Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:11 pm BST

PDB ID	:	2YHE
Title	:	Structure determination of the stereoselective inverting sec- alkylsulfatase Pisa1 from Pseudomonas sp.
Authors	:	Kepplinger, B.; Faber, K.; Macheroux, P.; Schober, M.; Knaus, T.; Wagner, U.G.
Deposited on	:	2011-04-29
Resolution	:	2.70 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:

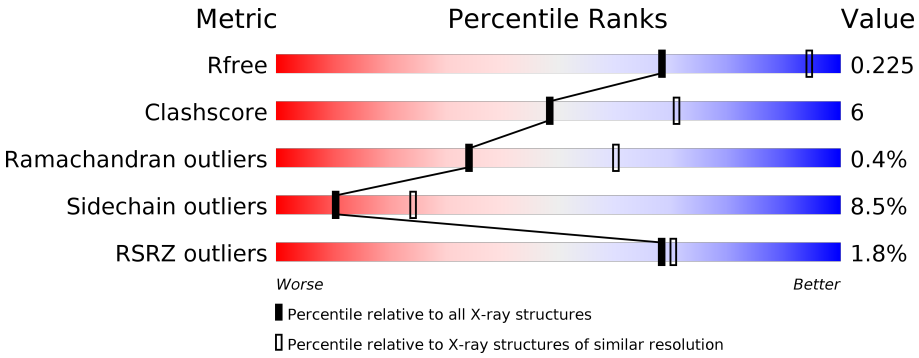
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	668	% 81% 13% • •
1	B	668	2% 80% 14% • 5%
1	C	668	2% 77% 16% • 5%
1	D	668	% 78% 15% • 5%
1	E	668	3% 77% 16% • 5%
1	F	668	% 79% 15% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31033 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 SEC-ALKYL SULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	10	0
			5044	3196	888	941	19			
1	B	634	Total	C	N	O	S	0	4	0
			4959	3142	863	935	19			
1	C	634	Total	C	N	O	S	0	2	0
			4948	3133	863	933	19			
1	D	634	Total	C	N	O	S	0	4	0
			4961	3145	867	930	19			
1	E	634	Total	C	N	O	S	0	5	0
			4959	3144	863	933	19			
1	F	634	Total	C	N	O	S	0	3	0
			4954	3137	865	933	19			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ARG	HIS	conflict	UNP F8KAY7
A	661	LEU	-	expression tag	UNP F8KAY7
A	662	GLU	-	expression tag	UNP F8KAY7
A	663	HIS	-	expression tag	UNP F8KAY7
A	664	HIS	-	expression tag	UNP F8KAY7
A	665	HIS	-	expression tag	UNP F8KAY7
A	666	HIS	-	expression tag	UNP F8KAY7
A	667	HIS	-	expression tag	UNP F8KAY7
A	668	HIS	-	expression tag	UNP F8KAY7
B	107	ARG	HIS	conflict	UNP F8KAY7
B	661	LEU	-	expression tag	UNP F8KAY7
B	662	GLU	-	expression tag	UNP F8KAY7
B	663	HIS	-	expression tag	UNP F8KAY7
B	664	HIS	-	expression tag	UNP F8KAY7
B	665	HIS	-	expression tag	UNP F8KAY7
B	666	HIS	-	expression tag	UNP F8KAY7
B	667	HIS	-	expression tag	UNP F8KAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	668	HIS	-	expression tag	UNP F8KAY7
C	107	ARG	HIS	conflict	UNP F8KAY7
C	661	LEU	-	expression tag	UNP F8KAY7
C	662	GLU	-	expression tag	UNP F8KAY7
C	663	HIS	-	expression tag	UNP F8KAY7
C	664	HIS	-	expression tag	UNP F8KAY7
C	665	HIS	-	expression tag	UNP F8KAY7
C	666	HIS	-	expression tag	UNP F8KAY7
C	667	HIS	-	expression tag	UNP F8KAY7
C	668	HIS	-	expression tag	UNP F8KAY7
D	107	ARG	HIS	conflict	UNP F8KAY7
D	661	LEU	-	expression tag	UNP F8KAY7
D	662	GLU	-	expression tag	UNP F8KAY7
D	663	HIS	-	expression tag	UNP F8KAY7
D	664	HIS	-	expression tag	UNP F8KAY7
D	665	HIS	-	expression tag	UNP F8KAY7
D	666	HIS	-	expression tag	UNP F8KAY7
D	667	HIS	-	expression tag	UNP F8KAY7
D	668	HIS	-	expression tag	UNP F8KAY7
E	107	ARG	HIS	conflict	UNP F8KAY7
E	661	LEU	-	expression tag	UNP F8KAY7
E	662	GLU	-	expression tag	UNP F8KAY7
E	663	HIS	-	expression tag	UNP F8KAY7
E	664	HIS	-	expression tag	UNP F8KAY7
E	665	HIS	-	expression tag	UNP F8KAY7
E	666	HIS	-	expression tag	UNP F8KAY7
E	667	HIS	-	expression tag	UNP F8KAY7
E	668	HIS	-	expression tag	UNP F8KAY7
F	107	ARG	HIS	conflict	UNP F8KAY7
F	661	LEU	-	expression tag	UNP F8KAY7
F	662	GLU	-	expression tag	UNP F8KAY7
F	663	HIS	-	expression tag	UNP F8KAY7
F	664	HIS	-	expression tag	UNP F8KAY7
F	665	HIS	-	expression tag	UNP F8KAY7
F	666	HIS	-	expression tag	UNP F8KAY7
F	667	HIS	-	expression tag	UNP F8KAY7
F	668	HIS	-	expression tag	UNP F8KAY7

