



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:28 AM UTC

PDB ID : 6DFK / pdb_00006dfk
Title : Crystal structure of the 11S subunit of the Plasmodium falciparum proteasome, PA28
Authors : Xie, S.C.; Metcalfe, R.D.; Gillett, D.L.; Tilley, L.; Griffin, M.D.W.
Deposited on : 2018-05-15
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

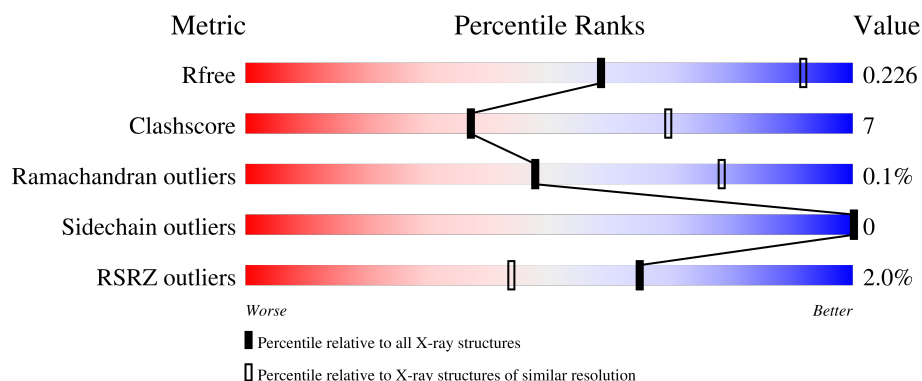
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	280	2% 61% 16% 23%
1	B	280	2% 66% 17% 17%
1	C	280	% 65% 14% 21%
1	D	280	% 70% 13% 17%
1	E	280	2% 60% 15% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	280	68% 14% 18%
1	G	280	59% 17% 24%
1	H	280	64% 14% 23%
1	I	280	70% 14% 16%
1	J	280	64% 13% 24%
1	K	280	61% 18% 20%
1	L	280	69% 14% 17%
1	M	280	64% 12% 24%
1	N	280	68% 16% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	303	-	-	X	-
2	SO4	B	303	-	-	X	-
2	SO4	C	302	-	-	X	-
2	SO4	D	303	-	-	X	-
2	SO4	E	303	-	-	X	-
2	SO4	G	303	-	-	X	-
2	SO4	H	302	-	-	X	-
2	SO4	J	303	-	-	X	-
2	SO4	M	303	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26498 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 Subunit of proteasome activator complex, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1813	1173	298	339	3			
1	B	232	Total	C	N	O	S	0	0	0
			1945	1255	321	366	3			
1	C	222	Total	C	N	O	S	0	0	0
			1862	1203	307	349	3			
1	D	233	Total	C	N	O	S	0	0	0
			1950	1258	323	366	3			
1	E	212	Total	C	N	O	S	0	0	0
			1777	1149	293	332	3			
1	F	229	Total	C	N	O	S	0	0	0
			1920	1241	315	361	3			
1	G	213	Total	C	N	O	S	0	0	0
			1789	1158	294	334	3			
1	H	216	Total	C	N	O	S	0	0	0
			1812	1173	298	338	3			
1	I	236	Total	C	N	O	S	0	0	0
			1974	1274	327	370	3			
1	J	214	Total	C	N	O	S	0	0	0
			1797	1162	296	336	3			
1	K	223	Total	C	N	O	S	0	0	0
			1868	1208	307	349	4			
1	L	233	Total	C	N	O	S	0	0	0
			1952	1262	321	366	3			
1	M	213	Total	C	N	O	S	0	0	0
			1785	1153	295	334	3			
1	N	233	Total	C	N	O	S	0	0	0
			1954	1262	323	366	3			

There are 14 discrepancies between the modelled and reference sequences:

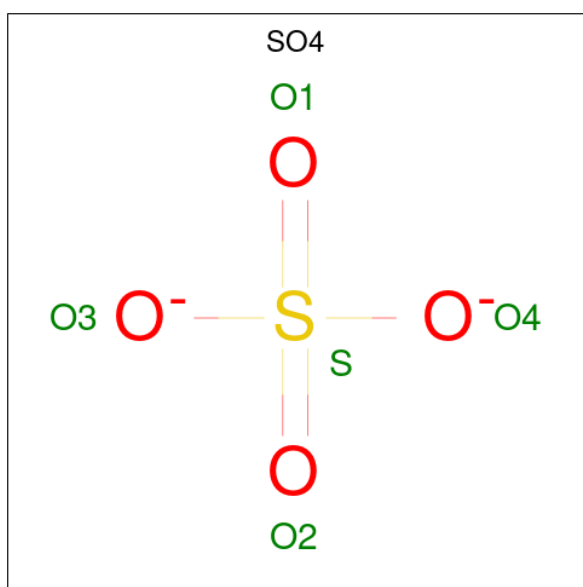
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8I374

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q8I374
C	0	GLY	-	expression tag	UNP Q8I374
D	0	GLY	-	expression tag	UNP Q8I374
E	0	GLY	-	expression tag	UNP Q8I374
F	0	GLY	-	expression tag	UNP Q8I374
G	0	GLY	-	expression tag	UNP Q8I374
H	0	GLY	-	expression tag	UNP Q8I374
I	0	GLY	-	expression tag	UNP Q8I374
J	0	GLY	-	expression tag	UNP Q8I374
K	0	GLY	-	expression tag	UNP Q8I374
L	0	GLY	-	expression tag	UNP Q8I374
M	0	GLY	-	expression tag	UNP Q8I374
N	0	GLY	-	expression tag	UNP Q8I374

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

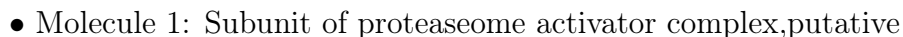
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

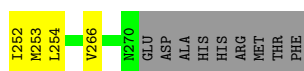
Continued on next page...

Continued from previous page...

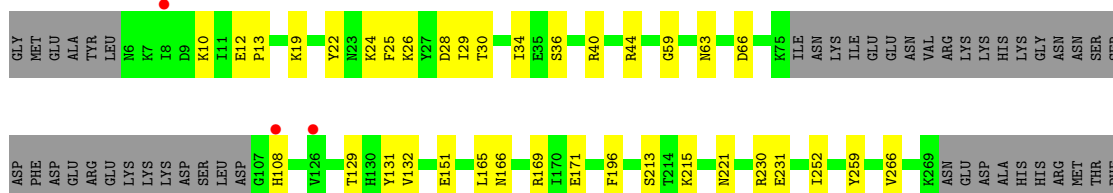
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 1: Subunit of proteasome activator complex,putative

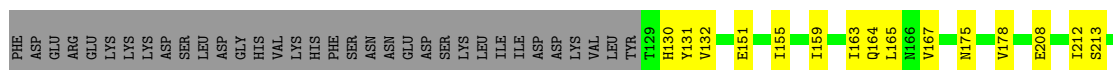
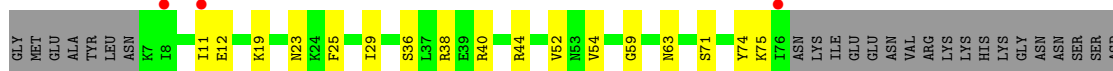




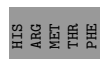
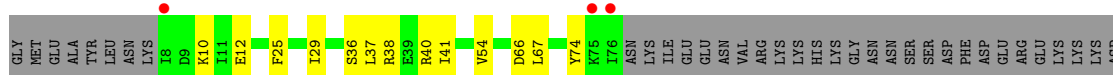
- Molecule 1: Subunit of proteasome activator complex,putative



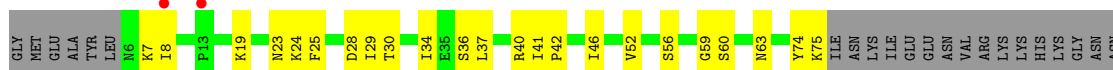
- Molecule 1: Subunit of proteasome activator complex,putative

