



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:00 pm BST

PDB ID : 1U10
Title : MEPA, active form with ZN in P1
Authors : Marcyjaniak, M.; Odintsov, S.G.; Sabala, I.; Bochtler, M.
Deposited on : 2004-07-14
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

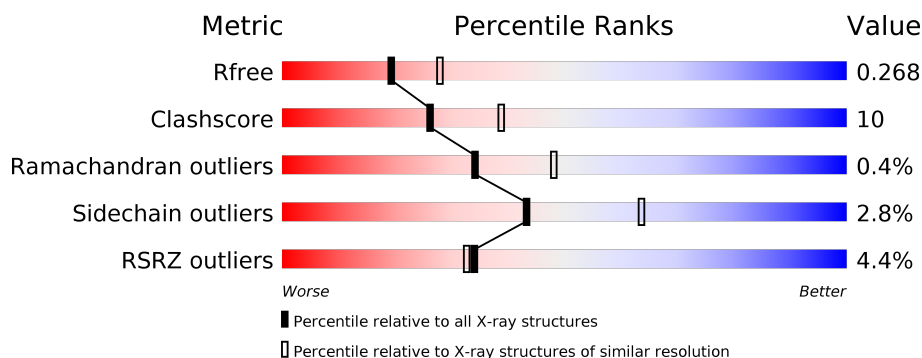
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	255	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 9%</div> </div> </div>
1	B	255	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	C	255	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	D	255	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	E	255	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	F	255	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11311 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 Penicillin-insensitive murein endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	0	0
			1813	1142	329	330	6	6			
1	B	239	Total	C	N	O	S	Se	0	0	0
			1871	1179	339	341	6	6			
1	C	241	Total	C	N	O	S	Se	0	0	0
			1885	1189	341	343	6	6			
1	D	241	Total	C	N	O	S	Se	0	0	0
			1885	1189	341	343	6	6			
1	E	241	Total	C	N	O	S	Se	0	0	0
			1885	1189	341	343	6	6			
1	F	240	Total	C	N	O	S	Se	0	0	0
			1878	1184	340	342	6	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
A	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
A	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
A	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
A	100	MSE	MET	MODIFIED RESIDUE	UNP P14007
A	210	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	100	MSE	MET	MODIFIED RESIDUE	UNP P14007
B	210	MSE	MET	MODIFIED RESIDUE	UNP P14007
C	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
C	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
C	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
C	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
C	100	MSE	MET	MODIFIED RESIDUE	UNP P14007

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Chain	Residue	Modelled	Actual	Comment	Reference
C	210	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	100	MSE	MET	MODIFIED RESIDUE	UNP P14007
D	210	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	100	MSE	MET	MODIFIED RESIDUE	UNP P14007
E	210	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	61	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	76	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	90	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	98	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	100	MSE	MET	MODIFIED RESIDUE	UNP P14007
F	210	MSE	MET	MODIFIED RESIDUE	UNP P14007

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

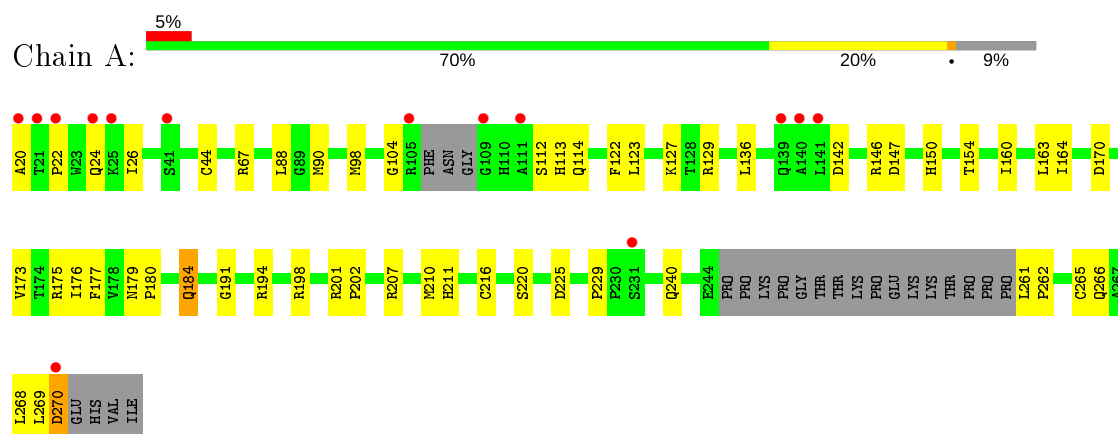
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	12	Total	O	0	0
			12	12		
4	C	9	Total	O	0	0
			9	9		
4	D	8	Total	O	0	0
			8	8		
4	E	12	Total	O	0	0
			12	12		
4	F	8	Total	O	0	0
			8	8		

