



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:26 PM UTC

PDB ID : 3L7Z / pdb_00003l7z
Title : Crystal structure of the S. solfataricus archaeal exosome
Authors : Lu, C.; Ding, F.; Ke, A.
Deposited on : 2009-12-29
Resolution : 2.41 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

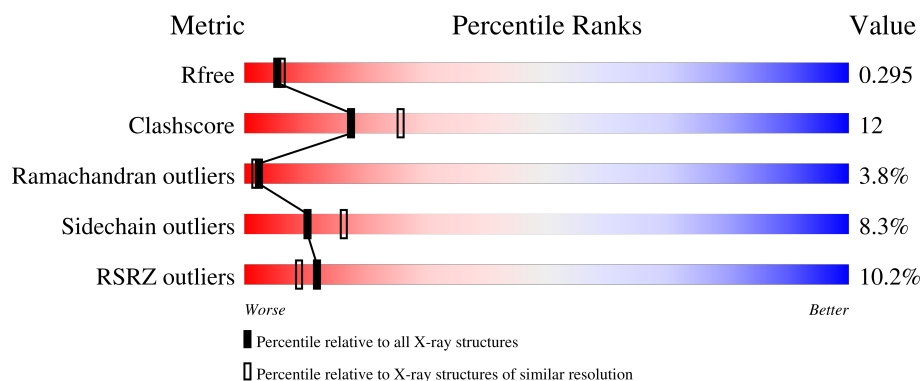
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 $\leq 5\%$. 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	271	5% 74% 15% 7%
1	D	271	13% 79% 15% • •
1	G	271	9% 72% 18% 8% •
2	B	245	2% 74% 17% • 5%
2	E	245	6% 74% 18% • •

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Mol	Chain	Length	Quality of chain
2	H	245	3% 73% 20% • • •
3	C	249	12% 57% 25% 6% • 11%
3	F	249	9% 57% 19% 9% 14%
3	I	249	27% 49% 24% 9% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16393 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 Probable exosome complex exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1926	1229	314	378	5			
1	D	261	Total	C	N	O	S	0	0	0
			1974	1260	321	388	5			
1	G	270	Total	C	N	O	S	0	0	0
			2082	1328	338	411	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	THR	GLU	engineered mutation	UNP Q9UXC0
A	?	-	HIS	deletion	UNP Q9UXC0
A	?	-	SER	deletion	UNP Q9UXC0
A	?	-	ASN	deletion	UNP Q9UXC0
A	?	-	GLY	deletion	UNP Q9UXC0
D	96	THR	GLU	engineered mutation	UNP Q9UXC0
D	?	-	HIS	deletion	UNP Q9UXC0
D	?	-	SER	deletion	UNP Q9UXC0
D	?	-	ASN	deletion	UNP Q9UXC0
D	?	-	GLY	deletion	UNP Q9UXC0
G	96	THR	GLU	engineered mutation	UNP Q9UXC0
G	?	-	HIS	deletion	UNP Q9UXC0
G	?	-	SER	deletion	UNP Q9UXC0
G	?	-	ASN	deletion	UNP Q9UXC0
G	?	-	GLY	deletion	UNP Q9UXC0

- Molecule 2 is a protein called Probable exosome complex exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1774	1122	309	334	9			

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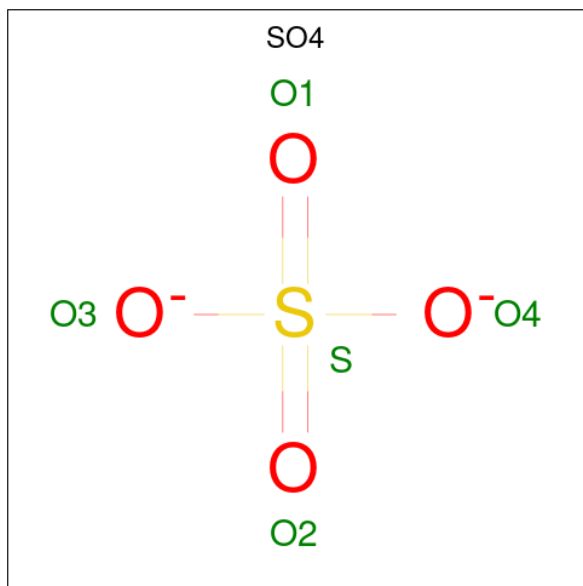
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	237	Total	C	N	O	S	0	0	0
			1832	1157	319	346	10			
2	H	234	Total	C	N	O	S	0	0	0
			1810	1142	316	342	10			

- Molecule 3 is a protein called Probable exosome complex RNA-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	222	Total	C	N	O	S	0	0	0
			1697	1096	279	319	3			
3	F	215	Total	C	N	O	S	0	0	0
			1705	1104	281	316	4			
3	I	206	Total	C	N	O	S	0	0	0
			1578	1029	250	296	3			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

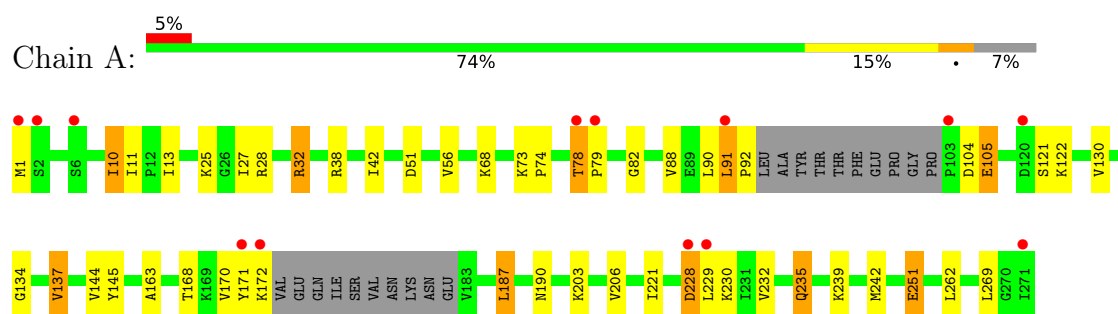


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

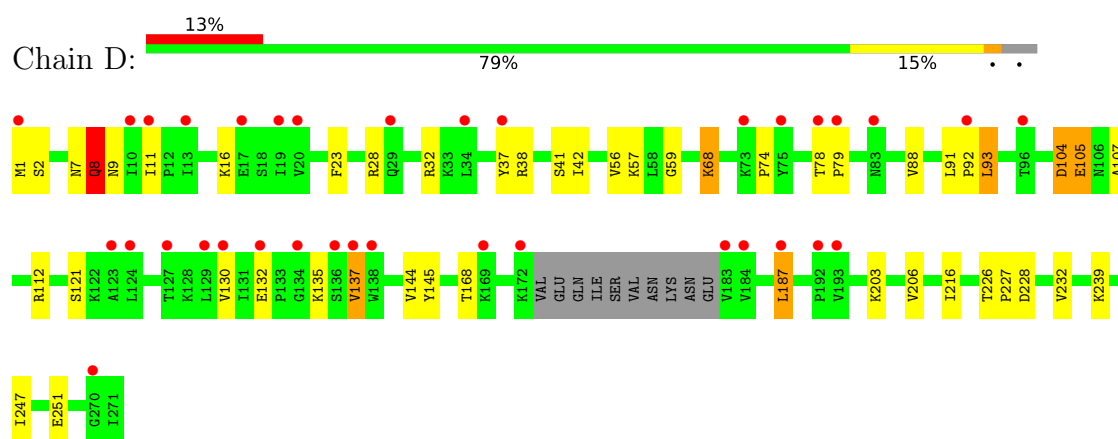
3 Residue-property plots [i](#)

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.