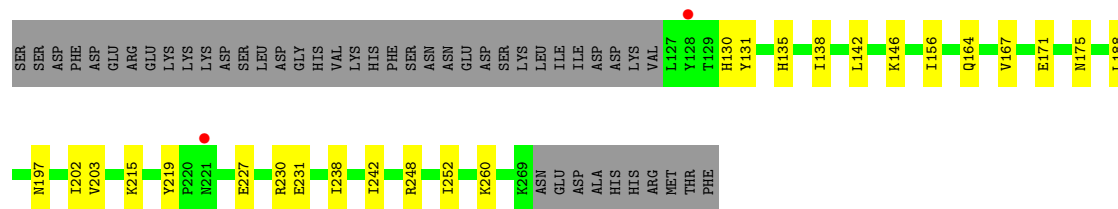


- Molecule 1: Subunit of proteasome activator complex,putative

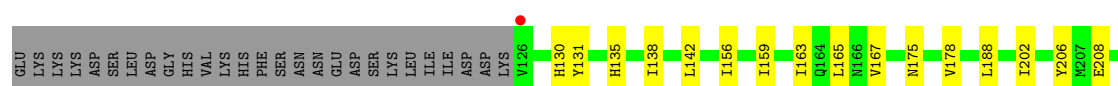
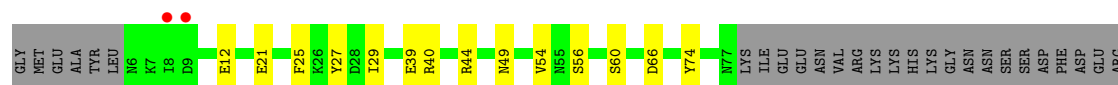


- Molecule 1: Subunit of proteasome activator complex,putative

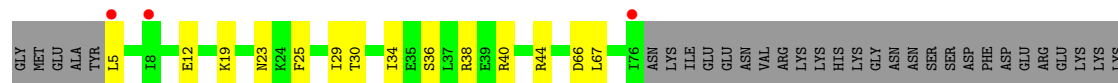




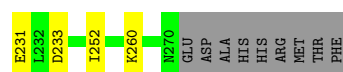
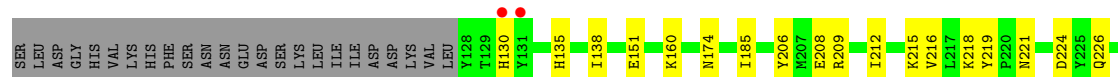
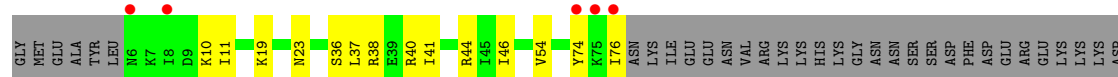
- Molecule 1: Subunit of proteasome activator complex, putative



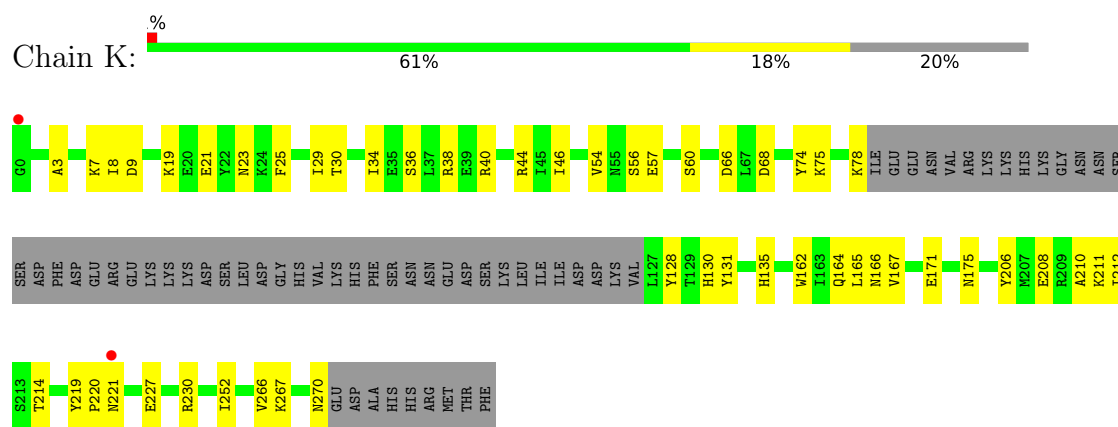
- Molecule 1: Subunit of proteasome activator complex, putative



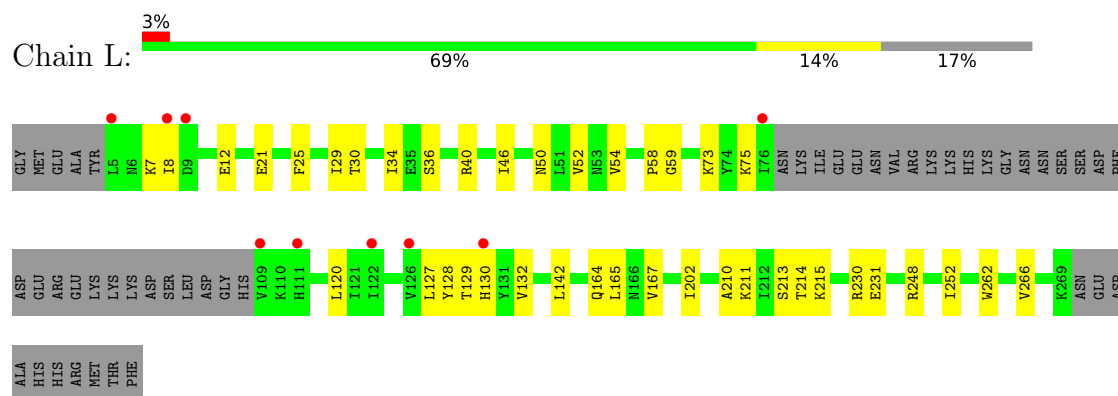
- Molecule 1: Subunit of proteasome activator complex, putative



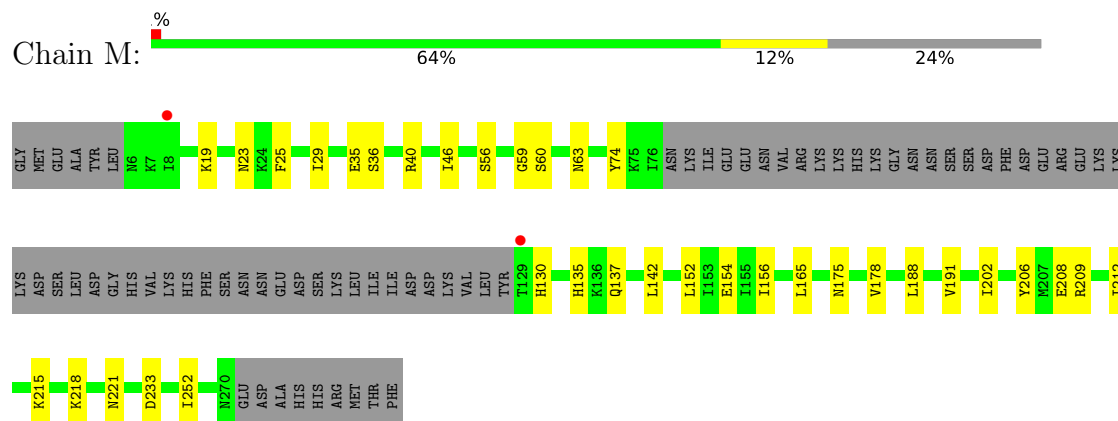
- Molecule 1: Subunit of proteasome activator complex, putative