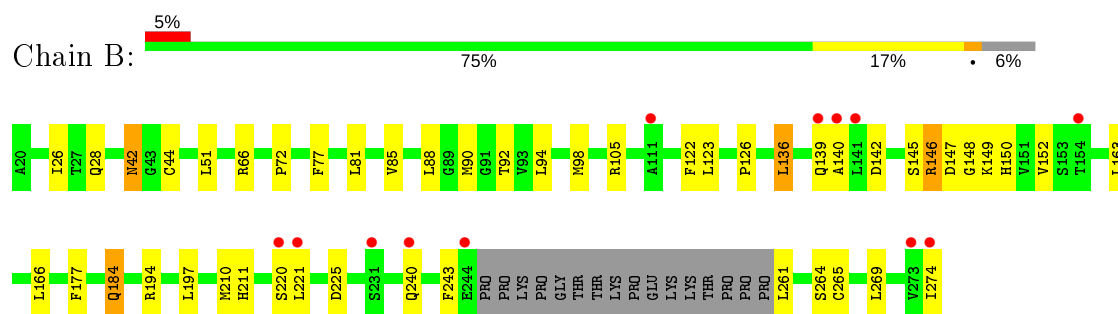
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

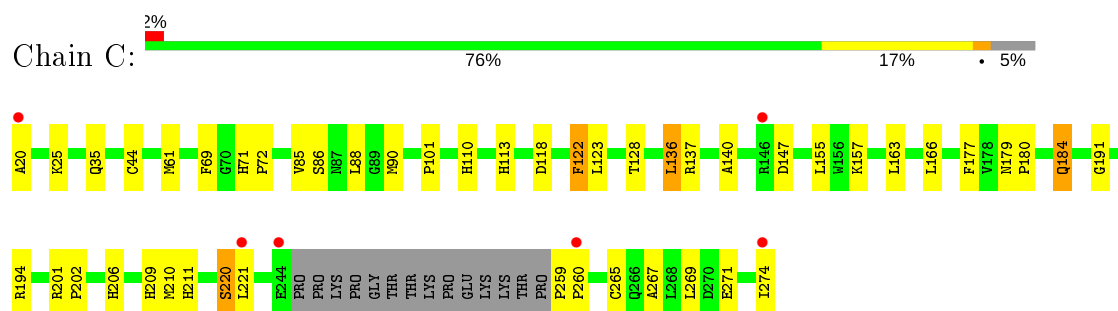
- Molecule 1: Penicillin-insensitive murein endopeptidase




- Molecule 1: Penicillin-insensitive murein endopeptidase

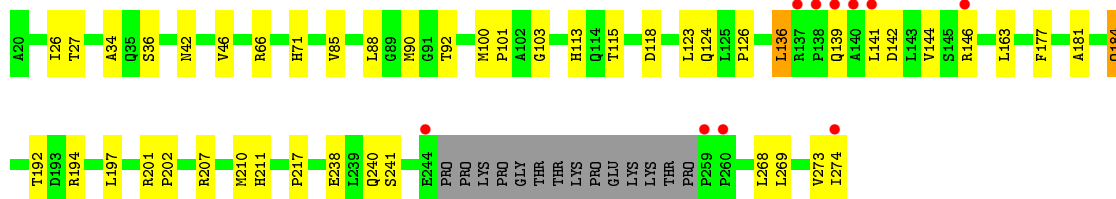


- Molecule 1: Penicillin-insensitive murein endopeptidase



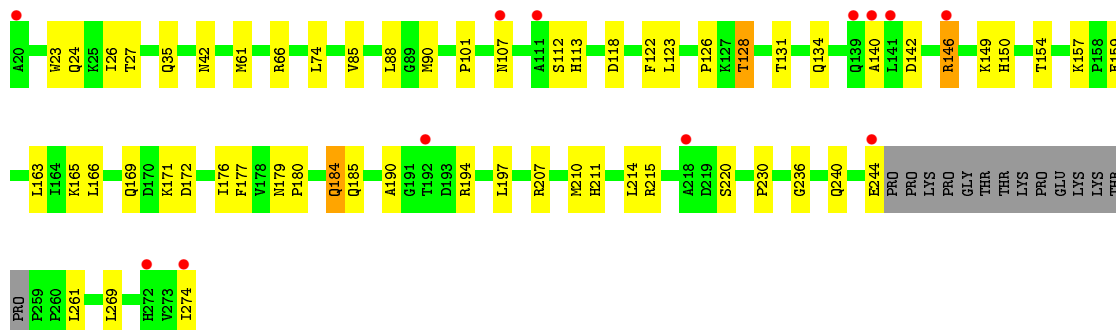
- Molecule 1: Penicillin-insensitive murein endopeptidase