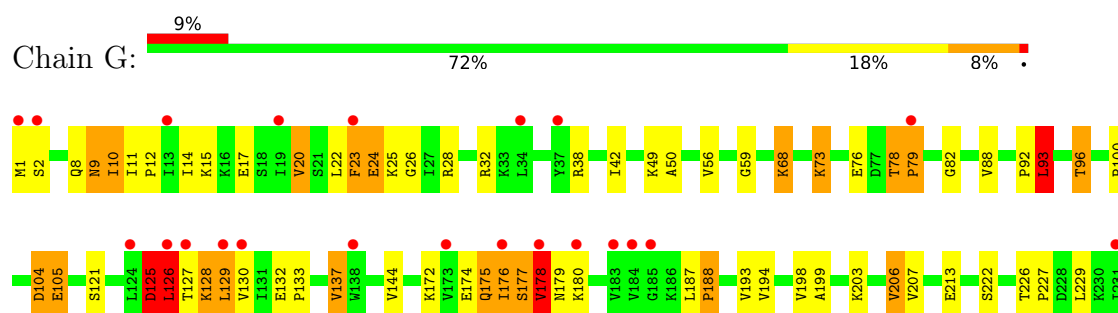
- Molecule 1: Probable exosome complex exonuclease 2



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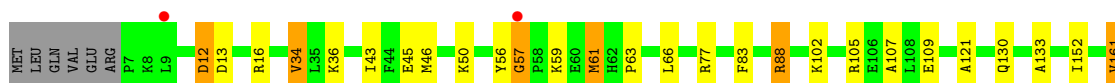
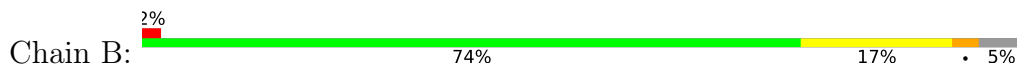


- Molecule 1: Probable exosome complex exonuclease 2

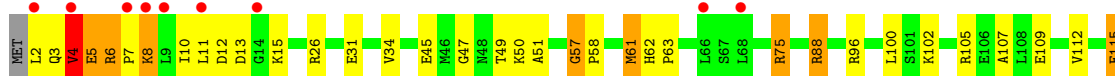
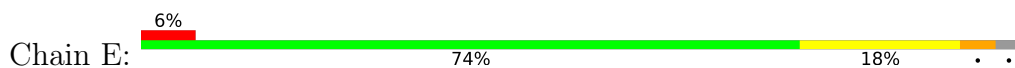




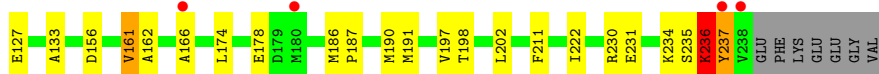
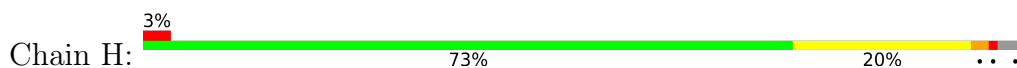
- Molecule 2: Probable exosome complex exonuclease 1



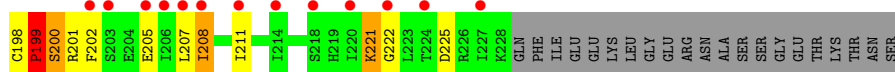
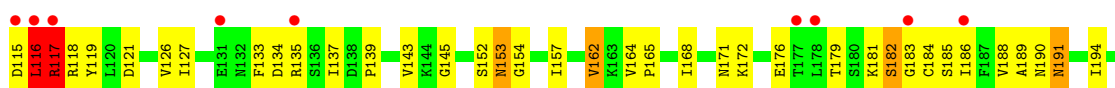
- Molecule 2: Probable exosome complex exonuclease 1



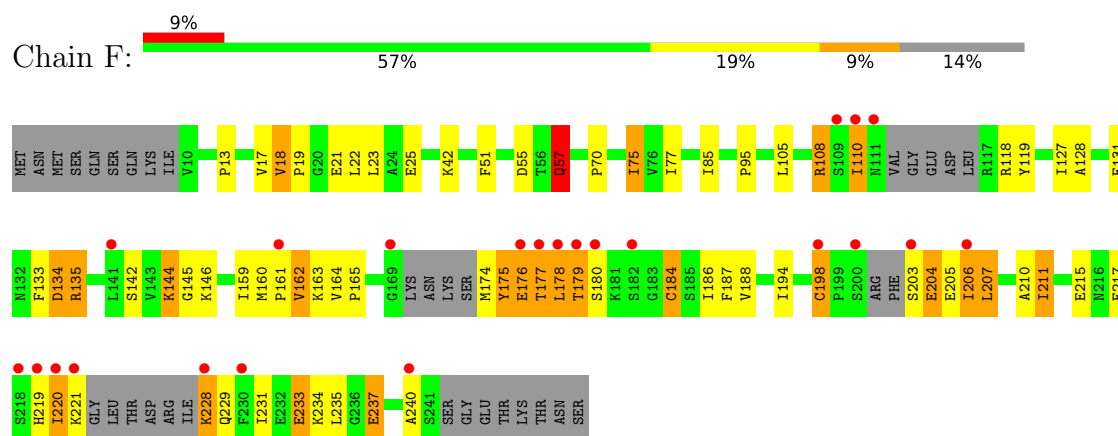
- Molecule 2: Probable exosome complex exonuclease 1



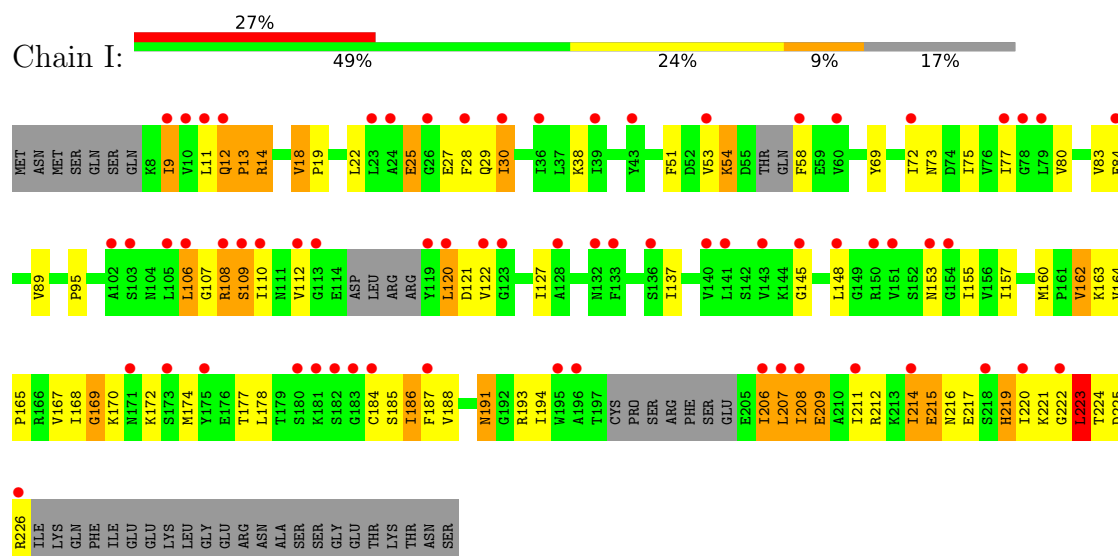
- Molecule 3: Probable exosome complex RNA-binding protein 1



• Molecule 3: Probable exosome complex RNA-binding protein 1



• Molecule 3: Probable exosome complex RNA-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.12Å 145.48Å 97.25Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.41 20.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.41) 92.2 (20.00-2.41)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.263 , 0.289 0.263 , 0.295	Depositor DCC
R_{free} test set	7505 reflections (9.34%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16393	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.47	0/1952	0.78	0/2646
1	D	0.45	0/2004	0.83	2/2724 (0.1%)
1	G	0.50	0/2114	0.87	1/2873 (0.0%)
2	B	0.48	0/1802	0.82	0/2439
2	E	0.49	0/1859	0.86	1/2512 (0.0%)
2	H	0.47	0/1838	0.84	1/2484 (0.0%)
3	C	0.55	0/1732	0.92	7/2362 (0.3%)
3	F	0.51	0/1737	0.84	2/2351 (0.1%)
3	I	0.56	0/1609	0.92	7/2188 (0.3%)
All	All	0.50	0/16647	0.85	21/22579 (0.1%)

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	G	0	2
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	116	LEU	N-CA-C	-8.97	101.58	111.36
3	I	208	ILE	N-CA-C	8.55	124.41	112.35
3	F	175	TYR	N-CA-C	8.12	123.66	113.43
3	C	181	LYS	N-CA-C	-8.07	101.46	112.03
2	E	236	LYS	N-CA-C	-6.72	96.49	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	208	ILE	CA-C-N	6.27	132.98	121.70
3	I	208	ILE	C-N-CA	6.27	132.98	121.70
3	C	112	VAL	N-CA-C	6.11	112.75	106.21
2	H	11	LEU	N-CA-C	-5.99	102.20	110.35
1	G	126	LEU	N-CA-C	5.94	123.44	110.80
3	I	169	GLY	N-CA-C	-5.71	105.49	112.68
3	I	69	TYR	CA-C-N	5.49	125.76	119.83
3	I	69	TYR	C-N-CA	5.49	125.76	119.83
3	F	145	GLY	N-CA-C	5.29	117.15	110.38
3	C	69	TYR	CA-C-N	5.27	125.52	119.83
3	C	69	TYR	C-N-CA	5.27	125.52	119.83
1	D	132	GLU	CA-C-N	5.13	125.42	119.93
1	D	132	GLU	C-N-CA	5.13	125.42	119.93
3	I	153	ASN	N-CA-C	5.13	115.01	108.24
3	C	199	PRO	CA-C-N	5.02	130.74	121.70
3	C	199	PRO	C-N-CA	5.02	130.74	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	125	ASP	Peptide
1	G	76	GLU	Peptide
2	H	11	LEU	Peptide

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	1926	0	1997	32	0
1	D	1974	0	2008	29	0
1	G	2082	0	2151	68	0
2	B	1774	0	1801	37	0
2	E	1832	0	1882	38	0
2	H	1810	0	1850	52	0
3	C	1697	0	1667	56	0
3	F	1705	0	1733	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1578	0	1555	78	0
4	B	5	0	0	0	0
4	E	5	0	0	0	0
4	H	5	0	0	0	0
All	All	16393	0	16644	408	0

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 12.