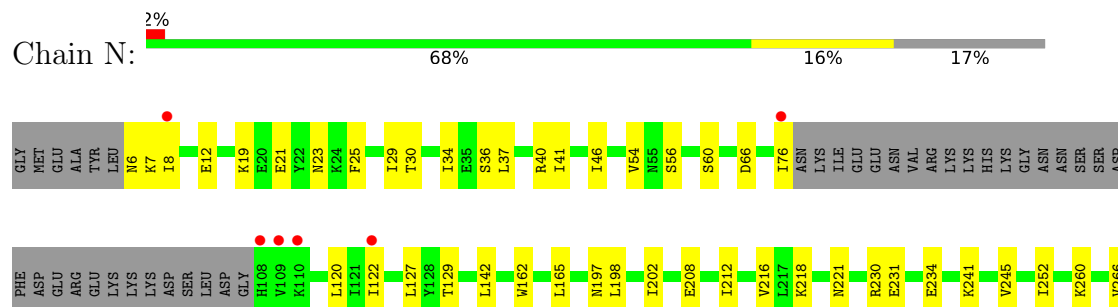
- Molecule 1: Subunit of proteasome activator complex, putative



- Molecule 1: Subunit of proteasome activator complex,putative



- Molecule 1: Subunit of proteasome activator complex, putative



K269
ASN
GLU
ASP
ALA
HIS
HIS
ARG
MET
THR
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.49Å 166.49Å 399.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 3.10 48.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.89-3.10) 100.0 (48.89-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.182 , 0.225 0.184 , 0.226	Depositor DCC
R_{free} test set	3535 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26498	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/1848	0.37	0/2493
1	B	0.16	0/1982	0.37	0/2673
1	C	0.15	0/1897	0.38	0/2559
1	D	0.14	0/1988	0.38	0/2681
1	E	0.14	0/1811	0.34	0/2443
1	F	0.13	0/1957	0.35	0/2640
1	G	0.14	0/1824	0.35	0/2461
1	H	0.15	0/1847	0.39	0/2493
1	I	0.16	0/2012	0.38	0/2714
1	J	0.15	0/1832	0.39	0/2472
1	K	0.15	0/1904	0.36	0/2568
1	L	0.14	0/1989	0.37	0/2683
1	M	0.14	0/1819	0.38	0/2454
1	N	0.15	0/1992	0.37	0/2687
All	All	0.15	0/26702	0.37	0/36021

There are no bond length outliers.

There are no bond angle outliers.

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	1813	0	1841	32	0
1	B	1945	0	1969	41	0
1	C	1862	0	1892	30	0
1	D	1950	0	1971	33	0
1	E	1777	0	1806	32	0
1	F	1920	0	1944	30	0
1	G	1789	0	1815	33	0
1	H	1812	0	1841	30	0
1	I	1974	0	1999	34	0
1	J	1797	0	1821	30	0
1	K	1868	0	1897	44	0
1	L	1952	0	1983	30	0
1	M	1785	0	1812	30	0
1	N	1954	0	1979	34	0
2	A	20	0	0	3	0
2	B	25	0	0	3	0
2	C	20	0	0	2	0
2	D	20	0	0	3	0
2	E	20	0	0	2	0
2	F	25	0	0	1	0
2	G	20	0	0	3	0
2	H	15	0	0	2	0
2	I	25	0	0	2	0
2	J	25	0	0	4	0
2	K	20	0	0	2	0
2	L	20	0	0	1	0
2	M	25	0	0	3	0
2	N	20	0	0	1	0
All	All	26498	0	26570	379	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 7.