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

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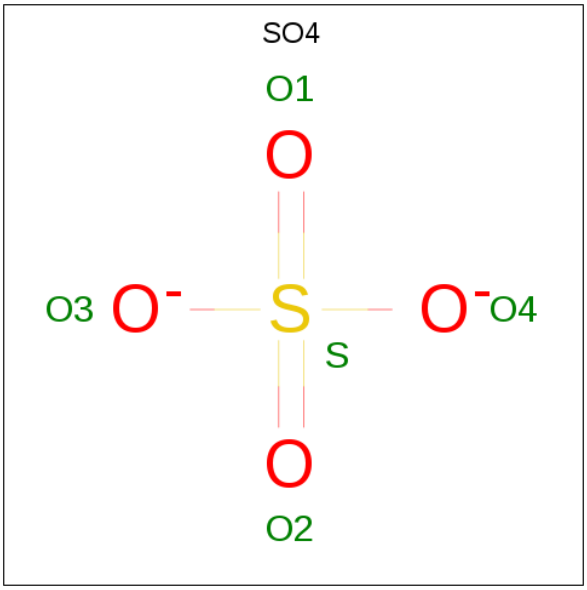
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

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	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

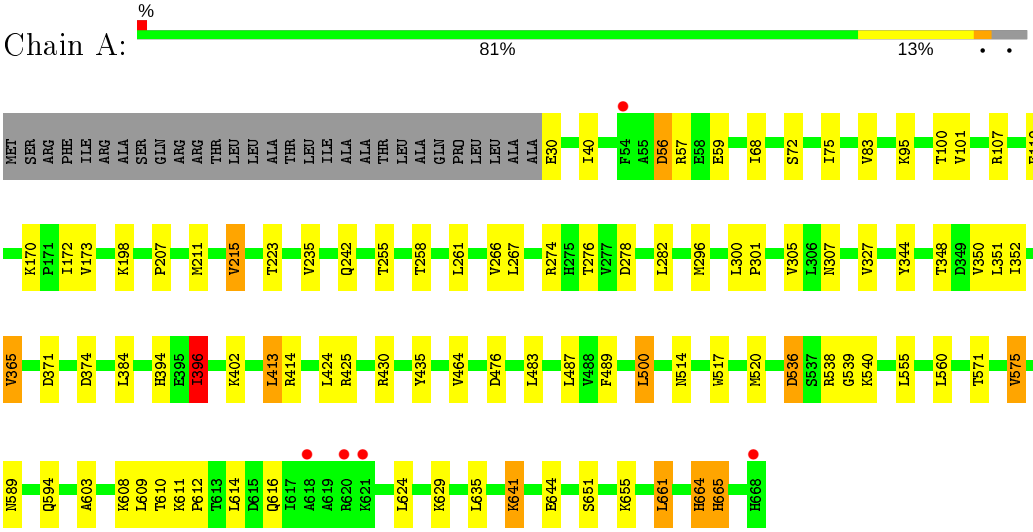
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	257	Total O 257 257	0	0
4	B	225	Total O 225 225	0	0
4	C	181	Total O 181 181	0	0
4	D	178	Total O 178 178	0	0
4	E	166	Total O 166 166	0	0
4	F	159	Total O 159 159	0	0

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.