All (408) 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)
3:I:221:LYS:HB3	3:I:222:GLY:HA2	1.21	1.18
3:I:224:THR:HB	3:I:225:ASP:HB3	1.25	1.18
3:C:221:LYS:HG3	3:C:222:GLY:HA2	1.28	1.14
2:H:236:LYS:O	2:H:237:TYR:CD2	2.02	1.12
3:I:208:ILE:N	3:I:209:GLU:HB3	1.67	1.10
1:G:125:ASP:HB3	1:G:127:THR:HA	1.34	1.09
3:I:224:THR:HB	3:I:225:ASP:CB	1.83	1.08
1:G:127:THR:CB	1:G:128:LYS:HB2	1.86	1.05
3:I:174:MET:HE2	3:I:214:ILE:HD12	1.39	1.03
2:H:237:TYR:HD2	3:I:219:HIS:CD2	1.76	1.02
2:H:237:TYR:CD2	3:I:219:HIS:NE2	2.28	1.02
3:C:117:ARG:HD3	3:C:118:ARG:H	1.22	1.00
2:H:237:TYR:CD2	3:I:219:HIS:CD2	2.50	1.00
1:G:127:THR:HB	1:G:128:LYS:CB	1.92	0.99
3:F:134:ASP:CG	3:F:135:ARG:H	1.69	0.99
1:D:7:ASN:CA	1:D:8:GLN:HB2	1.92	0.98
3:I:224:THR:HB	3:I:225:ASP:CA	1.93	0.98
1:G:127:THR:HB	1:G:128:LYS:HB2	0.99	0.96
3:I:224:THR:CB	3:I:225:ASP:HB3	1.96	0.96
1:G:1:MET:N	2:H:77:ARG:HH12	1.65	0.94
1:A:235:GLN:HE22	2:B:201:GLN:HE21	1.16	0.93
3:I:221:LYS:CB	3:I:222:GLY:HA2	2.01	0.90
3:F:178:LEU:O	3:F:180:SER:N	2.05	0.88
3:I:221:LYS:HB3	3:I:222:GLY:CA	2.06	0.85
3:I:53:VAL:HG22	3:I:54:LYS:H	1.40	0.84
1:G:174:GLU:O	1:G:175:GLN:HB2	1.76	0.84
1:G:1:MET:H1	2:H:77:ARG:HH12	1.22	0.83
2:B:88:ARG:HH11	2:B:88:ARG:CG	1.92	0.82
2:B:59:LYS:NZ	1:G:96:THR:HG22	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:LEU:O	1:G:129:LEU:HG	1.78	0.82
1:G:125:ASP:CB	1:G:127:THR:HA	2.08	0.82
3:I:18:VAL:HG22	3:I:19:PRO:HD2	1.63	0.81
2:E:45:GLU:HG2	2:E:50:LYS:HG3	1.61	0.80
3:C:221:LYS:CG	3:C:222:GLY:HA2	2.12	0.79
3:F:75:ILE:HG12	3:F:187:PHE:HZ	1.48	0.79
3:I:208:ILE:N	3:I:209:GLU:CB	2.46	0.79
1:G:73:LYS:HE2	1:G:73:LYS:H	1.48	0.78
3:C:18:VAL:HG22	3:C:19:PRO:HD2	1.64	0.78
3:I:224:THR:HB	3:I:225:ASP:HA	1.64	0.77
2:E:88:ARG:HH11	2:E:88:ARG:HG2	1.49	0.77
3:I:222:GLY:O	3:I:223:LEU:HB3	1.86	0.75
3:C:198:CYS:SG	3:C:205:GLU:HB3	2.27	0.75
1:G:127:THR:OG1	1:G:188:PRO:CB	2.35	0.74
3:I:108:ARG:O	3:I:109:SER:HB2	1.88	0.74
3:C:85:ILE:HG12	3:I:137:ILE:HG22	1.67	0.74
3:F:18:VAL:HG22	3:F:19:PRO:HD2	1.69	0.74
1:D:130:VAL:HA	1:D:137:VAL:HG23	1.68	0.74
3:F:220:ILE:HG22	3:F:221:LYS:H	1.52	0.73
3:F:75:ILE:HD11	3:F:127:ILE:HG22	1.71	0.73
3:C:75:ILE:H	3:C:190:ASN:HD22	1.36	0.72
3:F:134:ASP:CG	3:F:135:ARG:N	2.40	0.72
3:I:72:ILE:O	3:I:73:ASN:HB2	1.88	0.72
3:C:221:LYS:HG3	3:C:222:GLY:CA	2.16	0.72
1:A:1:MET:HG2	2:B:77:ARG:HG3	1.71	0.71
1:G:1:MET:N	2:H:77:ARG:NH1	2.39	0.71
2:B:59:LYS:HZ3	1:G:96:THR:HG22	1.52	0.71
3:F:203:SER:O	3:F:204:GLU:HB2	1.90	0.71
3:C:205:GLU:O	3:C:205:GLU:HG2	1.89	0.70
1:G:176:ILE:O	1:G:177:SER:O	2.08	0.70
3:C:184:CYS:CB	3:C:185:SER:HA	2.20	0.70
2:H:11:LEU:HB3	2:H:12:ASP:HB2	1.74	0.70
2:E:88:ARG:HH11	2:E:88:ARG:CG	2.04	0.70
3:I:53:VAL:HA	3:I:58:PHE:HA	1.72	0.70
1:A:228:ASP:O	1:A:229:LEU:HB2	1.90	0.70
1:G:127:THR:OG1	1:G:188:PRO:HB3	1.93	0.69
3:C:157:ILE:HD12	3:C:194:ILE:HD11	1.73	0.69
2:E:161:VAL:HG22	2:E:222:ILE:HG13	1.76	0.68
2:B:63:PRO:HG2	2:B:66:LEU:HD12	1.75	0.68
3:F:204:GLU:HG3	3:F:205:GLU:H	1.58	0.67
3:I:188:VAL:HA	3:I:194:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:208:ILE:H	3:I:209:GLU:HB3	1.53	0.67
3:I:216:ASN:O	3:I:219:HIS:CE1	2.48	0.67
1:D:121:SER:HA	1:D:232:VAL:HG21	1.77	0.67
2:H:161:VAL:HG22	2:H:222:ILE:HG13	1.75	0.67
3:I:207:LEU:C	3:I:209:GLU:HB3	2.20	0.67
3:F:159:ILE:HG21	3:F:211:ILE:HG22	1.75	0.66
1:A:91:LEU:N	1:A:92:PRO:HD2	2.10	0.66
1:A:91:LEU:HD11	1:A:145:TYR:HD2	1.60	0.66
3:C:152:SER:O	3:C:153:ASN:HB3	1.94	0.66
2:E:75:ARG:HH11	2:E:75:ARG:HG2	1.59	0.66
1:G:127:THR:OG1	1:G:188:PRO:HB2	1.94	0.66
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.62	0.65
3:I:217:GLU:HA	3:I:219:HIS:HE1	1.60	0.65
2:H:11:LEU:CA	2:H:12:ASP:HB2	2.26	0.65
1:D:88:VAL:HG22	1:D:144:VAL:HB	1.79	0.64
3:C:199:PRO:HB2	3:C:200:SER:HA	1.79	0.64
2:H:75:ARG:HG2	2:H:75:ARG:HH11	1.62	0.64
2:H:236:LYS:O	2:H:237:TYR:CG	2.50	0.64
1:G:127:THR:H	1:G:128:LYS:HB3	1.62	0.64
1:D:104:ASP:O	1:D:105:GLU:HB2	1.98	0.63
3:C:117:ARG:CD	3:C:118:ARG:H	2.05	0.63
2:B:88:ARG:HH11	2:B:88:ARG:HG3	1.64	0.63
3:I:211:ILE:O	3:I:215:GLU:HB2	1.98	0.63
1:G:8:GLN:C	1:G:10:ILE:H	2.07	0.63
1:D:91:LEU:C	1:D:93:LEU:H	2.06	0.62
3:C:182:SER:HB2	3:C:183:GLY:HA3	1.81	0.62
3:C:75:ILE:H	3:C:190:ASN:ND2	1.97	0.62
1:G:92:PRO:O	1:G:93:LEU:HD12	1.98	0.62
1:G:121:SER:HA	1:G:232:VAL:HG21	1.80	0.62
3:I:217:GLU:HA	3:I:219:HIS:CE1	2.35	0.62
3:F:75:ILE:HG12	3:F:187:PHE:CZ	2.34	0.62
2:H:11:LEU:HA	2:H:12:ASP:HB2	1.80	0.62
2:B:105:ARG:O	2:B:109:GLU:HG2	2.00	0.61
3:I:53:VAL:HG22	3:I:54:LYS:N	2.13	0.61
3:I:208:ILE:H	3:I:209:GLU:CB	2.11	0.61
1:D:105:GLU:HG2	2:E:102:LYS:HD2	1.83	0.61
2:E:58:PRO:HB2	3:F:95:PRO:HB3	1.82	0.61
3:I:164:VAL:HB	3:I:165:PRO:HD3	1.82	0.60
1:D:7:ASN:CA	1:D:8:GLN:CB	2.70	0.60
2:B:186:MET:HE3	2:B:202:LEU:HD13	1.84	0.60
1:A:122:LYS:O	1:A:190:ASN:ND2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:VAL:O	2:E:4:VAL:HG13	2.02	0.59
3:C:199:PRO:N	3:C:200:SER:HB2	2.17	0.59
1:G:1:MET:H1	2:H:77:ARG:NH1	1.95	0.59
3:F:188:VAL:HA	3:F:194:ILE:HG22	1.83	0.59
2:H:186:MET:HE3	2:H:202:LEU:HD13	1.84	0.59
1:A:121:SER:HA	1:A:232:VAL:HG21	1.84	0.59
1:G:17:GLU:O	1:G:20:VAL:HG12	2.02	0.59
1:A:74:PRO:HB2	1:A:79:PRO:HA	1.85	0.59
1:G:1:MET:H2	2:H:77:ARG:HH12	1.48	0.59
3:F:144:LYS:O	3:F:144:LYS:HG2	2.02	0.59
3:I:157:ILE:HD12	3:I:194:ILE:HD11	1.84	0.59
2:E:6:ARG:HB3	2:E:7:PRO:HA	1.85	0.58
1:D:226:THR:HB	1:D:227:PRO:HD2	1.84	0.58
3:F:161:PRO:O	3:F:162:VAL:HB	2.03	0.58
2:H:123:ASP:HB3	2:H:125:PHE:CE1	2.38	0.58
3:I:224:THR:CB	3:I:225:ASP:CB	2.68	0.58
2:H:16:ARG:HD3	2:H:178:GLU:OE2	2.03	0.58
1:G:226:THR:HB	1:G:227:PRO:HD2	1.86	0.57
1:A:28:ARG:NH1	1:A:206:VAL:HG13	2.20	0.57
1:A:91:LEU:HD11	1:A:145:TYR:CD2	2.39	0.57
3:F:178:LEU:C	3:F:180:SER:H	2.09	0.57
3:C:117:ARG:HD3	3:C:118:ARG:N	2.07	0.57
2:E:4:VAL:O	2:E:5:GLU:HB2	2.05	0.57
2:E:105:ARG:O	2:E:109:GLU:HG2	2.05	0.57