Chain D:  4% 76% 18% • 5%




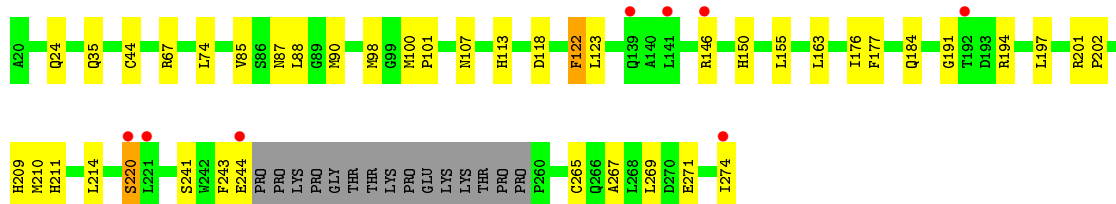
• Molecule 1: Penicillin-insensitive murein endopeptidase

Chain E:  5% 71% 22% • 5%



• Molecule 1: Penicillin-insensitive murein endopeptidase

Chain F:  3% 78% 16% • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.61Å 77.99Å 127.66Å 93.15° 95.93° 90.75°	Depositor
Resolution (Å)	20.00 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.40) 98.3 (19.95-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.234 , 0.266 0.235 , 0.268	Depositor DCC
R_{free} test set	2658 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11311	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 36.19 % 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 5.1911e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, 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	0.46	0/1851	0.64	0/2502
1	B	0.51	0/1912	0.66	0/2585
1	C	0.51	0/1928	0.66	0/2608
1	D	0.48	0/1928	0.68	0/2608
1	E	0.49	0/1928	0.68	0/2608
1	F	0.50	0/1920	0.65	0/2596
All	All	0.49	0/11467	0.66	0/15507

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	1788	40	0
1	B	1871	0	1840	40	0
1	C	1885	0	1855	39	0
1	D	1885	0	1855	38	0
1	E	1885	0	1855	51	0
1	F	1878	0	1848	28	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	6	0	0	1	0
4	B	12	0	0	3	0
4	C	9	0	0	1	0
4	D	8	0	0	0	0
4	E	12	0	0	1	0
4	F	8	0	0	0	0
All	All	11311	0	11041	227	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 10.