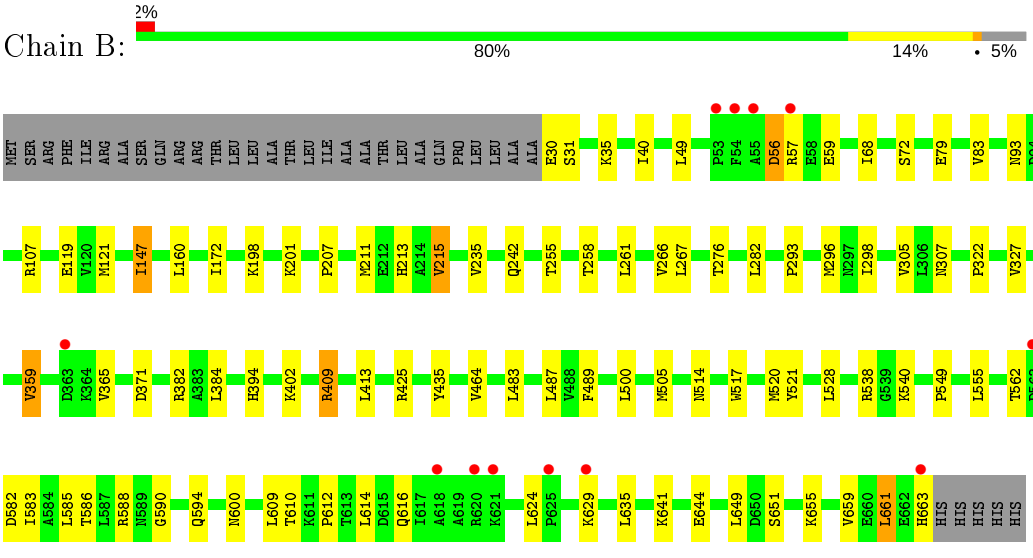
• Molecule 1: SEC-ALKYL SULFATASE

Chain A:



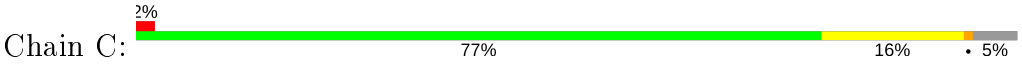
• Molecule 1: SEC-ALKYL SULFATASE

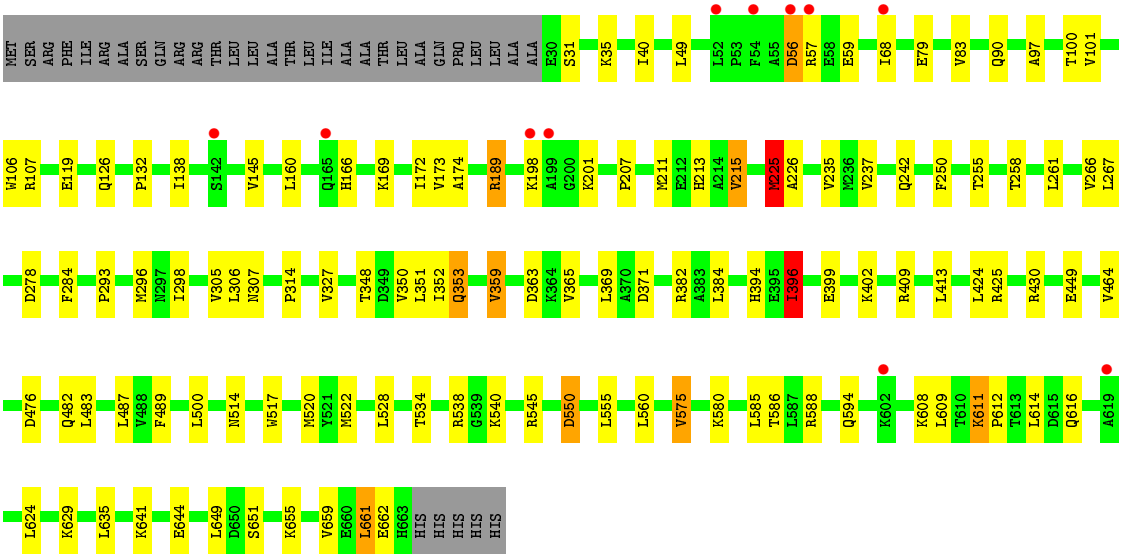
Chain B:



• Molecule 1: SEC-ALKYL SULFATASE

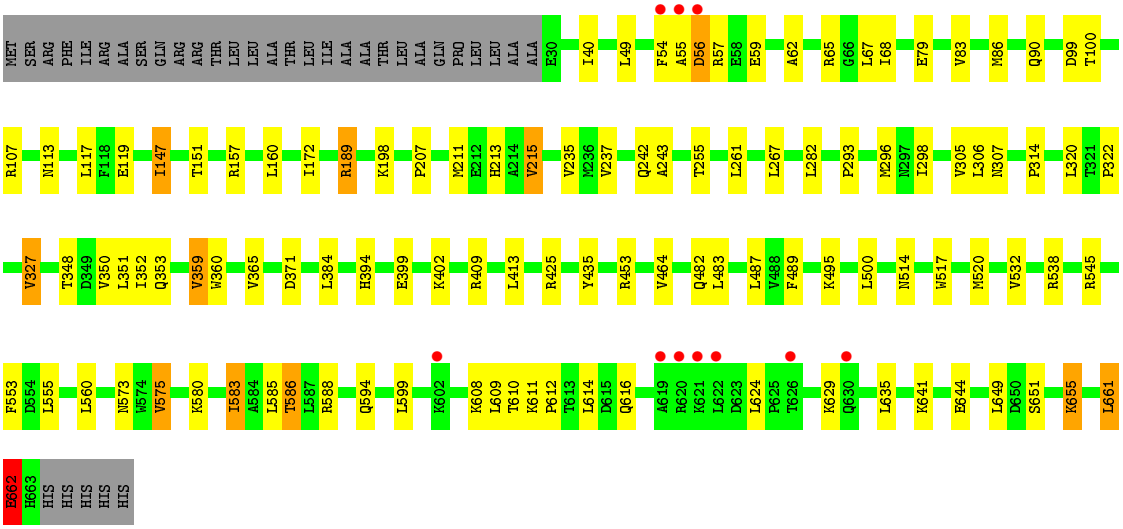
Chain C:





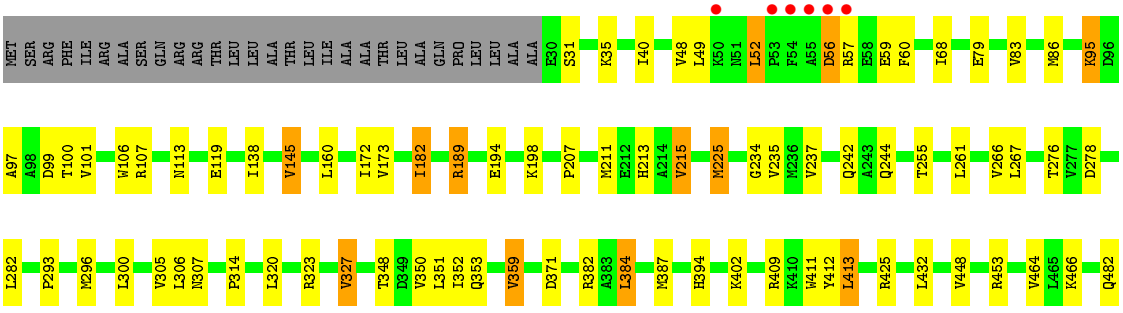
• Molecule 1: SEC-ALKYL SULFATASE

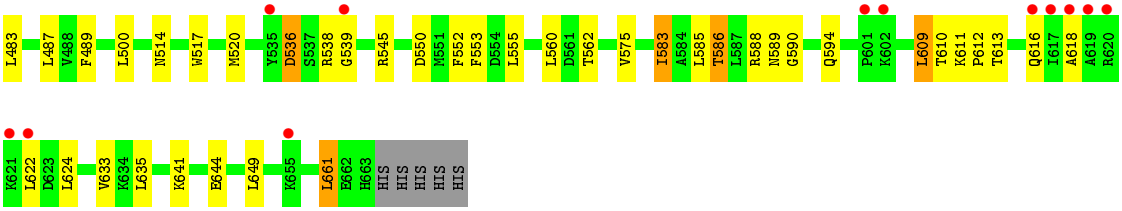
Chain D:



• Molecule 1: SEC-ALKYL SULFATASE

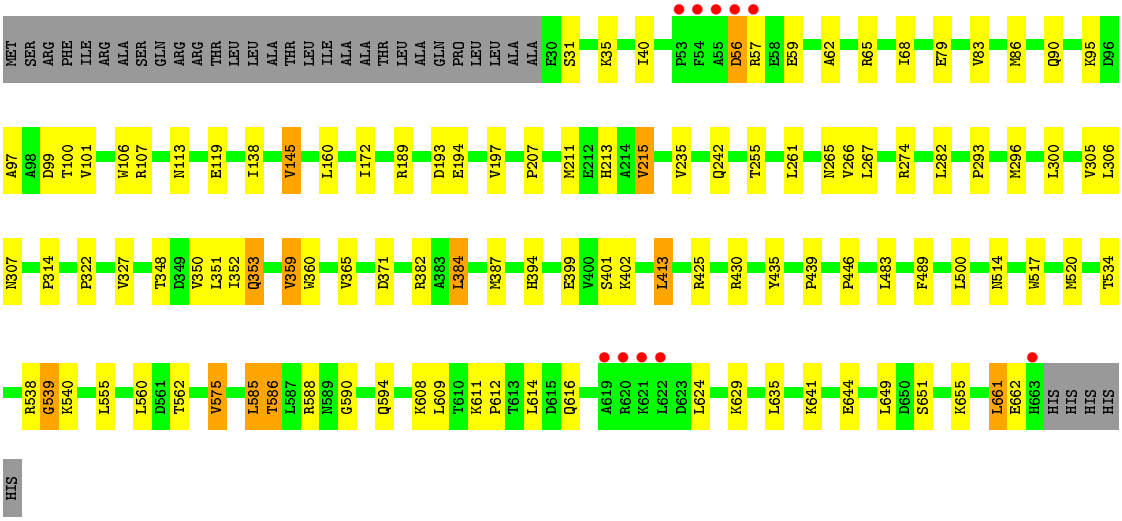
Chain E:





- Molecule 1: SEC-ALKYL SULFATASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.73Å 200.59Å 245.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.91-2.70) 100.0 (19.90-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.183 , 0.230 0.178 , 0.225	Depositor DCC
R_{free} test set	5090 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31033	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.50	0/5184	0.73	2/7031 (0.0%)
1	B	0.50	0/5076	0.72	2/6885 (0.0%)
1	C	0.50	0/5059	0.73	2/6862 (0.0%)
1	D	0.51	0/5078	0.72	1/6887 (0.0%)
1	E	0.51	0/5079	0.72	0/6891
1	F	0.50	0/5068	0.72	1/6874 (0.0%)
All	All	0.50	0/30544	0.72	8/41430 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	539	GLY	C-N-CA	10.21	147.24	121.70
1	D	662	GLU	C-N-CA	8.46	142.84	121.70
1	A	664	HIS	C-N-CA	7.62	140.75	121.70
1	C	396	ILE	CA-CB-CG2	5.41	121.73	110.90
1	C	225	MET	CG-SD-CE	-5.32	91.69	100.20
1	B	663	HIS	N-CA-CB	5.16	119.89	110.60
1	B	409	ARG	CB-CG-CD	5.09	124.84	111.60
1	A	396	ILE	CA-CB-CG2	5.03	120.97	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	353	GLN	Sidechain
1	D	662	GLU	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	5044	0	5016	57	0
1	B	4959	0	4918	52	0
1	C	4948	0	4901	55	0
1	D	4961	0	4934	67	0
1	E	4959	0	4923	78	0
1	F	4954	0	4911	62	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	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	257	0	0	10	0
4	B	225	0	0	6	0
4	C	181	0	0	11	0
4	D	178	0	0	7	0
4	E	166	0	0	8	0
4	F	159	0	0	3	0
All	All	31033	0	29603	355	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 6.