1:G:23:PHE:O	1:G:25:LYS:N	2.38	0.57
2:H:63:PRO:HG2	2:H:66:LEU:HD12	1.85	0.57
3:F:176:GLU:O	3:F:178:LEU:N	2.38	0.57
1:G:172:LYS:HE3	1:G:174:GLU:HB3	1.87	0.57
3:C:62:PRO:HB2	3:C:162:VAL:HG21	1.88	0.56
1:D:104:ASP:O	1:D:105:GLU:CB	2.54	0.56
2:H:186:MET:HE1	2:H:211:PHE:HD1	1.70	0.56
2:B:16:ARG:HD3	2:B:178:GLU:OE2	2.05	0.56
2:B:61:MET:HG2	2:B:121:ALA:HB2	1.88	0.56
2:B:234:LYS:C	2:B:236:LYS:H	2.12	0.56
1:A:130:VAL:HA	1:A:137:VAL:HG23	1.87	0.56
1:G:82:GLY:HA3	1:G:129:LEU:HB3	1.86	0.56
2:E:107:ALA:HB1	2:E:198:THR:HG23	1.88	0.56
3:F:77:ILE:HG22	3:F:127:ILE:HG23	1.86	0.56
3:C:205:GLU:C	3:C:207:LEU:H	2.14	0.55
1:D:1:MET:HG3	1:D:2:SER:H	1.72	0.55
1:A:42:ILE:HG12	1:A:56:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:118:ARG:H	3:F:118:ARG:CD	2.20	0.55
2:H:11:LEU:CB	2:H:12:ASP:HB2	2.35	0.55
3:C:188:VAL:HA	3:C:194:ILE:HG22	1.89	0.55
2:H:61:MET:HG2	2:H:121:ALA:HB2	1.89	0.55
1:D:91:LEU:HD11	1:D:145:TYR:HD2	1.72	0.54
3:F:194:ILE:HD11	3:F:211:ILE:HD13	1.88	0.54
3:F:159:ILE:HG21	3:F:211:ILE:CG2	2.37	0.54
1:G:82:GLY:HA2	1:G:137:VAL:HG13	1.89	0.54
2:E:26:ARG:HD2	2:E:47:GLY:HA3	1.88	0.54
1:A:88:VAL:HG22	1:A:144:VAL:HB	1.90	0.54
3:C:176:GLU:HA	3:C:179:THR:HB	1.88	0.54
1:G:28:ARG:HD3	1:G:213:GLU:OE2	2.08	0.54
1:G:127:THR:CB	1:G:128:LYS:CB	2.67	0.54
3:C:184:CYS:CB	3:C:185:SER:CA	2.86	0.54
2:E:3:GLN:O	2:E:4:VAL:HB	2.08	0.54
2:E:62:HIS:CB	2:E:63:PRO:HD3	2.38	0.53
1:A:51:ASP:HB3	1:A:168:THR:HG23	1.90	0.53
2:B:238:VAL:HA	3:C:16:ILE:HG13	1.91	0.53
1:D:68:LYS:HG2	2:H:88:ARG:HB2	1.91	0.53
3:F:118:ARG:H	3:F:118:ARG:HD2	1.73	0.53
3:F:210:ALA:HB2	3:F:235:LEU:HD21	1.91	0.53
3:I:162:VAL:HG12	3:I:163:LYS:HD2	1.91	0.53
1:G:125:ASP:CG	1:G:127:THR:HG23	2.34	0.53
2:B:161:VAL:HG22	2:B:222:ILE:HG13	1.91	0.52
3:F:17:VAL:HG21	3:F:23:LEU:HD21	1.90	0.52
2:B:209:ASP:O	2:B:213:GLN:HG3	2.09	0.52
3:C:199:PRO:HB2	3:C:200:SER:CA	2.39	0.52
2:H:237:TYR:C	3:I:220:ILE:HD11	2.34	0.52
2:H:45:GLU:HG2	2:H:50:LYS:HG3	1.92	0.52
1:A:91:LEU:N	1:A:92:PRO:CD	2.72	0.52
2:B:190:MET:HG2	2:B:222:ILE:HD13	1.92	0.52
2:H:58:PRO:HB2	3:I:95:PRO:HB3	1.92	0.52
3:I:53:VAL:CG2	3:I:54:LYS:H	2.17	0.52
3:I:225:ASP:O	3:I:226:ARG:HB2	2.10	0.52
3:I:174:MET:O	3:I:177:THR:HG22	2.09	0.52
1:A:163:ALA:HA	1:A:269:LEU:HD21	1.91	0.51
3:F:220:ILE:HG22	3:F:221:LYS:N	2.23	0.51
1:G:125:ASP:HB3	1:G:126:LEU:CA	2.40	0.51
2:B:59:LYS:HZ1	1:G:96:THR:HG22	1.74	0.51
3:C:164:VAL:HG11	3:C:190:ASN:HA	1.92	0.51
1:D:91:LEU:HD13	2:H:127:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:217:GLU:C	3:F:219:HIS:H	2.18	0.51
1:G:82:GLY:HA3	1:G:129:LEU:HD12	1.93	0.51
3:I:212:ARG:CA	3:I:215:GLU:HB2	2.40	0.51
2:E:61:MET:HG2	2:E:121:ALA:HB2	1.93	0.51
3:I:174:MET:O	3:I:178:LEU:HD12	2.10	0.51
3:I:221:LYS:CB	3:I:222:GLY:CA	2.78	0.51
2:E:231:GLU:HA	2:E:234:LYS:HB2	1.92	0.51
2:B:45:GLU:HG2	2:B:50:LYS:HG3	1.92	0.51
1:D:41:SER:HB3	1:D:57:LYS:HB2	1.92	0.51
3:F:177:THR:HB	3:F:179:THR:OG1	2.10	0.50
3:C:14:ARG:O	3:C:14:ARG:HG2	2.10	0.50
1:A:235:GLN:NE2	2:B:201:GLN:HE21	1.96	0.50
2:E:190:MET:HG2	2:E:222:ILE:HD13	1.94	0.50
1:G:92:PRO:HG3	1:G:100:PRO:HB3	1.94	0.50
3:C:179:THR:HG23	3:C:184:CYS:CB	2.42	0.50
1:D:74:PRO:HB2	1:D:79:PRO:HA	1.94	0.50
3:F:184:CYS:HB2	3:F:186:ILE:HD11	1.94	0.50
1:G:49:LYS:O	1:G:68:LYS:HE3	2.12	0.50
3:C:157:ILE:HG21	3:C:211:ILE:HG21	1.95	0.49
1:D:104:ASP:H	1:D:107:ALA:HB3	1.76	0.49
2:E:50:LYS:HD3	2:E:130:GLN:CD	2.36	0.49
2:E:88:ARG:CG	2:E:88:ARG:NH1	2.71	0.49
2:H:237:TYR:HB2	3:I:220:ILE:HD13	1.94	0.49
2:B:56:TYR:CD2	1:G:96:THR:HG23	2.47	0.49
2:B:164:GLY:HA3	2:B:174:LEU:HD21	1.95	0.49
3:F:108:ARG:NH1	3:F:110:ILE:H	2.10	0.49
1:G:194:VAL:HB	1:G:261:LEU:HD23	1.94	0.49
1:G:24:GLU:C	1:G:26:GLY:N	2.70	0.49
2:H:34:VAL:HG21	2:H:43:ILE:HG13	1.94	0.49
3:I:145:GLY:H	3:I:148:LEU:HD12	1.77	0.49
3:I:224:THR:CB	3:I:225:ASP:HA	2.35	0.49
1:D:91:LEU:HD11	1:D:145:TYR:CD2	2.47	0.49
2:E:4:VAL:O	2:E:5:GLU:CB	2.61	0.49
3:F:204:GLU:HG3	3:F:205:GLU:N	2.25	0.49
3:I:80:VAL:HG21	3:I:120:LEU:HD13	1.94	0.49
3:C:186:ILE:HG13	3:C:194:ILE:HD13	1.94	0.49
3:F:75:ILE:HD12	3:F:128:ALA:O	2.13	0.49
3:I:14:ARG:HB3	3:I:51:PHE:O	2.13	0.49
2:H:190:MET:HB3	2:H:197:VAL:HA	1.95	0.49
1:G:12:PRO:C	1:G:14:ILE:H	2.21	0.48
3:C:154:GLY:O	1:G:14:ILE:HD11	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:236:LYS:C	2:H:237:TYR:CD2	2.87	0.48
3:C:157:ILE:HB	3:C:194:ILE:HG13	1.96	0.48
2:E:237:TYR:O	2:E:237:TYR:CG	2.66	0.48
3:F:217:GLU:C	3:F:219:HIS:N	2.71	0.48
1:G:38:ARG:HD2	1:G:59:GLY:HA3	1.94	0.48
3:C:106:LEU:HD11	3:C:119:TYR:CZ	2.49	0.48
3:C:201:ARG:HA	3:C:202:PHE:HA	1.67	0.48
3:C:205:GLU:C	3:C:207:LEU:N	2.71	0.48
1:G:8:GLN:C	1:G:10:ILE:N	2.68	0.48
2:E:31:GLU:HG3	2:E:34:VAL:HG13	1.95	0.47
3:I:168:ILE:C	3:I:174:MET:HB2	2.39	0.47
3:I:211:ILE:HA	3:I:214:ILE:HG22	1.95	0.47
2:E:8:LYS:HG2	2:E:11:LEU:HD23	1.95	0.47
3:I:208:ILE:HA	3:I:211:ILE:HG22	1.96	0.47
2:E:161:VAL:HG13	2:E:225:ILE:HD12	1.95	0.47
3:I:29:GLN:CA	3:I:30:ILE:HB	2.45	0.47
3:I:223:LEU:HG	3:I:224:THR:HG23	1.95	0.47
3:C:116:LEU:C	3:C:117:ARG:HG3	2.39	0.47
2:B:50:LYS:HB2	2:B:130:GLN:HB2	1.95	0.47
1:G:1:MET:H2	2:H:77:ARG:NH1	2.08	0.47
1:A:25:LYS:HE2	1:A:27:ILE:HG21	1.97	0.47
1:A:79:PRO:HB2	1:A:134:GLY:HA2	1.96	0.47
3:C:168:ILE:HG22	3:C:172:LYS:HA	1.97	0.47
1:D:38:ARG:HD2	1:D:59:GLY:HA3	1.97	0.47
3:F:142:SER:HB2	3:F:144:LYS:HD2	1.97	0.47
1:G:199:ALA:HB3	1:G:206:VAL:HG12	1.97	0.47
2:B:88:ARG:CG	2:B:88:ARG:NH1	2.63	0.46
3:C:7:GLN:O	3:C:8:LYS:HG3	2.15	0.46
2:B:234:LYS:C	2:B:236:LYS:N	2.74	0.46
1:G:12:PRO:HB2	1:G:15:LYS:HB2	1.97	0.46
1:G:121:SER:HB3	1:G:232:VAL:HG11	1.97	0.46
3:I:77:ILE:HD11	3:I:193:ARG:HB3	1.97	0.46
3:F:221:LYS:HD3	3:F:228:LYS:HE3	1.98	0.46
2:H:230:ARG:HG2	3:I:18:VAL:HG11	1.97	0.46
3:I:224:THR:CB	3:I:225:ASP:CA	2.74	0.46
1:A:32:ARG:CZ	1:A:38:ARG:HG3	2.46	0.46
2:E:51:ALA:HB3	2:E:138:VAL:HG12	1.98	0.46
3:I:184:CYS:O	3:I:186:ILE:N	2.49	0.46