All (379) 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:G:74:TYR:HH	1:G:130:HIS:HD1	1.21	0.88
1:K:221:ASN:ND2	1:L:129:THR:O	2.13	0.80
1:L:54:VAL:HG21	1:M:29:ILE:HG12	1.64	0.80
1:A:128:TYR:OH	1:B:125:LYS:NZ	2.21	0.74
1:E:221:ASN:ND2	1:F:129:THR:O	2.18	0.73
1:K:162:TRP:HH2	1:K:266:VAL:HG12	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:ILE:HG12	1:N:54:VAL:HG21	1.70	0.72
1:B:215:LYS:NZ	2:B:303:SO4:O2	2.23	0.71
1:J:215:LYS:NZ	2:J:303:SO4:O2	2.23	0.70
1:L:73:LYS:O	1:L:75:LYS:NZ	2.25	0.70
1:B:162:TRP:HH2	1:B:266:VAL:HG12	1.57	0.69
1:F:36:SER:HA	1:F:40:ARG:HB2	1.74	0.69
1:A:38:ARG:HH22	1:B:8:ILE:HD12	1.57	0.69
1:M:215:LYS:NZ	2:M:303:SO4:O2	2.27	0.68
1:I:38:ARG:HD3	1:J:11:ILE:HA	1.76	0.68
1:N:197:ASN:ND2	2:N:304:SO4:O2	2.25	0.68
1:J:76:ILE:HA	1:J:130:HIS:CE1	2.29	0.67
1:C:174:ASN:O	1:C:174:ASN:ND2	2.28	0.67
1:I:25:PHE:HE2	1:I:29:ILE:HD11	1.59	0.66
1:A:215:LYS:NZ	2:A:303:SO4:O4	2.27	0.66
1:H:219:TYR:OH	2:H:302:SO4:O3	2.13	0.65
1:G:197:ASN:ND2	2:G:304:SO4:O4	2.29	0.64
1:L:215:LYS:NZ	2:L:303:SO4:O3	2.28	0.64
1:L:59:GLY:N	1:M:154:GLU:OE1	2.24	0.64
1:M:36:SER:HA	1:M:40:ARG:HB2	1.79	0.64
1:H:221:ASN:ND2	1:I:129:THR:O	2.22	0.64
1:N:19:LYS:O	1:N:23:ASN:ND2	2.31	0.64
1:J:174:ASN:O	1:J:174:ASN:ND2	2.30	0.63
1:F:197:ASN:ND2	2:F:305:SO4:O1	2.31	0.63
1:D:215:LYS:NZ	2:D:303:SO4:O4	2.29	0.63
1:J:221:ASN:HB3	1:K:131:TYR:HA	1.80	0.63
1:K:19:LYS:O	1:K:23:ASN:ND2	2.31	0.63
1:N:162:TRP:HH2	1:N:266:VAL:HG12	1.62	0.63
1:B:54:VAL:HG21	1:C:29:ILE:HG12	1.79	0.63
1:D:36:SER:HA	1:D:40:ARG:HB2	1.79	0.63
1:K:267:LYS:HE2	1:K:270:ASN:HB2	1.79	0.63
1:E:19:LYS:O	1:E:23:ASN:ND2	2.31	0.63
1:N:230:ARG:NH1	1:N:234:GLU:OE2	2.32	0.63
1:E:52:VAL:O	1:E:248:ARG:NH1	2.32	0.62
1:N:36:SER:HA	1:N:40:ARG:HB2	1.80	0.62
1:K:36:SER:HA	1:K:40:ARG:HB2	1.81	0.62
1:K:54:VAL:HG21	1:L:29:ILE:HG12	1.82	0.61
1:D:169:ARG:NH2	1:D:171:GLU:OE2	2.26	0.61
1:M:221:ASN:ND2	1:N:129:THR:O	2.24	0.61
1:D:108:HIS:ND1	1:D:131:TYR:OH	2.34	0.60
1:D:259:TYR:HA	1:E:11:ILE:HD11	1.81	0.60
1:H:215:LYS:NZ	2:H:302:SO4:O4	2.29	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:SER:HA	1:L:40:ARG:HB2	1.83	0.59
1:D:13:PRO:O	1:D:19:LYS:HE2	2.03	0.59
1:B:19:LYS:O	1:B:23:ASN:ND2	2.36	0.59
1:J:74:TYR:OH	1:J:226:GLN:NE2	2.36	0.58
1:C:54:VAL:HG21	1:D:29:ILE:HG12	1.84	0.58
1:J:19:LYS:O	1:J:23:ASN:ND2	2.31	0.58
1:E:44:ARG:NH1	1:E:151:GLU:OE1	2.36	0.58
1:I:231:GLU:HG3	1:J:206:TYR:CE2	2.38	0.58
1:I:12:GLU:N	1:I:12:GLU:OE1	2.36	0.58
1:M:252:ILE:HG12	1:N:165:LEU:HD21	1.85	0.58
1:K:74:TYR:CE1	1:K:130:HIS:HB2	2.39	0.58
1:L:58:PRO:HG2	1:M:40:ARG:HD3	1.86	0.57
1:I:169:ARG:NH2	1:I:171:GLU:OE2	2.37	0.57
1:J:36:SER:HA	1:J:40:ARG:HB2	1.85	0.57
1:N:122:ILE:HD12	1:N:127:LEU:HG	1.86	0.57
1:I:25:PHE:CE2	1:I:29:ILE:HD11	2.40	0.57
1:L:142:LEU:HD13	1:L:202:ILE:HG23	1.86	0.57
1:A:126:VAL:HG12	1:A:127:LEU:H	1.70	0.56
1:I:38:ARG:NH1	1:J:10:LYS:O	2.38	0.56
1:M:209:ARG:NH1	1:M:233:ASP:OD2	2.38	0.56
1:G:36:SER:HA	1:G:40:ARG:HB2	1.88	0.56
1:H:74:TYR:OH	1:H:130:HIS:ND1	2.28	0.56
1:A:19:LYS:O	1:A:23:ASN:ND2	2.37	0.56
1:F:221:ASN:HB3	1:G:131:TYR:HA	1.87	0.56
1:D:259:TYR:OH	1:E:12:GLU:OE2	2.23	0.56
1:F:38:ARG:HH22	1:G:8:ILE:HD12	1.71	0.56
1:C:19:LYS:O	1:C:23:ASN:ND2	2.37	0.56
1:D:12:GLU:N	1:D:12:GLU:OE1	2.38	0.56
1:G:7:LYS:HG3	1:G:8:ILE:H	1.71	0.56
1:M:19:LYS:O	1:M:23:ASN:ND2	2.36	0.56
1:D:215:LYS:NZ	2:D:303:SO4:S	2.78	0.55
1:J:54:VAL:HG21	1:K:29:ILE:HG12	1.88	0.55
1:A:44:ARG:NH2	1:A:151:GLU:OE1	2.27	0.55
1:D:24:LYS:NZ	1:D:28:ASP:OD2	2.37	0.55
1:K:74:TYR:HE1	1:K:130:HIS:HB2	1.72	0.55
1:I:36:SER:HA	1:I:40:ARG:HB2	1.88	0.55
1:G:215:LYS:NZ	2:G:303:SO4:O4	2.39	0.55
1:K:220:PRO:HD2	1:L:128:TYR:O	2.06	0.55
1:B:230:ARG:NH2	1:B:231:GLU:HG2	2.22	0.54
1:D:44:ARG:NH2	2:D:301:SO4:O3	2.40	0.54
1:F:162:TRP:HH2	1:F:266:VAL:HG12	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:ILE:HG23	1:H:188:LEU:HD22	1.88	0.54
1:F:12:GLU:OE1	1:F:12:GLU:N	2.40	0.54
1:J:218:LYS:NZ	2:J:303:SO4:O3	2.39	0.54
1:L:164:GLN:O	1:L:167:VAL:HG22	2.08	0.54
1:D:25:PHE:HE2	1:D:29:ILE:HD11	1.72	0.54
1:M:175:ASN:HB2	1:M:178:VAL:HG22	1.89	0.54
1:G:25:PHE:CE2	1:G:29:ILE:HD11	2.43	0.54
1:C:169:ARG:NH2	1:C:171:GLU:OE2	2.37	0.54
1:N:6:ASN:HB3	1:N:7:LYS:HD3	1.89	0.54
1:E:40:ARG:O	1:E:44:ARG:HG2	2.08	0.54
1:A:25:PHE:HE2	1:A:29:ILE:HD11	1.73	0.54
1:K:162:TRP:CH2	1:K:266:VAL:HG12	2.39	0.53
1:C:12:GLU:OE1	1:C:12:GLU:N	2.39	0.53
1:D:221:ASN:HB3	1:E:131:TYR:HA	1.89	0.53
1:D:40:ARG:O	1:D:44:ARG:HG2	2.09	0.53
1:F:25:PHE:CE2	1:F:29:ILE:HD11	2.44	0.53
1:H:131:TYR:HA	1:N:221:ASN:HB3	1.92	0.52
1:A:165:LEU:HD21	1:G:252:ILE:HG22	1.91	0.52
1:K:171:GLU:O	1:K:175:ASN:ND2	2.42	0.52
1:B:110:LYS:HE3	1:B:113:SER:HB3	1.92	0.52
1:G:156:ILE:HG23	1:G:188:LEU:HD22	1.92	0.52
1:C:162:TRP:HH2	1:C:266:VAL:HG22	1.74	0.52
1:F:231:GLU:OE2	1:G:146:LYS:NZ	2.31	0.52
1:C:221:ASN:ND2	1:D:129:THR:O	2.22	0.52
1:D:44:ARG:NH1	1:D:151:GLU:OE1	2.42	0.52
1:L:12:GLU:OE1	1:L:12:GLU:N	2.43	0.52
1:L:252:ILE:HG22	1:M:165:LEU:HD21	1.92	0.52
1:K:219:TYR:OH	2:K:303:SO4:O4	2.26	0.52
1:M:56:SER:HB3	1:M:60:SER:OG	2.10	0.52
1:A:165:LEU:O	1:G:260:LYS:NZ	2.42	0.51
1:N:212:ILE:O	1:N:216:VAL:HG23	2.10	0.51
1:B:231:GLU:HB3	1:C:203:VAL:HG22	1.91	0.51
1:C:171:GLU:O	1:C:175:ASN:ND2	2.44	0.51
1:F:231:GLU:HB3	1:G:203:VAL:HG22	1.92	0.51
1:I:132:VAL:HG11	1:I:213:SER:HB3	1.93	0.51
1:C:38:ARG:NH2	1:D:10:LYS:O	2.38	0.51
1:E:54:VAL:HG21	1:F:29:ILE:HG12	1.92	0.51
1:J:44:ARG:NH1	1:J:151:GLU:OE1	2.43	0.51
1:G:59:GLY:O	1:G:63:ASN:HB3	2.10	0.51
1:N:37:LEU:HD23	1:N:41:ILE:HD12	1.92	0.51
1:A:221:ASN:HB2	1:B:130:HIS:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:HD13	1:C:202:ILE:HG23	1.92	0.50
1:E:231:GLU:HG3	1:F:206:TYR:CE2	2.46	0.50