All (355) 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:E:40:ILE:CD1	1:E:40:ILE:CG1	1.74	1.58
1:E:552:PHE:CE1	1:E:618:ALA:HB2	1.77	1.19
1:D:661:LEU:HD23	1:D:661:LEU:H	1.00	1.15
1:D:67:LEU:HD12	4:D:2011:HOH:O	1.46	1.15
1:E:661:LEU:H	1:E:661:LEU:HD23	0.98	1.13
1:A:661:LEU:H	1:A:661:LEU:HD23	1.05	1.10
1:F:661:LEU:H	1:F:661:LEU:HD23	1.00	1.10
1:C:661:LEU:HD23	1:C:661:LEU:H	0.97	1.09
1:E:552:PHE:HE1	1:E:618:ALA:HB2	0.92	1.08
1:B:661:LEU:H	1:B:661:LEU:HD23	0.96	1.07
1:E:552:PHE:HE1	1:E:618:ALA:CB	1.68	1.07
1:E:237:VAL:HG23	1:E:244:GLN:HB2	1.44	0.98
1:B:661:LEU:H	1:B:661:LEU:CD2	1.77	0.97
1:C:661:LEU:CD2	1:C:661:LEU:H	1.78	0.96
1:B:661:LEU:HD23	1:B:661:LEU:N	1.80	0.95
1:C:661:LEU:HD23	1:C:661:LEU:N	1.80	0.95
1:F:661:LEU:H	1:F:661:LEU:CD2	1.79	0.94
1:E:661:LEU:N	1:E:661:LEU:HD23	1.80	0.93
1:D:661:LEU:HD23	1:D:661:LEU:N	1.84	0.93
1:F:661:LEU:N	1:F:661:LEU:HD23	1.83	0.93
1:E:237:VAL:CG2	1:E:244:GLN:HB2	2.00	0.90
1:E:661:LEU:CD2	1:E:661:LEU:H	1.77	0.89
1:A:661:LEU:N	1:A:661:LEU:HD23	1.88	0.88
1:C:138:ILE:HB	1:C:145:VAL:HG23	1.58	0.86
1:D:661:LEU:H	1:D:661:LEU:CD2	1.81	0.85
1:B:505:MET:HE2	1:B:521:TYR:HA	1.56	0.85
1:E:616:GLN:NE2	1:E:622:LEU:HD12	1.91	0.85
1:C:258:THR:HG22	1:C:540:LYS:HB3	1.60	0.83
1:A:661:LEU:H	1:A:661:LEU:CD2	1.84	0.83
1:A:258:THR:HG22	1:A:540:LYS:HB3	1.58	0.83
1:C:296:MET:HG3	4:C:2060:HOH:O	1.81	0.81
1:E:536:ASP:OD1	1:E:539:GLY:CA	2.29	0.80
1:A:464:VAL:HG22	1:A:487:LEU:HD22	1.64	0.80
1:E:611:LYS:HD3	4:E:2144:HOH:O	1.79	0.79
1:C:145:VAL:HG12	1:C:174:ALA:HB3	1.64	0.79
1:F:138:ILE:HB	1:F:145:VAL:HG13	1.64	0.79
1:C:464:VAL:HG22	1:C:487:LEU:HD22	1.64	0.78
1:D:464:VAL:HG22	1:D:487:LEU:HD22	1.65	0.78
1:E:138:ILE:HB	1:E:145:VAL:HG13	1.65	0.77
1:B:464:VAL:HG22	1:B:487:LEU:HD22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:464:VAL:HG22	1:E:487:LEU:HD22	1.67	0.76
1:D:67:LEU:CD1	4:D:2011:HOH:O	2.16	0.75
1:B:505:MET:CE	1:B:521:TYR:HA	2.17	0.74
1:A:536:ASP:OD1	1:A:539:GLY:CA	2.38	0.72
1:B:489:PHE:HA	1:B:661:LEU:HD22	1.72	0.72
1:C:68:ILE:HD11	1:C:119:GLU:HB2	1.71	0.72
1:D:489:PHE:HA	1:D:661:LEU:HD22	1.72	0.71
1:E:489:PHE:HA	1:E:661:LEU:HD22	1.73	0.70
1:D:68:ILE:HD11	1:D:119:GLU:HB2	1.74	0.69
1:B:68:ILE:HD11	1:B:119:GLU:HB2	1.74	0.69
1:E:68:ILE:HD11	1:E:119:GLU:HB2	1.75	0.69
1:A:489:PHE:HA	1:A:661:LEU:HD22	1.74	0.68
1:D:55:ALA:O	1:D:56:ASP:O	2.10	0.68
1:F:68:ILE:HD11	1:F:119:GLU:HB2	1.76	0.68
1:C:489:PHE:HA	1:C:661:LEU:HD22	1.74	0.68
1:D:532:VAL:HG12	1:D:655:LYS:HE3	1.76	0.68
1:F:489:PHE:HA	1:F:661:LEU:HD22	1.75	0.68
1:A:68:ILE:HD11	1:A:119:GLU:HB2	1.74	0.67
1:F:194:GLU:O	1:F:197:VAL:HG22	1.94	0.67
1:A:374:ASP:OD1	4:A:2143:HOH:O	2.11	0.67
1:A:476:ASP:OD1	4:A:2200:HOH:O	2.12	0.66
1:E:536:ASP:OD1	1:E:539:GLY:N	2.29	0.65
1:D:62:ALA:HA	1:D:360:TRP:CZ3	2.32	0.65
1:C:550:ASP:HB3	4:C:2157:HOH:O	1.97	0.65
1:B:505:MET:HE3	1:F:439:PRO:HB2	1.78	0.64
1:F:40:ILE:HD12	1:F:40:ILE:H	1.62	0.64
1:C:476:ASP:OD2	1:E:453:ARG:NH1	2.30	0.64
1:D:189:ARG:NE	1:D:545:ARG:HH21	1.96	0.63
1:D:189:ARG:HE	1:D:545:ARG:HH21	1.46	0.63