3:C:205:GLU:O	3:C:205:GLU:CG	2.63	0.46
3:F:110:ILE:HG21	3:F:119:TYR:CE2	2.51	0.46
3:F:164:VAL:N	3:F:165:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:23:LEU:HD22	3:F:51:PHE:CD1	2.51	0.45
2:H:78:TYR:CE2	2:H:100:LEU:HD12	2.52	0.45
3:I:106:LEU:HB3	3:I:107:GLY:H	1.35	0.45
3:C:189:ALA:C	3:C:191:ASN:H	2.24	0.45
3:F:70:PRO:HB2	3:F:133:PHE:CD2	2.50	0.45
1:G:42:ILE:HG12	1:G:56:VAL:HG22	1.99	0.45
3:I:28:PHE:CD2	3:I:58:PHE:HE2	2.35	0.45
3:I:29:GLN:HA	3:I:30:ILE:HB	1.96	0.45
2:B:107:ALA:HB1	2:B:198:THR:HG23	1.97	0.45
2:B:186:MET:HE1	2:B:211:PHE:HD1	1.81	0.45
3:F:108:ARG:HH12	3:F:110:ILE:H	1.63	0.45
3:C:69:TYR:HA	3:C:70:PRO:HD3	1.79	0.45
3:C:105:LEU:HD23	3:C:143:VAL:HG21	1.98	0.45
1:G:32:ARG:CZ	1:G:38:ARG:HG3	2.47	0.45
2:H:237:TYR:O	3:I:220:ILE:HD11	2.17	0.45
3:I:77:ILE:HG22	3:I:127:ILE:HG12	1.98	0.45
3:C:92:ILE:O	3:C:191:ASN:ND2	2.44	0.45
1:G:132:GLU:HA	1:G:133:PRO:HD3	1.84	0.45
1:A:90:LEU:C	1:A:92:PRO:HD2	2.42	0.45
1:G:104:ASP:O	1:G:105:GLU:HB2	2.17	0.45
2:H:234:LYS:O	2:H:236:LYS:N	2.40	0.45
1:D:42:ILE:HG12	1:D:56:VAL:HG22	1.98	0.45
2:H:234:LYS:C	2:H:236:LYS:H	2.24	0.45
3:I:157:ILE:HB	3:I:194:ILE:HG13	1.99	0.45
3:I:219:HIS:ND1	3:I:219:HIS:N	2.64	0.45
3:F:131:GLU:HG3	3:F:142:SER:HB3	1.98	0.44
2:H:10:ILE:HD13	2:H:166:ALA:HB3	2.00	0.44
2:B:165:LYS:HE3	2:B:168:GLY:HA2	1.98	0.44
2:E:6:ARG:HB3	2:E:7:PRO:CA	2.47	0.44
2:E:11:LEU:HB3	2:E:12:ASP:H	1.65	0.44
1:G:222:SER:O	1:G:234:ILE:HA	2.17	0.44
3:C:77:ILE:HG22	3:C:127:ILE:HG12	1.99	0.44
1:D:32:ARG:CZ	1:D:38:ARG:HG3	2.48	0.44
1:G:82:GLY:HA2	1:G:137:VAL:CG1	2.48	0.44
2:H:156:ASP:HB3	2:H:191:MET:HB3	2.00	0.44
1:G:28:ARG:NH2	1:G:207:VAL:O	2.39	0.44
3:C:84:GLU:HG2	3:C:85:ILE:H	1.83	0.44
3:F:25:GLU:HG2	3:F:42:LYS:HG2	1.99	0.44
2:H:234:LYS:C	2:H:236:LYS:N	2.76	0.44
1:A:91:LEU:O	1:A:92:PRO:C	2.60	0.44
1:G:78:THR:HA	1:G:79:PRO:HD3	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:29:GLN:N	3:I:30:ILE:HB	2.33	0.44
1:A:251:GLU:OE2	2:B:212:ARG:NH2	2.51	0.44
3:F:219:HIS:HB2	3:F:220:ILE:HD12	2.00	0.44
1:A:168:THR:HB	1:A:187:LEU:CD2	2.48	0.43
2:E:2:LEU:O	2:E:3:GLN:C	2.61	0.43
1:G:127:THR:CA	1:G:128:LYS:CB	2.97	0.43
2:B:34:VAL:HG21	2:B:43:ILE:HG13	1.99	0.43
1:G:88:VAL:HG22	1:G:144:VAL:HB	1.99	0.43
3:I:224:THR:OG1	3:I:225:ASP:HB3	2.16	0.43
1:A:228:ASP:HB2	1:A:230:LYS:HB2	1.99	0.43
3:F:178:LEU:C	3:F:180:SER:N	2.75	0.43
1:A:105:GLU:HG2	2:B:102:LYS:HD2	2.01	0.43
2:E:112:VAL:HA	2:E:154:MET:HG2	1.99	0.43
3:F:198:CYS:HB3	3:F:205:GLU:HB3	1.99	0.43
2:E:197:VAL:HG11	2:E:200:PHE:HD1	1.84	0.43
2:H:29:LYS:HB3	2:H:45:GLU:HB2	1.99	0.43
2:H:62:HIS:CB	2:H:63:PRO:HD3	2.48	0.43
3:I:107:GLY:O	3:I:108:ARG:HB2	2.19	0.43
1:A:221:ILE:HB	1:A:242:MET:HE1	2.00	0.43
1:D:121:SER:CA	1:D:232:VAL:HG21	2.46	0.43
1:G:127:THR:H	1:G:128:LYS:CB	2.31	0.43
3:I:169:GLY:HA2	3:I:170:LYS:CG	2.48	0.43
2:E:100:LEU:HD21	2:E:136:ARG:CZ	2.49	0.43
3:F:186:ILE:HD12	3:F:207:LEU:HD11	2.01	0.43
3:I:121:ASP:CG	3:I:122:VAL:H	2.27	0.43
3:I:187:PHE:O	3:I:194:ILE:HA	2.19	0.43
1:D:91:LEU:C	1:D:93:LEU:N	2.75	0.43
1:G:28:ARG:CZ	1:G:206:VAL:HG22	2.48	0.43
2:H:8:LYS:HE3	2:H:11:LEU:HD23	2.00	0.43
2:E:115:GLU:CD	2:E:115:GLU:H	2.27	0.43
3:C:208:ILE:O	3:C:211:ILE:HG22	2.18	0.42
3:F:18:VAL:HG12	3:F:21:GLU:HB2	2.00	0.42
3:F:75:ILE:HD11	3:F:127:ILE:CG2	2.45	0.42
1:G:178:VAL:HG12	1:G:179:ASN:H	1.84	0.42
2:H:96:ARG:O	2:H:100:LEU:HG	2.19	0.42
3:I:11:LEU:HB2	3:I:12:GLN:HE21	1.83	0.42
3:C:12:GLN:HA	3:C:13:PRO:HD3	1.88	0.42
3:F:206:ILE:O	3:F:206:ILE:HG23	2.18	0.42
1:G:227:PRO:C	1:G:229:LEU:H	2.27	0.42
3:I:84:GLU:CD	3:I:89:VAL:HG23	2.44	0.42
1:G:198:VAL:HG22	1:G:207:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:167:VAL:O	3:I:167:VAL:HG12	2.19	0.42
2:B:163:VAL:HB	2:B:218:ALA:HB2	2.01	0.42
3:I:167:VAL:HA	3:I:214:ILE:HD13	2.01	0.42
3:C:82:ASP:OD1	2:H:119:ARG:NH2	2.52	0.42
2:B:236:LYS:HE3	3:C:63:LEU:HB3	2.00	0.42
3:C:164:VAL:HB	3:C:165:PRO:HD3	2.02	0.42
1:G:82:GLY:HA3	1:G:129:LEU:CD1	2.49	0.42
2:H:10:ILE:HG23	2:H:11:LEU:O	2.19	0.42
2:B:83:PHE:HB2	1:G:50:ALA:HB2	2.02	0.42
3:F:57:GLN:HE21	3:F:57:GLN:HB3	1.63	0.42
3:I:9:ILE:HG23	3:I:25:GLU:OE2	2.19	0.42
1:D:112:ARG:HH22	2:E:96:ARG:NH1	2.18	0.42
3:I:211:ILE:O	3:I:215:GLU:CB	2.68	0.42
3:C:171:ASN:O	3:C:171:ASN:CG	2.62	0.41
1:D:168:THR:HB	1:D:187:LEU:HD22	2.00	0.41
1:G:22:LEU:C	1:G:23:PHE:O	2.62	0.41
1:G:24:GLU:C	1:G:26:GLY:H	2.27	0.41
3:C:16:ILE:HD12	3:C:63:LEU:HD11	2.02	0.41
1:D:11:ILE:HG21	1:D:216:ILE:CG2	2.50	0.41
2:H:74:LEU:HD23	2:H:122:ILE:HB	2.02	0.41
2:B:57:GLY:HA2	2:B:152:ILE:HD11	2.02	0.41
3:C:111:ASN:HB2	3:C:114:GLU:HG3	2.02	0.41
1:D:121:SER:HA	1:D:232:VAL:CG2	2.48	0.41
1:G:121:SER:CA	1:G:232:VAL:HG21	2.49	0.41
2:H:31:GLU:HG3	2:H:34:VAL:HG13	2.02	0.41
2:H:162:ALA:HA	2:H:187:PRO:HA	2.02	0.41
2:H:231:GLU:HA	2:H:234:LYS:HB2	2.02	0.41
1:A:1:MET:CG	2:B:77:ARG:HG3	2.44	0.41
3:I:13:PRO:HB2	3:I:14:ARG:H	1.72	0.41
3:F:17:VAL:HG21	3:F:23:LEU:CD2	2.51	0.41
3:F:110:ILE:HG21	3:F:119:TYR:HE2	1.84	0.41
3:F:179:THR:HG23	3:F:186:ILE:HG12	2.01	0.41
1:D:68:LYS:HD3	2:H:83:PHE:HA	2.02	0.41
1:A:78:THR:HA	1:A:79:PRO:HD3	1.91	0.41
3:C:117:ARG:HE	3:C:121:ASP:CG	2.29	0.41
1:A:51:ASP:CB	1:A:168:THR:HG23	2.51	0.41
3:C:137:ILE:HG22	3:F:85:ILE:HG21	2.03	0.41
3:F:163:LYS:HD2	3:F:215:GLU:OE2	2.21	0.41
3:I:191:ASN:HD22	3:I:191:ASN:HA	1.64	0.41
2:B:36:LYS:HD3	2:B:36:LYS:HA	1.92	0.41
2:H:190:MET:HG2	2:H:222:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:HA2	1:A:137:VAL:HG22	2.03	0.40
1:A:170:VAL:HG12	1:A:171:TYR:N	2.36	0.40
2:E:57:GLY:O	2:E:58:PRO:C	2.63	0.40
1:D:23:PHE:HE1	1:D:28:ARG:HG2	1.86	0.40
3:I:160:MET:C	3:I:162:VAL:H	2.29	0.40
2:E:49:THR:C	2:E:50:LYS:HD2	2.47	0.40
3:F:233:GLU:O	3:F:237:GLU:HB3	2.20	0.40
3:C:133:PHE:CD1	3:C:139:PRO:HG3	2.56	0.40
2:E:165:LYS:HE3	2:E:168:GLY:HA2	2.04	0.40
2:E:4:VAL:O	2:E:4:VAL:CG1	2.69	0.40