1:H:27:TYR:HD1	1:I:5:LEU:N	2.09	0.50
1:N:66:ASP:OD1	1:N:66:ASP:N	2.37	0.50
1:H:12:GLU:OE1	1:H:12:GLU:N	2.37	0.50
1:I:230:ARG:NH2	1:I:231:GLU:HG2	2.27	0.50
1:A:208:GLU:O	1:A:212:ILE:HG13	2.11	0.50
1:B:259:TYR:HA	1:C:11:ILE:HD11	1.92	0.50
1:B:221:ASN:HB3	1:C:131:TYR:HA	1.93	0.50
1:L:262:TRP:O	1:L:266:VAL:HG23	2.11	0.50
1:A:227:GLU:OE1	1:A:230:ARG:NH2	2.35	0.50
1:K:74:TYR:OH	1:K:130:HIS:ND1	2.41	0.50
1:L:211:LYS:O	1:L:214:THR:OG1	2.22	0.50
1:B:36:SER:HA	1:B:40:ARG:HB2	1.93	0.50
1:J:40:ARG:O	1:J:44:ARG:HG2	2.11	0.49
1:B:132:VAL:HG11	1:B:213:SER:HB3	1.94	0.49
1:N:7:LYS:HG2	1:N:8:ILE:H	1.76	0.49
1:J:260:LYS:NZ	1:K:165:LEU:O	2.42	0.49
1:D:59:GLY:O	1:D:63:ASN:HB3	2.12	0.49
1:G:171:GLU:O	1:G:175:ASN:ND2	2.46	0.49
1:K:130:HIS:H	1:K:130:HIS:CD2	2.31	0.49
1:A:25:PHE:CE2	1:A:29:ILE:HD11	2.47	0.49
1:F:37:LEU:HD23	1:F:41:ILE:HD12	1.95	0.49
1:J:76:ILE:HG12	1:J:130:HIS:CD2	2.48	0.49
1:N:30:THR:O	1:N:34:ILE:HG12	2.13	0.49
1:K:221:ASN:HB2	1:L:130:HIS:O	2.13	0.49
1:H:165:LEU:HD21	1:N:252:ILE:HG22	1.96	0.48
1:E:219:TYR:OH	2:E:303:SO4:O3	2.31	0.48
1:B:30:THR:O	1:B:34:ILE:HG12	2.13	0.48
1:C:253:MET:HG3	1:C:254:LEU:N	2.27	0.48
1:I:66:ASP:OD1	1:I:66:ASP:N	2.37	0.48
1:J:231:GLU:HG3	1:K:206:TYR:CE2	2.49	0.48
1:N:7:LYS:CG	1:N:8:ILE:H	2.27	0.48
1:C:36:SER:HA	1:C:40:ARG:HB2	1.96	0.48
1:E:36:SER:HA	1:E:40:ARG:HB2	1.94	0.48
1:I:188:LEU:HD23	1:I:254:LEU:HD13	1.95	0.48
1:J:208:GLU:O	1:J:212:ILE:HG13	2.13	0.48
1:B:119:LYS:HE2	1:B:128:TYR:OH	2.13	0.48
1:I:118:SER:H	1:I:129:THR:HG23	1.79	0.48
1:E:164:GLN:O	1:E:167:VAL:HG22	2.14	0.48
1:J:252:ILE:HG22	1:K:165:LEU:HD21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:GLU:HG3	1:M:206:TYR:CE2	2.49	0.47
1:A:24:LYS:NZ	1:A:28:ASP:OD2	2.46	0.47
1:B:44:ARG:NH1	2:B:301:SO4:O2	2.43	0.47
1:E:218:LYS:NZ	2:E:303:SO4:O1	2.46	0.47
1:F:74:TYR:CD1	1:F:132:VAL:HG22	2.50	0.47
1:F:208:GLU:O	1:F:212:ILE:HG13	2.15	0.47
1:M:74:TYR:OH	1:M:130:HIS:ND1	2.37	0.47
1:B:10:LYS:HB3	1:B:12:GLU:OE1	2.15	0.47
1:I:219:TYR:OH	2:I:303:SO4:O2	2.24	0.47
1:K:68:ASP:O	1:K:135:HIS:NE2	2.45	0.47
1:H:167:VAL:O	1:N:260:LYS:NZ	2.29	0.47
1:K:3:ALA:O	1:K:7:LYS:HG3	2.13	0.47
1:F:120:LEU:HB2	1:F:127:LEU:HB3	1.96	0.47
1:M:218:LYS:NZ	2:M:303:SO4:O4	2.42	0.47
1:F:173:GLY:O	1:F:174:ASN:ND2	2.47	0.47
1:H:227:GLU:OE1	1:H:230:ARG:NH2	2.46	0.47
2:M:304:SO4:O4	1:N:218:LYS:NZ	2.45	0.47
1:J:135:HIS:ND1	1:J:138:ILE:HG13	2.30	0.47
1:L:25:PHE:CE2	1:L:29:ILE:HD11	2.50	0.47
1:D:66:ASP:OD1	1:D:66:ASP:N	2.43	0.47
1:H:54:VAL:HG21	1:I:29:ILE:HG12	1.96	0.47
1:D:25:PHE:CE2	1:D:29:ILE:HD11	2.49	0.47
1:I:208:GLU:O	1:I:212:ILE:HG13	2.15	0.47
1:M:175:ASN:HB2	1:M:178:VAL:CG2	2.44	0.47
1:A:221:ASN:HB3	1:B:131:TYR:HA	1.97	0.46
1:D:252:ILE:HG12	1:E:165:LEU:HD21	1.96	0.46
1:N:230:ARG:NH2	1:N:231:GLU:HG2	2.30	0.46
1:A:30:THR:O	1:A:34:ILE:HG12	2.15	0.46
1:B:120:LEU:HB2	1:B:127:LEU:HB3	1.97	0.46
1:B:252:ILE:HG22	1:C:165:LEU:HD21	1.96	0.46
1:K:252:ILE:HG22	1:L:165:LEU:HD21	1.96	0.46
1:L:120:LEU:HB2	1:L:127:LEU:HB3	1.98	0.46
1:A:36:SER:HA	1:A:40:ARG:HB2	1.97	0.46
1:E:25:PHE:CE2	1:E:29:ILE:HD11	2.49	0.46
1:M:59:GLY:O	1:M:63:ASN:HB3	2.15	0.46
1:C:57:GLU:O	1:C:60:SER:OG	2.33	0.46
1:E:220:PRO:HD2	1:F:128:TYR:O	2.15	0.46
1:B:252:ILE:HD13	1:C:25:PHE:CE2	2.51	0.46
1:C:219:TYR:OH	2:C:302:SO4:O4	2.27	0.46
1:B:208:GLU:O	1:B:212:ILE:HG13	2.16	0.46
1:M:74:TYR:CE1	1:M:130:HIS:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:HD23	1:G:41:ILE:HD12	1.98	0.46
1:N:120:LEU:HB2	1:N:127:LEU:HB3	1.98	0.46
1:L:7:LYS:HA	1:L:7:LYS:HE2	1.97	0.46
1:G:24:LYS:NZ	1:G:28:ASP:OD2	2.47	0.46
1:M:208:GLU:O	1:M:212:ILE:HG13	2.16	0.46
1:A:187:GLU:OE2	1:A:190:ARG:NH2	2.40	0.45
1:D:166:ASN:ND2	1:D:266:VAL:O	2.49	0.45
1:E:175:ASN:HB3	1:E:269:LYS:NZ	2.32	0.45
1:N:142:LEU:HD13	1:N:202:ILE:HG23	1.99	0.45
1:B:231:GLU:HG3	1:C:206:TYR:CE2	2.52	0.45
1:F:67:LEU:HD13	1:F:237:TRP:CE3	2.51	0.45
1:K:208:GLU:O	1:K:212:ILE:HG13	2.16	0.45
1:G:19:LYS:O	1:G:23:ASN:ND2	2.49	0.45
1:K:38:ARG:HH22	1:L:8:ILE:HG23	1.81	0.45
1:F:159:ILE:O	1:F:163:ILE:HG13	2.15	0.45
1:H:142:LEU:HD13	1:H:202:ILE:HG23	1.97	0.45
1:I:110:LYS:HZ1	1:I:113:SER:HA	1.81	0.45
1:A:231:GLU:OE2	1:B:146:LYS:NZ	2.35	0.45
1:D:10:LYS:HB2	1:D:12:GLU:OE1	2.16	0.45
1:E:74:TYR:OH	1:E:130:HIS:ND1	2.34	0.45
1:A:219:TYR:OH	2:A:303:SO4:O2	2.29	0.45
1:H:159:ILE:O	1:H:163:ILE:HG13	2.16	0.45
1:G:52:VAL:O	1:G:248:ARG:NH1	2.50	0.45
1:H:25:PHE:CE2	1:N:252:ILE:HD13	2.52	0.45
1:D:22:TYR:CE2	1:D:26:LYS:HD2	2.52	0.44
1:E:71:SER:O	1:E:75:LYS:NZ	2.38	0.44
1:G:75:LYS:HG3	1:G:131:TYR:CZ	2.52	0.44
1:M:156:ILE:HG23	1:M:188:LEU:HD22	1.98	0.44
1:F:262:TRP:O	1:F:266:VAL:HG22	2.17	0.44
1:I:38:ARG:HH12	1:J:10:LYS:HG3	1.81	0.44
1:L:52:VAL:O	1:L:248:ARG:NH1	2.50	0.44
1:A:231:GLU:HG3	1:B:206:TYR:CE2	2.52	0.44
1:L:132:VAL:HG11	1:L:213:SER:HB3	1.98	0.44
1:N:25:PHE:CE2	1:N:29:ILE:HD11	2.53	0.44
1:B:57:GLU:CD	1:B:57:GLU:H	2.26	0.44
1:G:219:TYR:OH	2:G:303:SO4:O3	2.33	0.44
1:E:208:GLU:O	1:E:212:ILE:HG13	2.17	0.44
1:I:118:SER:H	1:I:129:THR:CG2	2.30	0.44
1:K:75:LYS:HD2	1:K:75:LYS:HA	1.70	0.44
1:F:252:ILE:HD13	1:G:25:PHE:CE2	2.52	0.44
1:G:227:GLU:OE1	1:G:230:ARG:NH2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HG11	1:D:213:SER:HB3	1.99	0.44
1:I:125:LYS:HB2	1:I:125:LYS:HE2	1.81	0.44
1:J:160:LYS:HG3	1:J:185:ILE:HG23	2.00	0.44
1:K:78:LYS:NZ	1:K:128:TYR:OH	2.42	0.44
1:L:210:ALA:O	1:L:214:THR:HG23	2.17	0.44
1:G:142:LEU:HD13	1:G:202:ILE:HG23	2.00	0.44
1:H:66:ASP:OD1	1:H:66:ASP:N	2.45	0.44
1:N:208:GLU:O	1:N:212:ILE:HG13	2.18	0.44
1:K:211:LYS:O	1:K:214:THR:OG1	2.31	0.43
1:C:252:ILE:HG22	1:D:165:LEU:HD21	2.00	0.43
1:D:44:ARG:HH12	1:D:151:GLU:HB3	1.83	0.43
1:E:175:ASN:O	1:E:178:VAL:HG22	2.16	0.43
1:F:66:ASP:OD1	1:F:66:ASP:N	2.37	0.43