1:D:435:TYR:HA	4:D:2118:HOH:O	1.99	0.63
1:B:575:VAL:HG13	1:B:582:ASP:OD1	1.98	0.63
1:C:40:ILE:HD12	1:C:40:ILE:H	1.64	0.62
1:B:371:ASP:OD1	1:F:588:ARG:NH2	2.31	0.62
1:B:40:ILE:HD12	1:B:40:ILE:H	1.65	0.62
1:D:40:ILE:H	1:D:40:ILE:HD12	1.65	0.62
1:C:348:THR:HB	4:C:2061:HOH:O	2.01	0.61
1:F:62:ALA:HA	1:F:360:TRP:CZ3	2.36	0.61
1:A:571:THR:HG22	1:A:603:ALA:HA	1.82	0.60
1:B:588:ARG:NH2	1:F:371:ASP:OD1	2.34	0.60
1:C:396:ILE:HD11	1:C:424:LEU:HD22	1.82	0.60
1:C:225:MET:HG3	1:C:226:ALA:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HD11	1:A:424:LEU:HD22	1.83	0.60
1:B:93:ASN:O	4:B:2016:HOH:O	2.17	0.60
1:D:322:PRO:HB3	1:D:520:MET:CE	2.32	0.59
1:B:371:ASP:HB3	1:B:413[A]:LEU:HD11	1.84	0.59
1:E:40:ILE:HD12	1:E:40:ILE:H	1.67	0.59
1:F:62:ALA:O	1:F:360:TRP:CH2	2.57	0.58
1:A:40:ILE:H	1:A:40:ILE:HD12	1.67	0.58
1:A:489:PHE:HA	1:A:661:LEU:CD2	2.34	0.58
1:E:489:PHE:HA	1:E:661:LEU:CD2	2.33	0.58
1:C:258:THR:CG2	1:C:540:LYS:HB3	2.32	0.58
1:C:588:ARG:NH2	1:E:371:ASP:OD1	2.37	0.58
1:F:489:PHE:HA	1:F:661:LEU:CD2	2.33	0.58
1:A:536:ASP:OD1	1:A:539:GLY:N	2.37	0.58
1:B:322:PRO:HB3	1:B:520:MET:CE	2.33	0.58
1:D:322:PRO:HB3	1:D:520:MET:HE1	1.86	0.58
1:D:62:ALA:O	1:D:360:TRP:CH2	2.57	0.58
1:B:489:PHE:HA	1:B:661:LEU:CD2	2.33	0.58
1:D:489:PHE:HA	1:D:661:LEU:CD2	2.33	0.58
1:A:371:ASP:OD1	1:D:588:ARG:NH2	2.37	0.58
1:D:211:MET:O	1:D:215:VAL:HG12	2.04	0.57
1:D:305:VAL:HG22	1:D:350:VAL:HG13	1.85	0.57
1:F:351:LEU:HB3	1:F:359:VAL:HG13	1.86	0.57
1:C:489:PHE:HA	1:C:661:LEU:CD2	2.34	0.56
1:D:371:ASP:HB3	1:D:413[A]:LEU:HD11	1.87	0.56
1:D:62:ALA:CA	1:D:360:TRP:HZ3	2.18	0.56
1:D:532:VAL:CG1	1:D:655:LYS:HE3	2.34	0.56
1:A:258:THR:CG2	1:A:540:LYS:HB3	2.34	0.56
1:E:616:GLN:CD	1:E:622:LEU:HD12	2.25	0.56
1:A:173:VAL:HG11	1:A:278:ASP:HB2	1.86	0.55
1:D:117:LEU:N	4:D:2011:HOH:O	2.39	0.55
1:E:40:ILE:CD1	1:E:40:ILE:CB	2.78	0.55
4:A:2180:HOH:O	1:D:520:MET:HE2	2.06	0.55
1:F:59:GLU:HB2	1:F:107:ARG:HH22	1.71	0.55
1:A:571:THR:HG23	4:A:2234:HOH:O	2.05	0.55
1:D:189:ARG:HG2	1:D:189:ARG:NH1	2.22	0.55
1:E:211:MET:O	1:E:215:VAL:HG13	2.06	0.55
1:E:552:PHE:CE1	1:E:618:ALA:CB	2.60	0.55
1:B:585:LEU:HD23	1:B:594:GLN:HB3	1.90	0.54
1:F:585:LEU:HD23	1:F:594:GLN:HB3	1.88	0.54
1:D:351:LEU:HB3	1:D:359:VAL:HG13	1.89	0.54
1:F:322:PRO:HB3	1:F:520:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:HD23	1:A:594:GLN:HB3	1.89	0.54
1:E:173:VAL:HG11	1:E:278:ASP:HB2	1.88	0.54
1:B:505:MET:HE3	1:B:521:TYR:HD1	1.73	0.54
1:B:211:MET:O	1:B:215:VAL:HG13	2.07	0.54
1:F:586:THR:HG22	4:F:2148:HOH:O	2.08	0.54
1:E:562:THR:HG22	1:E:590:GLY:O	2.08	0.54
1:B:305:VAL:HG22	1:B:350:VAL:HG13	1.89	0.53
1:F:211:MET:O	1:F:215:VAL:HG13	2.09	0.53
1:B:562:THR:HG22	1:B:590:GLY:O	2.08	0.53
1:F:62:ALA:CA	1:F:360:TRP:HZ3	2.22	0.53
1:B:351:LEU:HB3	1:B:359:VAL:HG13	1.91	0.53
1:B:520:MET:HE2	4:F:2111:HOH:O	2.08	0.53
1:D:586:THR:HG22	4:D:2166:HOH:O	2.08	0.53
1:A:274[A]:ARG:HH21	1:A:301:PRO:HG2	1.74	0.53
1:A:589:ASN:HB2	4:A:2238:HOH:O	2.09	0.53
1:D:147[A]:ILE:HD13	1:D:298:ILE:HD13	1.90	0.52
1:E:411:TRP:O	4:E:2086:HOH:O	2.19	0.52