All (227) 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:B:146:ARG:N	1:B:146:ARG:HD3	1.58	1.09
1:B:146:ARG:H	1:B:146:ARG:CD	1.64	1.08
1:E:146:ARG:NH2	1:F:146:ARG:HH21	1.64	0.95
1:C:269:LEU:HD23	1:C:274:ILE:HD12	1.46	0.94
1:E:146:ARG:HH21	1:F:146:ARG:HH21	1.16	0.94
1:E:184:GLN:HE22	1:E:240:GLN:HE22	1.11	0.93
1:B:146:ARG:H	1:B:146:ARG:HD3	0.79	0.92
1:B:221:LEU:HB2	4:B:507:HOH:O	1.69	0.92
1:A:22:PRO:HB2	1:A:269:LEU:HD22	1.52	0.92
1:C:44:CYS:HG	1:C:265:CYS:HG	0.94	0.85
1:F:44:CYS:HG	1:F:265:CYS:HG	1.15	0.85
1:A:44:CYS:HG	1:A:265:CYS:HG	0.87	0.85
1:F:163:LEU:HG	1:F:210:MSE:HE1	1.61	0.82
1:B:66:ARG:HD2	4:B:509:HOH:O	1.80	0.80
1:E:24:GLN:NE2	1:E:107:ASN:HB2	1.99	0.77
1:A:177:PHE:HB2	1:A:211:HIS:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD21	1:B:210:MSE:HB3	1.67	0.75
1:D:123:LEU:HD21	1:D:210:MSE:HB3	1.67	0.75
1:B:44:CYS:HG	1:B:265:CYS:HG	0.90	0.74
1:D:88:LEU:HD12	1:D:90:MSE:HE2	1.69	0.74
1:A:127:LYS:HD2	1:C:221:LEU:HD13	1.68	0.73
1:F:123:LEU:HD21	1:F:210:MSE:HB3	1.69	0.71
1:F:194:ARG:HB2	1:F:197:LEU:HD12	1.72	0.71
1:B:88:LEU:HD12	1:B:90:MSE:HE2	1.73	0.70
1:B:163:LEU:HG	1:B:210:MSE:HE1	1.74	0.70
1:B:177:PHE:HB2	1:B:211:HIS:HB3	1.73	0.70
1:C:191:GLY:O	1:C:194:ARG:HD2	1.90	0.70
1:C:85:VAL:HA	1:C:90:MSE:HE3	1.72	0.70
1:C:35:GLN:OE1	1:C:220:SER:HA	1.91	0.70
1:E:85:VAL:HA	1:E:90:MSE:HE3	1.72	0.70
1:C:20:ALA:O	1:C:25:LYS:HE3	1.92	0.69
1:E:146:ARG:NH2	1:F:146:ARG:NH2	2.37	0.69
1:F:269:LEU:HD23	1:F:274:ILE:HD12	1.74	0.68
1:F:244:GLU:HA	1:F:244:GLU:OE2	1.93	0.68
1:A:191:GLY:O	1:A:194:ARG:HD2	1.93	0.68
1:A:104:GLY:C	1:A:114:GLN:HG2	2.14	0.67
1:E:150:HIS:CD2	1:F:150:HIS:CD2	2.83	0.67
1:C:269:LEU:CD2	1:C:274:ILE:HD12	2.25	0.66
1:E:190:ALA:HB3	1:E:194:ARG:NH1	2.12	0.65
1:E:90:MSE:HE1	1:E:166:LEU:CD1	2.27	0.65
1:B:146:ARG:NH1	1:B:152:VAL:HG22	2.12	0.64
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.61	0.64
1:A:146:ARG:HG3	1:A:146:ARG:HH11	1.63	0.63
1:E:194:ARG:HB2	1:E:197:LEU:HD12	1.80	0.62
1:E:244:GLU:HA	1:E:244:GLU:OE2	1.97	0.62
1:E:269:LEU:CD2	1:E:274:ILE:HD12	2.29	0.62
1:C:110:HIS:HE1	1:C:209:HIS:NE2	1.97	0.62
1:B:146:ARG:HH11	1:B:152:VAL:HG22	1.62	0.62
1:D:26:ILE:HB	1:D:274:ILE:OXT	2.00	0.61
1:E:149:LYS:HB2	1:E:150:HIS:CD2	2.36	0.61
1:A:170:ASP:HB3	1:A:173:VAL:HG23	1.82	0.61
1:D:163:LEU:HG	1:D:210:MSE:HE1	1.82	0.60
1:A:22:PRO:HB2	1:A:269:LEU:CD2	2.30	0.60
1:A:22:PRO:CB	1:A:269:LEU:HD22	2.31	0.60
1:A:146:ARG:NH1	4:A:603:HOH:O	2.35	0.59
1:B:85:VAL:HA	1:B:90:MSE:CE	2.33	0.58
1:E:112:SER:O	1:E:113:HIS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:VAL:HA	1:D:90:MSE:CE	2.34	0.58
1:D:268:LEU:HB2	1:D:274:ILE:HD11	1.86	0.57
1:C:267:ALA:O	1:C:271:GLU:HG3	2.04	0.57
1:E:35:GLN:OE1	1:E:220:SER:HA	2.05	0.57
1:D:142:ASP:OD1	1:D:207:ARG:HD3	2.05	0.56
1:C:88:LEU:HD12	1:C:90:MSE:HE2	1.87	0.56
1:F:88:LEU:HD12	1:F:90:MSE:HE2	1.88	0.55
1:E:177:PHE:HB2	1:E:211:HIS:HB3	1.89	0.55
1:C:221:LEU:HB2	4:C:507:HOH:O	2.05	0.55
1:E:23:TRP:CH2	1:E:274:ILE:HD11	2.41	0.55
1:B:194:ARG:HB2	1:B:197:LEU:HD12	1.89	0.55
1:D:163:LEU:HG	1:D:210:MSE:CE	2.37	0.55
1:A:142:ASP:OD1	1:A:207:ARG:HD3	2.07	0.54
1:C:137:ARG:NH1	1:C:137:ARG:HG3	2.20	0.54
1:D:146:ARG:HG3	1:D:146:ARG:HH11	1.72	0.54
1:A:210:MSE:O	1:A:210:MSE:HG3	2.08	0.54
1:B:26:ILE:HD11	1:B:28:GLN:O	2.07	0.54
1:D:177:PHE:HB2	1:D:211:HIS:HB3	1.89	0.54
1:F:35:GLN:OE1	1:F:220:SER:HA	2.08	0.54
1:E:123:LEU:HD21	1:E:210:MSE:HB3	1.90	0.54
1:E:163:LEU:HG	1:E:210:MSE:HE1	1.88	0.54