There are no symmetry-related clashes.

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	245/271 (90%)	229 (94%)	12 (5%)	4 (2%)	7	10
1	D	257/271 (95%)	242 (94%)	10 (4%)	5 (2%)	6	7
1	G	268/271 (99%)	238 (89%)	13 (5%)	17 (6%)	1	0
2	B	230/245 (94%)	212 (92%)	12 (5%)	6 (3%)	4	4
2	E	235/245 (96%)	219 (93%)	9 (4%)	7 (3%)	3	3
2	H	232/245 (95%)	215 (93%)	12 (5%)	5 (2%)	5	5
3	C	220/249 (88%)	184 (84%)	24 (11%)	12 (6%)	1	1
3	F	205/249 (82%)	169 (82%)	24 (12%)	12 (6%)	1	0
3	I	198/249 (80%)	163 (82%)	24 (12%)	11 (6%)	1	0
All	All	2090/2295 (91%)	1871 (90%)	140 (7%)	79 (4%)	2	2

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
2	B	13	ASP
3	C	8	LYS
3	C	182	SER
1	D	8	GLN
1	D	78	THR
2	E	4	VAL
2	E	5	GLU
2	E	13	ASP
2	E	236	LYS
3	F	162	VAL
3	F	177	THR
3	F	179	THR
3	F	204	GLU
3	F	220	ILE
1	G	23	PHE
1	G	105	GLU
1	G	126	LEU
1	G	175	GLN
1	G	177	SER
2	H	13	ASP
2	H	236	LYS
2	H	237	TYR
3	I	13	PRO
3	I	108	ARG
3	I	112	VAL
3	I	185	SER
3	I	206	ILE
3	I	209	GLU
3	I	223	LEU
1	A	10	ILE
3	C	13	PRO
3	C	117	ARG
3	C	208	ILE
1	D	16	LYS
1	D	105	GLU
3	F	13	PRO
3	F	57	GLN
1	G	24	GLU
1	G	78	THR
1	G	93	LEU
1	G	128	LYS
1	G	180	LYS