1:H:49:ASN:CG	1:I:25:PHE:HE1	2.26	0.43
1:N:198:LEU:HA	1:N:198:LEU:HD23	1.74	0.43
1:J:209:ARG:NH1	1:J:233:ASP:OD2	2.52	0.43
1:A:21:GLU:HB3	1:G:46:ILE:HD12	2.01	0.43
1:D:230:ARG:NH2	1:D:231:GLU:HG2	2.33	0.43
1:D:259:TYR:HD1	1:D:259:TYR:O	2.01	0.43
1:K:25:PHE:CE2	1:K:29:ILE:HD11	2.54	0.43
1:N:12:GLU:OE1	1:N:12:GLU:N	2.45	0.43
1:B:12:GLU:OE1	1:B:12:GLU:N	2.47	0.43
1:I:171:GLU:HB2	1:I:269:LYS:NZ	2.34	0.43
1:K:46:ILE:HD12	1:L:21:GLU:HB3	2.01	0.43
1:K:57:GLU:O	1:K:60:SER:OG	2.31	0.43
1:M:35:GLU:HG2	1:M:40:ARG:NH1	2.34	0.43
1:N:76:ILE:HD12	1:N:76:ILE:H	1.84	0.43
1:E:74:TYR:CE1	1:E:130:HIS:HB2	2.54	0.43
1:E:159:ILE:O	1:E:163:ILE:HG13	2.19	0.43
1:E:36:SER:HB3	1:E:155:ILE:HG23	2.00	0.43
1:H:56:SER:HB3	1:H:60:SER:OG	2.18	0.43
1:K:227:GLU:OE1	1:K:230:ARG:NH2	2.49	0.43
1:K:164:GLN:O	1:K:167:VAL:HG12	2.19	0.43
1:A:38:ARG:NH2	1:B:10:LYS:O	2.38	0.42
1:B:221:ASN:ND2	1:C:128:TYR:CG	2.87	0.42
1:E:130:HIS:CD2	1:E:130:HIS:H	2.35	0.42
1:H:249:ASN:CG	1:I:161:LEU:HD22	2.44	0.42
1:H:252:ILE:HG22	1:I:165:LEU:HD21	2.01	0.42
1:C:70:VAL:HB	1:H:39:GLU:HG2	2.01	0.42
1:I:30:THR:O	1:I:34:ILE:HG12	2.18	0.42
1:I:44:ARG:NH1	2:I:301:SO4:O2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:TYR:OH	2:J:303:SO4:O1	2.32	0.42
1:M:135:HIS:CE1	1:M:137:GLN:HB3	2.54	0.42
1:N:241:LYS:O	1:N:245:VAL:HG23	2.19	0.42
1:A:132:VAL:HG11	1:A:213:SER:HB3	2.00	0.42
1:B:135:HIS:ND1	1:B:138:ILE:HG13	2.33	0.42
1:B:215:LYS:NZ	2:B:303:SO4:S	2.92	0.42
1:J:38:ARG:HH21	1:K:8:ILE:HG21	1.84	0.42
1:M:25:PHE:CE2	1:M:29:ILE:HD11	2.54	0.42
1:J:224:ASP:HB2	1:K:210:ALA:HB2	2.01	0.42
1:I:118:SER:O	1:I:129:THR:HG22	2.20	0.42
1:J:44:ARG:NH2	2:J:301:SO4:O2	2.49	0.42
1:C:25:PHE:CE2	1:C:29:ILE:HD11	2.54	0.42
1:C:215:LYS:NZ	2:C:302:SO4:O2	2.53	0.42
1:E:227:GLU:OE1	1:E:230:ARG:NH2	2.49	0.42
1:G:42:PRO:O	1:G:46:ILE:HG12	2.19	0.42
1:K:78:LYS:HG2	1:K:128:TYR:CE2	2.55	0.42
1:B:36:SER:HB3	1:B:155:ILE:HG23	2.02	0.42
1:C:74:TYR:CE1	1:C:130:HIS:HB2	2.54	0.42
1:H:21:GLU:HB3	1:N:46:ILE:HD12	2.00	0.42
1:H:175:ASN:O	1:H:178:VAL:HG22	2.20	0.42
1:H:208:GLU:O	1:H:212:ILE:HG13	2.20	0.42
1:M:130:HIS:CD2	1:M:130:HIS:H	2.37	0.42
1:A:42:PRO:O	1:A:46:ILE:HG12	2.19	0.42
1:H:40:ARG:O	1:H:44:ARG:HG2	2.20	0.42
1:L:46:ILE:O	1:L:50:ASN:ND2	2.53	0.42
1:A:130:HIS:HB3	1:A:217:LEU:HD22	2.02	0.42
1:B:135:HIS:CE1	1:B:137:GLN:HB3	2.55	0.42
1:C:59:GLY:O	1:C:63:ASN:HB3	2.20	0.42
1:F:135:HIS:ND1	1:F:138:ILE:HG13	2.35	0.42
1:G:135:HIS:ND1	1:G:138:ILE:HG13	2.35	0.42
1:C:239:HIS:CE1	1:D:196:PHE:CE1	3.08	0.41
1:I:19:LYS:O	1:I:23:ASN:ND2	2.51	0.41
1:J:37:LEU:HD23	1:J:41:ILE:HD12	2.02	0.41
1:N:56:SER:HB3	1:N:60:SER:OG	2.20	0.41
1:C:66:ASP:OD1	1:C:66:ASP:N	2.44	0.41
1:I:142:LEU:HD23	1:I:142:LEU:HA	1.91	0.41
1:K:25:PHE:HE2	1:K:29:ILE:HD11	1.85	0.41
1:K:56:SER:HB3	1:K:60:SER:OG	2.20	0.41
1:M:175:ASN:O	1:M:178:VAL:HG22	2.20	0.41
1:B:57:GLU:OE2	1:H:131:TYR:OH	2.29	0.41
1:B:159:ILE:O	1:B:163:ILE:HG13	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:THR:O	1:D:34:ILE:HG12	2.19	0.41
1:E:59:GLY:O	1:E:63:ASN:HB3	2.20	0.41
1:A:56:SER:HB3	1:A:60:SER:OG	2.21	0.41
1:K:9:ASP:OD1	1:K:9:ASP:N	2.53	0.41
1:F:54:VAL:HG21	1:G:29:ILE:HG12	2.03	0.41
1:G:164:GLN:O	1:G:167:VAL:HG12	2.21	0.41
1:H:206:TYR:CE2	1:N:231:GLU:HG3	2.56	0.41
1:L:230:ARG:NH2	1:L:231:GLU:HG2	2.36	0.41
1:M:35:GLU:HG2	1:M:40:ARG:CZ	2.51	0.41
1:A:159:ILE:O	1:A:163:ILE:HG13	2.21	0.41
1:J:46:ILE:HD12	1:K:21:GLU:HB3	2.01	0.41
1:K:30:THR:O	1:K:34:ILE:HG12	2.20	0.41
1:B:210:ALA:O	1:B:214:THR:HG23	2.21	0.41
1:H:221:ASN:HB3	1:I:131:TYR:HA	2.03	0.41
1:J:212:ILE:O	1:J:216:VAL:HG23	2.19	0.41
1:K:44:ARG:NH1	2:K:301:SO4:O3	2.46	0.41
1:L:30:THR:O	1:L:34:ILE:HG12	2.20	0.41
1:A:152:LEU:HD21	1:A:191:VAL:HG12	2.03	0.41
1:E:238:ILE:O	1:E:242:ILE:HG13	2.21	0.41
1:A:169:ARG:NH2	1:A:171:GLU:OE2	2.37	0.41
1:B:211:LYS:O	1:B:214:THR:OG1	2.29	0.41
1:E:38:ARG:NH2	1:F:10:LYS:O	2.50	0.41
1:F:36:SER:HB3	1:F:155:ILE:HG23	2.03	0.41
1:F:259:TYR:HD1	1:F:259:TYR:O	2.03	0.41
1:I:135:HIS:CE1	1:I:137:GLN:HB3	2.56	0.41
1:M:46:ILE:HD12	1:N:21:GLU:HB3	2.03	0.41
1:E:132:VAL:HG11	1:E:213:SER:HB3	2.03	0.41
1:E:221:ASN:HB2	1:F:130:HIS:O	2.21	0.41
1:G:238:ILE:O	1:G:242:ILE:HG13	2.21	0.41
1:H:135:HIS:ND1	1:H:138:ILE:HG13	2.36	0.41
1:I:67:LEU:HD13	1:I:237:TRP:CE3	2.56	0.41
1:M:142:LEU:HD13	1:M:202:ILE:HG23	2.03	0.41
1:B:67:LEU:HD13	1:B:237:TRP:CE3	2.57	0.40
1:K:166:ASN:ND2	1:K:266:VAL:O	2.53	0.40
1:B:66:ASP:OD1	1:B:66:ASP:N	2.37	0.40
1:G:30:THR:O	1:G:34:ILE:HG12	2.21	0.40
1:G:230:ARG:NH2	1:G:231:GLU:HG2	2.36	0.40
1:F:10:LYS:HA	1:F:10:LYS:HD3	1.95	0.40
1:L:252:ILE:HD13	1:M:25:PHE:CE2	2.57	0.40
1:A:224:ASP:HB2	1:B:210:ALA:HB2	2.02	0.40
1:G:56:SER:HB3	1:G:60:SER:OG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:ASP:OD1	1:K:66:ASP:N	2.38	0.40
1:A:218:LYS:NZ	2:A:303:SO4:O3	2.48	0.40
1:D:259:TYR:C	1:D:259:TYR:CD1	3.00	0.40
1:M:152:LEU:HD21	1:M:191:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	212/280 (76%)	200 (94%)	12 (6%)	0	100	100
1	B	228/280 (81%)	216 (95%)	12 (5%)	0	100	100
1	C	218/280 (78%)	206 (94%)	11 (5%)	1 (0%)	24	57
1	D	229/280 (82%)	217 (95%)	12 (5%)	0	100	100
1	E	208/280 (74%)	199 (96%)	9 (4%)	0	100	100
1	F	225/280 (80%)	215 (96%)	10 (4%)	0	100	100
1	G	209/280 (75%)	198 (95%)	11 (5%)	0	100	100
1	H	212/280 (76%)	202 (95%)	10 (5%)	0	100	100
1	I	232/280 (83%)	220 (95%)	11 (5%)	1 (0%)	30	61
1	J	210/280 (75%)	198 (94%)	12 (6%)	0	100	100
1	K	219/280 (78%)	210 (96%)	9 (4%)	0	100	100
1	L	229/280 (82%)	217 (95%)	12 (5%)	0	100	100
1	M	209/280 (75%)	199 (95%)	10 (5%)	0	100	100
1	N	229/280 (82%)	218 (95%)	11 (5%)	0	100	100
All	All	3069/3920 (78%)	2915 (95%)	152 (5%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	124	ASP
1	I	130	HIS