1:F:113:HIS:HA	1:F:118:ASP:HB2	1.88	0.54
1:B:147:ASP:OD1	1:B:147:ASP:C	2.47	0.53
1:E:184:GLN:NE2	1:E:240:GLN:HE22	1.94	0.53
1:C:163:LEU:HG	1:C:210:MSE:HE1	1.89	0.53
1:E:165:LYS:O	1:E:169:GLN:HG3	2.09	0.53
1:F:267:ALA:O	1:F:271:GLU:HG3	2.08	0.53
1:D:113:HIS:HA	1:D:118:ASP:HB2	1.89	0.53
1:C:110:HIS:CE1	1:C:209:HIS:NE2	2.76	0.53
1:E:269:LEU:HD23	1:E:274:ILE:HD12	1.90	0.53
1:C:85:VAL:HA	1:C:90:MSE:CE	2.39	0.52
1:B:142:ASP:N	4:B:511:HOH:O	2.41	0.52
1:D:273:VAL:HG12	1:D:273:VAL:O	2.09	0.52
1:E:149:LYS:HB2	1:E:150:HIS:HD2	1.73	0.52
1:A:269:LEU:O	1:A:270:ASP:HB2	2.08	0.52
1:E:88:LEU:HB2	1:E:90:MSE:HE2	1.91	0.52
1:A:163:LEU:HG	1:A:210:MSE:HE1	1.91	0.51
1:A:123:LEU:HD21	1:A:210:MSE:HB3	1.93	0.51
1:A:176:ILE:HA	1:A:211:HIS:O	2.10	0.51
1:B:269:LEU:HD23	1:B:274:ILE:HD12	1.92	0.51
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD12	1:A:262:PRO:CD	2.41	0.51
1:C:90:MSE:HE1	1:C:166:LEU:HD11	1.92	0.51
1:D:85:VAL:HA	1:D:90:MSE:HE3	1.93	0.51
1:E:171:LYS:O	1:E:215:ARG:NH2	2.43	0.51
1:C:177:PHE:HB2	1:C:211:HIS:HB3	1.92	0.50
1:C:123:LEU:HD21	1:C:210:MSE:HB3	1.92	0.50
1:D:194:ARG:HB2	1:D:197:LEU:HD12	1.91	0.50
1:B:90:MSE:HE1	1:B:166:LEU:CD1	2.41	0.50
1:E:27:THR:HA	1:E:66:ARG:NH1	2.26	0.50
1:E:26:ILE:HG23	1:E:101:PRO:HB2	1.93	0.50
1:E:176:ILE:HA	1:E:211:HIS:O	2.12	0.50
1:F:163:LEU:HG	1:F:210:MSE:CE	2.35	0.50
1:E:142:ASP:OD1	1:E:207:ARG:HD3	2.12	0.50
1:D:27:THR:HA	1:D:66:ARG:NH1	2.27	0.49
1:A:268:LEU:C	1:A:270:ASP:H	2.14	0.49
1:B:85:VAL:HG13	1:B:90:MSE:HE3	1.93	0.49
1:D:269:LEU:HD23	1:D:274:ILE:HD12	1.95	0.49
1:D:92:THR:O	1:D:126:PRO:HD2	2.12	0.48
1:E:90:MSE:HE1	1:E:166:LEU:HD12	1.93	0.48
1:A:20:ALA:N	1:A:24:GLN:OE1	2.46	0.48
1:C:71:HIS:CE1	1:C:72:PRO:HD2	2.49	0.48
1:D:71:HIS:CD2	1:D:217:PRO:HG2	2.48	0.48
1:C:71:HIS:ND1	1:C:72:PRO:HD2	2.29	0.47
1:E:88:LEU:HD12	1:E:90:MSE:HE2	1.95	0.47
1:F:184:GLN:NE2	1:F:243:PHE:CE2	2.81	0.47
1:E:171:LYS:NZ	1:E:172:ASP:OD1	2.31	0.47
1:A:201:ARG:HA	1:A:202:PRO:HD3	1.81	0.47
1:B:149:LYS:HA	1:B:243:PHE:CE1	2.50	0.47
1:E:163:LEU:HG	1:E:210:MSE:CE	2.45	0.47
1:C:147:ASP:C	1:C:147:ASP:OD1	2.53	0.47
1:C:90:MSE:HE1	1:C:166:LEU:CD1	2.45	0.47
1:A:112:SER:O	1:A:113:HIS:HB2	2.15	0.47
1:D:34:ALA:HA	1:D:46:VAL:O	2.15	0.47
1:E:113:HIS:HA	1:E:118:ASP:HB2	1.95	0.47
1:E:131:THR:OG1	1:E:134:GLN:HG3	2.15	0.47
1:E:88:LEU:CD1	1:E:90:MSE:HE2	2.44	0.47
1:F:177:PHE:HB2	1:F:211:HIS:HB3	1.97	0.46
1:A:216:CYS:HB2	1:A:225:ASP:OD2	2.14	0.46
1:B:147:ASP:OD1	1:B:148:GLY:N	2.49	0.46
1:A:160:ILE:O	1:A:164:ILE:HG13	2.15	0.46
1:C:194:ARG:CZ	1:D:194:ARG:CZ	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:VAL:HA	1:E:90:MSE:CE	2.42	0.46
1:A:147:ASP:OD1	1:A:147:ASP:C	2.54	0.46
1:B:139:GLN:NE2	1:B:140:ALA:O	2.47	0.46
1:D:274:ILE:OXT	1:D:274:ILE:HG22	2.16	0.46
1:F:85:VAL:HG13	1:F:90:MSE:HE3	1.98	0.46
1:A:88:LEU:HD13	1:A:90:MSE:HE2	1.98	0.45
1:B:51:LEU:HD22	1:B:98:MSE:SE	2.66	0.45
1:E:236:GLY:O	1:E:240:GLN:HG2	2.17	0.45
1:B:145:SER:HB3	1:B:150:HIS:O	2.16	0.45
1:C:69:PHE:CE2	1:C:101:PRO:HG3	2.51	0.45
1:D:184:GLN:HB3	1:D:184:GLN:HE21	1.58	0.45
1:B:88:LEU:HD12	1:B:90:MSE:CE	2.46	0.45
1:C:201:ARG:HA	1:C:202:PRO:HD3	1.83	0.45
1:E:190:ALA:HB3	1:E:194:ARG:HH12	1.82	0.45
1:D:269:LEU:HD13	1:F:87:ASN:HB3	1.99	0.45
1:A:184:GLN:HB3	1:A:184:GLN:HE21	1.51	0.44
1:B:85:VAL:HA	1:B:90:MSE:HE2	1.98	0.44
1:F:176:ILE:HA	1:F:211:HIS:O	2.17	0.44
1:F:191:GLY:O	1:F:194:ARG:HD2	2.17	0.44
1:E:118:ASP:HB3	1:E:211:HIS:CE1	2.52	0.44