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Mol	Chain	Res	Type
3	I	54	LYS
2	B	12	ASP
2	B	235	SER
3	C	40	ASN
3	C	115	ASP
3	C	145	GLY
3	C	200	SER
2	E	57	GLY
3	F	55	ASP
3	F	160	MET
3	F	240	ALA
1	G	2	SER
1	G	79	PRO
1	G	176	ILE
2	H	235	SER
3	I	109	SER
2	B	57	GLY
2	B	133	ALA
2	B	237	TYR
3	C	134	ASP
3	C	153	ASN
2	E	133	ALA
3	F	108	ARG
1	G	10	ILE
3	I	172	LYS
1	A	78	THR
3	C	199	PRO
2	E	6	ARG
3	F	206	ILE
2	H	133	ALA
1	G	9	ASN
3	I	30	ILE
1	G	188	PRO
1	G	178	VAL
1	A	91	LEU
1	D	92	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	218/239 (91%)	202 (93%)	16 (7%)	13	21
1	D	217/239 (91%)	202 (93%)	15 (7%)	14	23
1	G	237/239 (99%)	217 (92%)	20 (8%)	10	16
2	B	187/205 (91%)	178 (95%)	9 (5%)	23	38
2	E	197/205 (96%)	185 (94%)	12 (6%)	17	28
2	H	194/205 (95%)	182 (94%)	12 (6%)	16	27
3	C	180/222 (81%)	163 (91%)	17 (9%)	8	12
3	F	190/222 (86%)	166 (87%)	24 (13%)	4	6
3	I	167/222 (75%)	144 (86%)	23 (14%)	3	4
All	All	1787/1998 (89%)	1639 (92%)	148 (8%)	10	16

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	ILE
1	A	13	ILE
1	A	32	ARG
1	A	68	LYS
1	A	73	LYS
1	A	104	ASP
1	A	137	VAL
1	A	172	LYS
1	A	187	LEU
1	A	203	LYS
1	A	228	ASP
1	A	235	GLN
1	A	239	LYS
1	A	251	GLU
1	A	262	LEU
2	B	12	ASP
2	B	34	VAL
2	B	46	MET
2	B	61	MET
2	B	88	ARG
2	B	161	VAL
2	B	183	GLU

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Mol	Chain	Res	Type
2	B	198	THR
2	B	238	VAL
3	C	7	GLN
3	C	18	VAL
3	C	22	LEU
3	C	55	ASP
3	C	56	THR
3	C	72	ILE
3	C	83	VAL
3	C	85	ILE
3	C	106	LEU
3	C	116	LEU
3	C	117	ARG
3	C	126	VAL
3	C	135	ARG
3	C	162	VAL
3	C	191	ASN
3	C	221	LYS
3	C	225	ASP
1	D	8	GLN
1	D	9	ASN
1	D	37	TYR
1	D	68	LYS
1	D	93	LEU
1	D	104	ASP
1	D	135	LYS
1	D	137	VAL
1	D	187	LEU
1	D	203	LYS
1	D	206	VAL
1	D	228	ASP
1	D	239	LYS
1	D	247	ILE
1	D	251	GLU
2	E	4	VAL
2	E	8	LYS
2	E	10	ILE
2	E	15	LYS
2	E	61	MET
2	E	75	ARG
2	E	88	ARG
2	E	115	GLU

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Mol	Chain	Res	Type
2	E	126	THR
2	E	161	VAL
2	E	198	THR
2	E	227	ASN
3	F	18	VAL
3	F	22	LEU
3	F	57	GLN
3	F	75	ILE
3	F	105	LEU
3	F	110	ILE
3	F	134	ASP
3	F	135	ARG
3	F	144	LYS
3	F	146	LYS
3	F	174	MET
3	F	175	TYR
3	F	176	GLU
3	F	178	LEU
3	F	184	CYS
3	F	198	CYS
3	F	207	LEU
3	F	211	ILE
3	F	228	LYS
3	F	229	GLN
3	F	231	ILE
3	F	233	GLU
3	F	234	LYS
3	F	237	GLU
1	G	9	ASN
1	G	11	ILE
1	G	20	VAL
1	G	68	LYS
1	G	73	LYS
1	G	93	LEU
1	G	96	THR
1	G	104	ASP
1	G	125	ASP
1	G	129	LEU
1	G	130	VAL
1	G	137	VAL
1	G	178	VAL
1	G	187	LEU

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Mol	Chain	Res	Type
1	G	193	VAL
1	G	203	LYS
1	G	206	VAL
1	G	232	VAL
1	G	239	LYS
1	G	251	GLU
2	H	10	ILE
2	H	11	LEU
2	H	15	LYS
2	H	34	VAL
2	H	46	MET
2	H	61	MET
2	H	75	ARG
2	H	126	THR
2	H	161	VAL
2	H	174	LEU
2	H	198	THR
2	H	236	LYS
3	I	9	ILE
3	I	12	GLN
3	I	14	ARG
3	I	18	VAL
3	I	22	LEU
3	I	25	GLU
3	I	27	GLU
3	I	38	LYS
3	I	75	ILE
3	I	83	VAL
3	I	106	LEU
3	I	110	ILE
3	I	120	LEU
3	I	155	ILE
3	I	162	VAL
3	I	186	ILE
3	I	191	ASN
3	I	206	ILE
3	I	207	LEU
3	I	214	ILE
3	I	215	GLU
3	I	219	HIS
3	I	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	83	ASN
1	A	235	GLN
1	A	252	ASN
3	C	7	GLN
3	C	190	ASN
3	C	191	ASN
1	D	235	GLN
2	E	3	GLN
3	F	57	GLN
1	G	8	GLN
1	G	9	ASN
1	G	29	GLN
1	G	80	ASN
1	G	83	ASN
1	G	235	GLN
2	H	130	GLN
3	I	12	GLN
3	I	191	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](#)

