,49,59,60	0
2	NA	H	501	1/1	0.93	0.12	32,32,32,32	0
3	PG4	A	502	13/13	0.93	0.14	43,45,49,49	0
2	NA	G	501	1/1	0.93	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	B	501	1/1	0.95	0.16	29,29,29,29	0
2	NA	F	501	1/1	0.95	0.19	35,35,35,35	0
2	NA	D	501	1/1	0.98	0.17	25,25,25,25	0
2	NA	E	501	1/1	0.99	0.14	21,21,21,21	0
2	NA	A	501	1/1	0.99	0.09	19,19,19,19	0
2	NA	C	501	1/1	1.00	0.16	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.