1:A:261:LEU:HD23	1:A:266:GLN:OE1	2.17	0.43
1:C:269:LEU:HD23	1:C:274:ILE:CD1	2.34	0.43
1:F:201:ARG:HA	1:F:202:PRO:HD3	1.82	0.43
1:D:274:ILE:CG2	1:D:274:ILE:OXT	2.65	0.43
1:A:127:LYS:HD2	1:C:221:LEU:CD1	2.45	0.43
1:D:124:GLN:CD	1:D:141:LEU:HD22	2.39	0.43
1:F:100:MSE:HB3	1:F:101:PRO:HD2	2.01	0.43
1:D:27:THR:HG22	1:D:66:ARG:CZ	2.48	0.43
1:A:179:ASN:CG	1:A:180:PRO:HD2	2.39	0.43
1:E:122:PHE:HZ	1:E:140:ALA:HA	1.83	0.43
1:E:157:LYS:HB3	1:E:159:GLU:OE1	2.18	0.43
1:E:85:VAL:HG13	1:E:90:MSE:HB2	2.00	0.43
1:F:122:PHE:HD2	1:F:209:HIS:CD2	2.35	0.43
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.94	0.43
1:B:136:LEU:HA	1:B:136:LEU:HD12	1.86	0.43
1:B:85:VAL:HA	1:B:90:MSE:HE3	2.00	0.43
1:D:210:MSE:O	1:D:210:MSE:HG3	2.19	0.43
1:E:159:GLU:CD	1:E:159:GLU:H	2.22	0.43
1:F:74:LEU:HA	1:F:214:LEU:HD11	2.00	0.43
1:E:179:ASN:CG	1:E:180:PRO:HD2	2.39	0.42
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLN:HB3	1:B:184:GLN:HE21	1.62	0.42
1:C:259:PRO:HA	1:C:260:PRO:HD3	1.85	0.42
1:A:177:PHE:HD2	1:A:211:HIS:CD2	2.38	0.42
1:D:201:ARG:HA	1:D:202:PRO:HD3	1.80	0.42
1:F:67:ARG:O	1:F:98:MSE:HB2	2.20	0.42
1:A:67:ARG:O	1:A:98:MSE:HB2	2.19	0.42
1:A:163:LEU:HG	1:A:210:MSE:CE	2.50	0.42
1:B:92:THR:O	1:B:126:PRO:HD2	2.19	0.42
1:E:146:ARG:HG2	1:E:146:ARG:H	1.45	0.42
1:C:61:MSE:HE1	1:C:122:PHE:CD2	2.55	0.42
1:B:90:MSE:HE1	1:B:166:LEU:HD11	2.02	0.41
1:E:126:PRO:HB2	1:E:128:THR:O	2.20	0.41
1:F:24:GLN:NE2	1:F:107:ASN:HB2	2.35	0.41
1:A:150:HIS:CE1	1:B:149:LYS:HE3	2.55	0.41
1:C:179:ASN:CG	1:C:180:PRO:HD2	2.40	0.41
1:B:42:ASN:OD1	1:B:261:LEU:HD12	2.20	0.41
1:C:136:LEU:HD12	1:C:136:LEU:HA	1.91	0.41
1:D:238:GLU:O	1:D:241:SER:OG	2.26	0.41
1:D:85:VAL:HG13	1:D:90:MSE:HE3	2.01	0.41
1:D:100:MSE:HE3	1:D:103:GLY:O	2.20	0.41
1:D:100:MSE:HB3	1:D:101:PRO:HD2	2.03	0.41
1:D:192:THR:O	1:D:192:THR:HG22	2.20	0.41
1:E:185:GLN:HB2	4:E:615:HOH:O	2.21	0.41
1:E:74:LEU:HA	1:E:214:LEU:HD11	2.03	0.41
1:F:155:LEU:HD23	1:F:155:LEU:HA	1.86	0.41
1:C:163:LEU:HG	1:C:210:MSE:CE	2.50	0.41
1:D:144:VAL:HG22	1:D:181:ALA:HB3	2.02	0.41
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.93	0.41
1:B:85:VAL:HG13	1:B:90:MSE:HB2	2.02	0.41
1:A:104:GLY:O	1:A:114:GLN:HG2	2.21	0.41
1:C:184:GLN:HB3	1:C:184:GLN:HE21	1.70	0.41
1:B:146:ARG:N	1:B:146:ARG:CD	2.42	0.41
1:B:163:LEU:HG	1:B:210:MSE:CE	2.46	0.41
1:B:77:PHE:CZ	1:B:81:LEU:HD22	2.55	0.41
1:D:36:SER:HB3	1:D:115:THR:HB	2.03	0.41
1:D:136:LEU:HA	1:D:136:LEU:HD12	1.81	0.40
1:E:179:ASN:ND2	1:E:180:PRO:HD2	2.36	0.40
1:C:122:PHE:CZ	1:C:140:ALA:HA	2.56	0.40
1:D:124:GLN:OE1	1:D:141:LEU:HD22	2.22	0.40
1:C:155:LEU:O	1:C:157:LYS:HE2	2.21	0.40
1:B:147:ASP:OD1	1:B:149:LYS:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:MSE:HB3	1:D:101:PRO:CD	2.52	0.40
1:A:113:HIS:NE2	1:A:211:HIS:HE1	2.18	0.40
1:A:198:ARG:NH2	1:A:229:PRO:O	2.39	0.40
1:C:113:HIS:HA	1:C:118:ASP:HB2	2.03	0.40
1:C:206:HIS:HA	1:C:209:HIS:CE1	2.56	0.40
1:E:61:MSE:HE1	1:E:122:PHE:CD2	2.56	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	226/255 (89%)	216 (96%)	8 (4%)	2 (1%)	17	25
1	B	235/255 (92%)	227 (97%)	7 (3%)	1 (0%)	34	48
1	C	237/255 (93%)	226 (95%)	11 (5%)	0	100	100
1	D	237/255 (93%)	224 (94%)	12 (5%)	1 (0%)	34	48
1	E	237/255 (93%)	225 (95%)	10 (4%)	2 (1%)	19	29
1	F	236/255 (92%)	225 (95%)	11 (5%)	0	100	100
All	All	1408/1530 (92%)	1343 (95%)	59 (4%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	42	ASN
1	A	129	ARG
1	D	42	ASN
1	B	42	ASN
1	E	230	PRO
1	A	26	ILE