3 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	$\# Z > 2$
4	SO4	B	246	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	H	246	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	E	246	-	4,4,4	0.22	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	251/271 (92%)	0.11	13 (5%) 33 29	25, 42, 77, 90	0
1	D	261/271 (96%)	0.80	35 (13%) 7 5	28, 57, 112, 137	0
1	G	270/271 (99%)	0.73	24 (8%) 15 12	31, 55, 98, 114	0
2	B	232/245 (94%)	0.14	5 (2%) 62 59	20, 43, 91, 100	0
2	E	237/245 (96%)	0.23	14 (5%) 28 24	20, 40, 91, 106	0
2	H	234/245 (95%)	0.27	8 (3%) 48 44	25, 50, 80, 104	0
3	C	222/249 (89%)	1.02	29 (13%) 7 5	31, 64, 120, 144	0
3	F	215/249 (86%)	0.76	23 (10%) 11 8	28, 59, 84, 93	0
3	I	206/249 (82%)	1.60	66 (32%) 1 1	39, 85, 120, 131	0
All	All	2128/2295 (92%)	0.61	217 (10%) 12 9	20, 53, 109, 144	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	110	ILE	5.4
2	H	237	TYR	4.9
3	I	112	VAL	4.9
3	I	24	ALA	4.6
1	G	173	VAL	4.6
3	F	203	SER	4.5
3	I	181	LYS	4.5
3	C	186	ILE	4.4
1	G	126	LEU	4.4
3	C	9	ILE	4.1
3	I	28	PHE	4.1
3	I	214	ILE	4.0
3	F	180	SER	4.0
3	I	119	TYR	4.0
1	D	183	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	206	ILE	3.7
2	H	8	LYS	3.7
3	F	220	ILE	3.7
1	A	271	ILE	3.7
1	D	19	ILE	3.7
1	D	37	TYR	3.6
3	F	179	THR	3.6
3	C	202	PHE	3.6
1	D	134	GLY	3.5
3	I	151	VAL	3.4
3	C	135	ARG	3.4
2	B	238	VAL	3.4
3	C	207	LEU	3.4
3	I	23	LEU	3.4
3	F	111	ASN	3.3
2	E	9	LEU	3.3
1	G	184	VAL	3.3
3	C	115	ASP	3.3
2	E	7	PRO	3.2
3	I	143	VAL	3.2
3	F	228	LYS	3.2
3	I	11	LEU	3.2
2	H	166	ALA	3.2
3	C	131	GLU	3.2
3	I	153	ASN	3.2
3	I	58	PHE	3.1
1	G	124	LEU	3.1
3	C	112	VAL	3.1
1	D	169	LYS	3.0
3	C	25	GLU	3.0
3	I	103	SER	3.0
2	E	11	LEU	3.0
3	C	116	LEU	3.0
3	C	222	GLY	3.0
3	I	120	LEU	3.0
1	D	29	GLN	3.0
3	I	110	ILE	2.9
1	D	138	TRP	2.9
1	A	79	PRO	2.9
3	C	224	THR	2.9
3	C	218	SER	2.9
3	I	84	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	I	105	LEU	2.8
1	A	2	SER	2.8
3	I	141	LEU	2.8
3	I	222	GLY	2.8
2	E	4	VAL	2.8
3	F	161	PRO	2.8
1	D	132	GLU	2.8
1	D	172	LYS	2.8
1	D	13	ILE	2.8
3	C	203	SER	2.8
1	G	138	TRP	2.7
3	I	132	ASN	2.7
1	G	129	LEU	2.7
3	I	106	LEU	2.7
3	I	220	ILE	2.7
3	C	10	VAL	2.7
2	E	2	LEU	2.7
2	E	14	GLY	2.7
1	G	176	ILE	2.7
3	C	227	ILE	2.7
3	I	208	ILE	2.7
3	I	150	ARG	2.7
3	I	180	SER	2.7
3	I	148	LEU	2.6
3	I	175	TYR	2.6
3	I	206	ILE	2.6
1	G	178	VAL	2.6
3	I	109	SER	2.6
1	D	136	SER	2.6
3	F	218	SER	2.6
3	I	173	SER	2.6
2	E	166	ALA	2.6
2	H	62	HIS	2.6
2	E	237	TYR	2.6
1	D	73	LYS	2.6
1	A	229	LEU	2.6
3	I	53	VAL	2.6
1	G	259	VAL	2.5
3	F	169	GLY	2.5
1	G	231	ILE	2.5
3	C	220	ILE	2.5
2	B	215	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	178	LEU	2.5
3	C	29	GLN	2.5
1	G	37	TYR	2.5
3	I	9	ILE	2.5
1	G	1	MET	2.5
3	C	206	ILE	2.5
3	I	122	VAL	2.5
3	I	108	ARG	2.5
3	F	177	THR	2.5
3	I	136	SER	2.5
3	I	123	GLY	2.4
3	I	183	GLY	2.4
3	I	77	ILE	2.4
3	I	211	ILE	2.4
2	E	181	TRP	2.4
1	D	123	ALA	2.4
2	H	180	MET	2.4
2	E	236	LYS	2.4
3	I	12	GLN	2.4
3	I	187	PHE	2.4
1	G	183	VAL	2.4
3	I	10	VAL	2.4
1	D	1	MET	2.4
2	B	235	SER	2.4
1	D	11	ILE	2.4
2	H	11	LEU	2.4
3	I	79	LEU	2.4
3	C	28	PHE	2.4
1	D	130	VAL	2.4
1	A	103	PRO	2.4
1	G	34	LEU	2.4
3	F	219	HIS	2.4
3	I	184	CYS	2.4
1	D	96	THR	2.3
1	G	13	ILE	2.3
3	C	117	ARG	2.3
2	B	9	LEU	2.3
3	C	208	ILE	2.3
3	C	211	ILE	2.3
3	F	230	PHE	2.3
1	G	127	THR	2.3
1	G	2	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	109	SER	2.3
3	I	226	ARG	2.3
3	I	39	ILE	2.3
1	D	17	GLU	2.3
1	D	83	ASN	2.3
3	I	171	ASN	2.3
2	E	68	LEU	2.3
3	C	178	LEU	2.3
3	I	36	ILE	2.3
1	A	1	MET	2.3
1	A	228	ASP	2.3
2	H	238	VAL	2.3
1	G	79	PRO	2.3
3	C	177	THR	2.3
1	D	270	GLY	2.3
3	C	183	GLY	2.3
1	A	91	LEU	2.3
3	I	207	LEU	2.3
1	G	23	PHE	2.3
1	D	193	VAL	2.3
1	D	78	THR	2.2
1	D	10	ILE	2.2
2	E	8	LYS	2.2
3	I	72	ILE	2.2
3	I	182	SER	2.2
1	D	20	VAL	2.2
1	D	79	PRO	2.2
1	D	92	PRO	2.2
1	D	187	LEU	2.2
3	C	214	ILE	2.2
1	D	192	PRO	2.2
3	F	240	ALA	2.2
1	A	172	LYS	2.2
1	D	124	LEU	2.2
2	B	57	GLY	2.2
3	F	141	LEU	2.2
3	F	182	SER	2.2
3	I	195	TRP	2.2
3	I	140	VAL	2.2
1	D	75	TYR	2.2
3	I	78	GLY	2.2
3	F	200	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	218	SER	2.2
3	I	102	ALA	2.1
1	G	185	GLY	2.1
1	A	171	TYR	2.1
3	I	30	ILE	2.1
1	A	6	SER	2.1
3	I	113	GLY	2.1
3	F	176	GLU	2.1
3	F	221	LYS	2.1
3	I	128	ALA	2.1
1	G	244	LEU	2.1
1	A	78	THR	2.1
3	I	26	GLY	2.1
3	I	43	TYR	2.1
2	E	238	VAL	2.1
3	I	60	VAL	2.1
3	I	196	ALA	2.1
1	D	127	THR	2.1
3	C	205	GLU	2.1
1	G	180	LYS	2.1
3	C	52	ASP	2.1
3	F	198	CYS	2.1
1	D	137	VAL	2.0
1	G	130	VAL	2.0
3	I	133	PHE	2.0
3	I	145	GLY	2.0
3	I	154	GLY	2.0
1	G	19	ILE	2.0
1	D	184	VAL	2.0
1	D	34	LEU	2.0
1	D	129	LEU	2.0
2	E	66	LEU	2.0
2	H	17	THR	2.0
1	A	120	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	SO4	B	246	5/5	0.97	0.09	45,45,46,46	0
4	SO4	E	246	5/5	0.97	0.09	45,45,46,46	0
4	SO4	H	246	5/5	0.97	0.07	49,49,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.