5.3.2 Protein sidechains ⓘ

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	202/261 (77%)	202 (100%)	0	100	100
1	B	218/261 (84%)	218 (100%)	0	100	100
1	C	208/261 (80%)	208 (100%)	0	100	100
1	D	218/261 (84%)	218 (100%)	0	100	100
1	E	198/261 (76%)	198 (100%)	0	100	100
1	F	215/261 (82%)	215 (100%)	0	100	100
1	G	199/261 (76%)	199 (100%)	0	100	100
1	H	202/261 (77%)	202 (100%)	0	100	100
1	I	221/261 (85%)	221 (100%)	0	100	100
1	J	200/261 (77%)	200 (100%)	0	100	100
1	K	207/261 (79%)	207 (100%)	0	100	100
1	L	219/261 (84%)	219 (100%)	0	100	100
1	M	199/261 (76%)	199 (100%)	0	100	100
1	N	219/261 (84%)	219 (100%)	0	100	100
All	All	2925/3654 (80%)	2925 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	50	ASN
1	C	50	ASN
1	C	239	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	270	ASN
1	D	115	ASN
1	D	130	HIS
1	D	174	ASN
1	D	239	HIS
1	E	50	ASN
1	F	130	HIS
1	F	181	GLN
1	F	239	HIS
1	G	158	ASN
1	G	181	GLN
1	G	239	HIS
1	H	50	ASN
1	H	239	HIS
1	I	32	GLN
1	I	65	ASN
1	J	226	GLN
1	K	239	HIS
1	L	50	ASN
1	L	115	ASN
1	L	130	HIS
1	L	239	HIS
1	M	32	GLN
1	M	226	GLN
1	M	239	HIS
1	N	55	ASN
1	N	115	ASN
1	N	130	HIS
1	N	239	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