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	199/214 (93%)	192 (96%)	7 (4%)	36	55
1	B	205/214 (96%)	195 (95%)	10 (5%)	25	40
1	C	207/214 (97%)	201 (97%)	6 (3%)	42	62
1	D	207/214 (97%)	203 (98%)	4 (2%)	57	75
1	E	207/214 (97%)	202 (98%)	5 (2%)	49	68
1	F	206/214 (96%)	203 (98%)	3 (2%)	65	80
All	All	1231/1284 (96%)	1196 (97%)	35 (3%)	43	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	PHE
1	A	136	LEU
1	A	154	THR
1	A	184	GLN
1	A	220	SER
1	A	240	GLN
1	A	270	ASP
1	B	72	PRO
1	B	105	ARG
1	B	122	PHE
1	B	136	LEU
1	B	146	ARG
1	B	184	GLN
1	B	220	SER
1	B	225	ASP
1	B	240	GLN
1	B	264	SER
1	C	86	SER
1	C	122	PHE
1	C	128	THR
1	C	136	LEU
1	C	184	GLN

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Mol	Chain	Res	Type
1	C	220	SER
1	D	136	LEU
1	D	139	GLN
1	D	184	GLN
1	D	240	GLN
1	E	128	THR
1	E	146	ARG
1	E	154	THR
1	E	184	GLN
1	E	261	LEU
1	F	122	PHE
1	F	220	SER
1	F	241	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	184	GLN
1	A	185	GLN
1	B	139	GLN
1	B	169	GLN
1	B	185	GLN
1	B	240	GLN
1	C	124	GLN
1	C	205	GLN
1	D	184	GLN
1	D	185	GLN
1	E	57	HIS
1	E	65	GLN
1	E	184	GLN
1	F	169	GLN
1	F	185	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	SO4	D	503	-	4,4,4	0.92	0	6,6,6	1.11	0
3	SO4	E	504	-	4,4,4	1.02	0	6,6,6	1.15	0
3	SO4	B	501	-	4,4,4	0.94	0	6,6,6	1.19	0
3	SO4	A	500	-	4,4,4	0.87	0	6,6,6	1.16	0
3	SO4	F	505	-	4,4,4	0.84	0	6,6,6	1.17	0
3	SO4	C	502	-	4,4,4	0.92	0	6,6,6	1.06	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

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	226/255 (88%)	0.41	14 (6%)	20 19	11, 29, 48, 57	0
1	B	233/255 (91%)	0.23	12 (5%)	27 26	7, 25, 48, 59	0
1	C	235/255 (92%)	0.07	6 (2%)	56 54	8, 23, 42, 54	0
1	D	235/255 (92%)	0.16	10 (4%)	35 33	6, 23, 43, 56	0
1	E	235/255 (92%)	0.25	12 (5%)	28 26	10, 24, 46, 57	0
1	F	234/255 (91%)	0.15	8 (3%)	45 44	7, 22, 46, 53	0
All	All	1398/1530 (91%)	0.21	62 (4%)	34 33	6, 25, 46, 59	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	141	LEU	11.3
1	D	141	LEU	10.1
1	A	141	LEU	7.8
1	A	20	ALA	6.3
1	E	140	ALA	5.9
1	B	141	LEU	5.7
1	B	274	ILE	5.5
1	D	140	ALA	5.3
1	A	231	SER	5.2
1	F	221	LEU	5.1
1	E	139	GLN	4.9
1	D	274	ILE	4.5
1	B	221	LEU	4.4
1	D	139	GLN	4.4
1	E	274	ILE	4.4
1	B	244	GLU	4.3
1	F	274	ILE	4.0
1	C	274	ILE	3.7
1	F	141	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	146	ARG	3.6
1	E	192	THR	3.6
1	A	139	GLN	3.6
1	A	22	PRO	3.5
1	A	105	ARG	3.4
1	D	138	PRO	3.3
1	B	140	ALA	3.3
1	C	244	GLU	3.2
1	F	146	ARG	3.2
1	A	25	LYS	3.1
1	D	260	PRO	3.1
1	B	154	THR	3.1
1	D	137	ARG	3.0
1	A	24	GLN	2.9
1	C	260	PRO	2.9
1	F	192	THR	2.9
1	B	231	SER	2.8
1	E	20	ALA	2.8
1	E	146	ARG	2.8
1	B	139	GLN	2.8
1	B	220	SER	2.8
1	E	244	GLU	2.7
1	F	244	GLU	2.7
1	A	111	ALA	2.6
1	B	111	ALA	2.5
1	B	240	GLN	2.5
1	D	259	PRO	2.5
1	F	139	GLN	2.5
1	D	146	ARG	2.4
1	A	109	GLY	2.4
1	E	111	ALA	2.4
1	A	41	SER	2.4
1	D	244	GLU	2.3
1	F	220	SER	2.2
1	A	140	ALA	2.2
1	E	272	HIS	2.2
1	C	20	ALA	2.2
1	A	270	ASP	2.1
1	E	107	ASN	2.1
1	A	21	THR	2.1
1	E	218	ALA	2.1
1	B	273	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	221	LEU	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 carbohydrates 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	ZN	A	601	1/1	0.77	0.14	49,49,49,49	0
3	SO4	F	505	5/5	0.83	0.25	44,45,47,49	0
3	SO4	B	501	5/5	0.89	0.26	43,45,46,47	0
3	SO4	E	504	5/5	0.92	0.14	39,40,42,43	0
2	ZN	E	603	1/1	0.92	0.07	33,33,33,33	0
3	SO4	A	500	5/5	0.94	0.13	43,43,44,46	0
3	SO4	C	502	5/5	0.94	0.18	32,32,33,35	0
3	SO4	D	503	5/5	0.95	0.19	43,44,45,45	0
2	ZN	D	602	1/1	0.96	0.04	27,27,27,27	0
2	ZN	A	400	1/1	0.99	0.06	25,25,25,25	0
2	ZN	B	400	1/1	0.99	0.04	15,15,15,15	0
2	ZN	E	400	1/1	1.00	0.06	16,16,16,16	0
2	ZN	F	400	1/1	1.00	0.08	18,18,18,18	0
2	ZN	C	400	1/1	1.00	0.04	14,14,14,14	0
2	ZN	D	400	1/1	1.00	0.05	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.