60 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	$\# Z > 2$
2	SO4	B	305	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	F	303	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	J	301	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	E	304	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	G	301	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	F	304	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	L	301	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	L	302	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	F	302	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	M	303	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	K	303	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	L	304	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	I	302	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	K	304	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	I	305	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	N	303	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	N	302	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	L	303	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	301	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	J	303	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	J	305	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	303	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	K	302	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	C	304	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	304	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	J	302	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	M	302	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	302	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	N	301	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	E	303	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	I	304	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	K	301	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	D	302	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	F	305	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	G	303	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	H	302	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	M	301	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	N	304	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	M	304	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	I	301	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	H	303	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	M	305	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	J	304	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	B	304	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	I	303	-	4,4,4	0.24	0	6,6,6	0.08	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.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	SO4	1	0
2	M	303	SO4	2	0
2	K	303	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	SO4	3	0
2	C	302	SO4	2	0
2	L	303	SO4	1	0
2	J	303	SO4	3	0
2	B	303	SO4	2	0
2	E	303	SO4	2	0
2	K	301	SO4	1	0
2	F	305	SO4	1	0
2	G	303	SO4	2	0
2	H	302	SO4	2	0
2	N	304	SO4	1	0
2	M	304	SO4	1	0
2	D	301	SO4	1	0
2	G	304	SO4	1	0
2	I	301	SO4	1	0
2	B	301	SO4	1	0
2	D	303	SO4	2	0
2	I	303	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	216/280 (77%)	-0.35	5 (2%) 61 39	42, 66, 133, 175	0
1	B	232/280 (82%)	-0.36	6 (2%) 57 36	35, 62, 147, 186	0
1	C	222/280 (79%)	-0.44	2 (0%) 81 63	37, 63, 122, 167	0
1	D	233/280 (83%)	-0.27	3 (1%) 75 56	42, 70, 141, 173	0
1	E	212/280 (75%)	-0.32	5 (2%) 59 38	49, 79, 120, 162	0
1	F	229/280 (81%)	-0.21	4 (1%) 69 48	54, 85, 156, 192	0
1	G	213/280 (76%)	-0.32	4 (1%) 66 45	45, 76, 128, 186	0
1	H	216/280 (77%)	-0.45	3 (1%) 73 53	37, 61, 117, 153	0
1	I	236/280 (84%)	-0.31	6 (2%) 58 37	41, 64, 140, 177	0
1	J	214/280 (76%)	-0.40	7 (3%) 49 29	44, 64, 116, 170	0
1	K	223/280 (79%)	-0.39	2 (0%) 81 63	44, 69, 121, 155	0
1	L	233/280 (83%)	-0.26	9 (3%) 43 24	40, 68, 155, 196	0
1	M	213/280 (76%)	-0.44	2 (0%) 81 63	41, 66, 114, 158	0
1	N	233/280 (83%)	-0.35	6 (2%) 57 36	39, 66, 150, 203	0
All	All	3125/3920 (79%)	-0.35	64 (2%) 65 44	35, 69, 135, 203	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	VAL	6.1
1	N	109	VAL	4.3
1	L	111	HIS	4.1
1	L	122	ILE	4.0
1	L	5	LEU	3.9
1	F	126	VAL	3.7
1	E	76	ILE	3.7
1	I	76	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	76	ILE	3.5
1	M	8	ILE	3.5
1	I	8	ILE	3.5
1	F	76	ILE	3.4
1	B	126	VAL	3.3
1	J	76	ILE	3.3
1	G	8	ILE	3.2
1	N	108	HIS	3.2
1	B	128	TYR	3.2
1	E	8	ILE	3.2
1	H	126	VAL	3.1
1	H	8	ILE	3.1
1	A	127	LEU	3.0
1	D	8	ILE	3.0
1	E	221	ASN	3.0
1	B	8	ILE	3.0
1	N	8	ILE	3.0
1	L	126	VAL	2.9
1	G	128	TYR	2.8
1	I	5	LEU	2.8
1	J	8	ILE	2.8
1	N	110	LYS	2.7
1	G	221	ASN	2.7
1	L	8	ILE	2.7
1	A	128	TYR	2.7
1	A	130	HIS	2.6
1	L	130	HIS	2.6
1	I	125	LYS	2.6
1	B	76	ILE	2.5
1	J	75	LYS	2.5
1	H	9	ASP	2.5
1	A	126	VAL	2.5
1	B	121	ILE	2.4
1	K	221	ASN	2.4
1	J	130	HIS	2.4
1	A	8	ILE	2.4
1	J	6	ASN	2.4
1	J	74	TYR	2.4
1	B	125	LYS	2.3
1	F	75	LYS	2.3
1	C	122	ILE	2.3
1	L	9	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	121	ILE	2.3
1	L	76	ILE	2.3
1	I	108	HIS	2.3
1	D	126	VAL	2.2
1	E	11	ILE	2.2
1	F	8	ILE	2.2
1	E	253	MET	2.2
1	G	13	PRO	2.2
1	M	129	THR	2.1
1	N	122	ILE	2.1
1	J	131	TYR	2.1
1	C	127	LEU	2.1
1	D	108	HIS	2.1
1	K	0	GLY	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 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(Å ²)	Q<0.9
2	SO4	J	305	5/5	0.46	0.10	189,189,191,195	0
2	SO4	J	302	5/5	0.50	0.13	167,170,172,173	0
2	SO4	E	302	5/5	0.52	0.11	167,168,169,170	0
2	SO4	I	302	5/5	0.54	0.11	162,169,170,172	0
2	SO4	B	304	5/5	0.55	0.14	170,174,182,186	0
2	SO4	N	304	5/5	0.56	0.11	163,176,179,184	0
2	SO4	M	305	5/5	0.62	0.10	144,150,151,152	0
2	SO4	H	301	5/5	0.63	0.11	174,175,183,185	0
2	SO4	D	304	5/5	0.65	0.10	148,149,152,152	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	G	303	5/5	0.65	0.25	119,136,139,147	0
2	SO4	M	302	5/5	0.66	0.09	155,157,162,168	0
2	SO4	G	304	5/5	0.67	0.09	142,151,152,157	0
2	SO4	N	303	5/5	0.67	0.10	159,159,164,172	0
2	SO4	D	303	5/5	0.67	0.12	195,196,198,201	0
2	SO4	B	305	5/5	0.68	0.23	125,135,139,148	0
2	SO4	A	304	5/5	0.68	0.09	157,162,165,171	0
2	SO4	F	305	5/5	0.69	0.08	158,168,170,176	0
2	SO4	N	302	5/5	0.69	0.10	155,158,161,162	0
2	SO4	L	302	5/5	0.69	0.20	132,137,147,149	0
2	SO4	F	302	5/5	0.69	0.11	154,155,161,164	0
2	SO4	I	305	5/5	0.70	0.10	152,163,167,169	0
2	SO4	B	302	5/5	0.70	0.12	163,168,173,174	0
2	SO4	A	302	5/5	0.70	0.12	172,175,176,181	0
2	SO4	L	304	5/5	0.71	0.21	138,144,147,153	0
2	SO4	H	303	5/5	0.72	0.09	141,146,150,160	0
2	SO4	E	304	5/5	0.72	0.08	158,163,167,169	0
2	SO4	K	304	5/5	0.73	0.09	144,147,149,151	0
2	SO4	B	303	5/5	0.73	0.10	164,168,171,171	0
2	SO4	C	301	5/5	0.73	0.08	176,180,183,186	0
2	SO4	K	302	5/5	0.73	0.09	147,161,165,166	0
2	SO4	G	302	5/5	0.74	0.09	148,151,153,156	0
2	SO4	J	304	5/5	0.74	0.09	137,144,147,154	0
2	SO4	D	302	5/5	0.75	0.09	147,169,175,177	0
2	SO4	I	304	5/5	0.75	0.12	184,186,188,190	0
2	SO4	C	303	5/5	0.75	0.10	143,147,151,160	0
2	SO4	F	303	5/5	0.76	0.08	159,164,167,170	0
2	SO4	C	304	5/5	0.77	0.09	148,158,160,161	0
2	SO4	M	304	5/5	0.77	0.10	174,176,180,183	0
2	SO4	J	303	5/5	0.78	0.09	178,180,184,184	0
2	SO4	F	304	5/5	0.79	0.09	183,185,186,186	0
2	SO4	I	303	5/5	0.79	0.09	148,149,157,160	0
2	SO4	M	303	5/5	0.81	0.19	128,133,138,141	0
2	SO4	A	303	5/5	0.81	0.21	118,125,138,145	0
2	SO4	K	303	5/5	0.81	0.23	132,133,143,154	0
2	SO4	E	303	5/5	0.82	0.17	129,138,142,142	0
2	SO4	K	301	5/5	0.83	0.16	118,126,130,132	0
2	SO4	L	303	5/5	0.83	0.10	145,149,153,156	0
2	SO4	F	301	5/5	0.84	0.10	114,123,126,128	0
2	SO4	H	302	5/5	0.85	0.17	91,116,116,140	0
2	SO4	G	301	5/5	0.85	0.19	97,100,114,119	0
2	SO4	E	301	5/5	0.86	0.11	105,115,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	302	5/5	0.86	0.15	105,113,116,117	0
2	SO4	D	301	5/5	0.88	0.11	104,109,114,121	0
2	SO4	N	301	5/5	0.90	0.09	90,104,107,115	0
2	SO4	A	301	5/5	0.91	0.14	81,85,115,117	0
2	SO4	L	301	5/5	0.92	0.09	65,82,96,102	0
2	SO4	I	301	5/5	0.93	0.13	87,90,109,119	0
2	SO4	B	301	5/5	0.94	0.11	87,98,101,108	0
2	SO4	J	301	5/5	0.95	0.08	68,85,87,94	0
2	SO4	M	301	5/5	0.97	0.06	77,78,84,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.