1:D:189:ARG:HH11	1:D:189:ARG:HG2	1.73	0.52
1:D:641:LYS:HA	1:D:644:GLU:HG2	1.92	0.52
1:E:351:LEU:HB3	1:E:359:VAL:HG13	1.90	0.52
1:B:147:ILE:HD13	1:B:298:ILE:HD13	1.91	0.52
1:C:585:LEU:HD23	1:C:594:GLN:HB3	1.91	0.52
1:A:586:THR:HG22	4:A:2236:HOH:O	2.08	0.52
1:E:411:TRP:CE2	1:E:412:TYR:HD2	2.28	0.52
1:E:189:ARG:NH2	4:E:2053:HOH:O	2.31	0.52
1:E:586:THR:CG2	4:E:2154:HOH:O	2.58	0.52
1:C:173:VAL:HG11	1:C:278:ASP:HB2	1.91	0.51
1:B:520:MET:HE1	1:F:435:TYR:HE2	1.75	0.51
1:C:517:TRP:HA	1:C:520:MET:HE3	1.91	0.51
1:A:351:LEU:HB3	1:A:359:VAL:HG13	1.92	0.51
1:C:371:ASP:OD1	1:E:588:ARG:NH2	2.41	0.51
1:F:62:ALA:O	1:F:360:TRP:CZ3	2.64	0.51
1:E:517:TRP:HA	1:E:520:MET:HE3	1.92	0.51
1:A:59:GLU:HB2	1:A:107:ARG:HH22	1.76	0.51
1:E:641:LYS:HA	1:E:644:GLU:HG2	1.92	0.51
1:E:225:MET:HE3	1:E:323:ARG:HB2	1.92	0.50
1:D:59:GLU:HB2	1:D:107:ARG:HH22	1.76	0.50
1:D:62:ALA:HA	1:D:360:TRP:HZ3	1.72	0.50
1:E:585:LEU:HD23	1:E:594:GLN:HB3	1.94	0.50
1:B:520:MET:HE1	1:F:435:TYR:CE2	2.46	0.50
1:E:536:ASP:OD1	1:E:539:GLY:HA3	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLU:HB2	1:C:107:ARG:HH22	1.77	0.50
1:A:641:LYS:HA	1:A:644:GLU:HG2	1.93	0.50
1:C:351:LEU:HB3	1:C:359:VAL:HG13	1.93	0.50
1:C:211:MET:O	1:C:215:VAL:HG13	2.11	0.49
1:E:189:ARG:NH2	1:E:545:ARG:HB2	2.27	0.49
1:E:234:GLY:O	1:E:237:VAL:HG22	2.13	0.49
1:E:189:ARG:NH1	4:E:2053:HOH:O	2.37	0.49
1:E:60:PHE:CD2	1:E:107:ARG:NH2	2.81	0.49
1:A:211:MET:O	1:A:215:VAL:HG13	2.13	0.49
1:A:571:THR:CG2	1:A:603:ALA:HA	2.43	0.49
1:E:613:THR:O	1:E:616:GLN:HG2	2.13	0.49
1:B:59:GLU:HB2	1:B:107:ARG:HH22	1.78	0.48
1:B:435:TYR:HE2	1:F:520:MET:HE1	1.78	0.48
1:D:62:ALA:O	1:D:360:TRP:HH2	1.96	0.48
1:E:60:PHE:HE2	1:E:107:ARG:CZ	2.26	0.48
1:E:586:THR:HG22	4:E:2154:HOH:O	2.13	0.48
1:D:211:MET:O	1:D:215:VAL:CG1	2.61	0.48
1:C:394:HIS:ND1	1:C:425:ARG:HD3	2.29	0.48
1:A:664:HIS:HA	1:A:665:HIS:HB2	1.96	0.48
1:E:83:VAL:HA	1:E:255:THR:O	2.14	0.48
1:D:585:LEU:HD23	1:D:594:GLN:HB3	1.94	0.48
1:F:371:ASP:HB3	1:F:413:LEU:HD21	1.95	0.48
1:B:435:TYR:CE2	1:F:520:MET:HE1	2.48	0.47
1:E:610:THR:HB	1:E:612:PRO:HD2	1.96	0.47
1:C:189:ARG:NH2	1:C:545:ARG:HB2	2.30	0.47
1:B:505:MET:CE	1:F:439:PRO:HB2	2.42	0.47
1:F:83:VAL:HA	1:F:255:THR:O	2.15	0.47
1:C:641:LYS:HA	1:C:644:GLU:HG2	1.96	0.47
1:B:641:LYS:HA	1:B:644:GLU:HG2	1.96	0.47
1:C:298:ILE:HG13	4:C:2060:HOH:O	2.14	0.47
1:D:62:ALA:O	1:D:360:TRP:CZ3	2.68	0.47
1:D:207:PRO:HG3	1:D:296:MET:HG2	1.98	0.46
1:A:588:ARG:NH2	1:D:371:ASP:OD1	2.47	0.46
1:B:121:MET:HE1	4:B:2096:HOH:O	2.15	0.46
1:D:83:VAL:HA	1:D:255:THR:O	2.15	0.46
1:F:305:VAL:HG12	1:F:350:VAL:HG13	1.97	0.46
1:A:476:ASP:OD2	1:D:453:ARG:NH1	2.42	0.46
1:A:83:VAL:HA	1:A:255:THR:O	2.16	0.46
4:C:2085:HOH:O	1:E:589:ASN:HB2	2.15	0.46
1:F:62:ALA:O	1:F:360:TRP:HH2	1.98	0.46
1:A:611:LYS:HD3	4:A:2217:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ILE:CD1	1:E:119:GLU:HB2	2.45	0.46
1:E:48:VAL:O	1:E:52:LEU:HG	2.16	0.46
1:F:641:LYS:HA	1:F:644:GLU:HG2	1.96	0.46
1:C:83:VAL:HA	1:C:255:THR:O	2.16	0.46
1:B:83:VAL:HA	1:B:255:THR:O	2.16	0.46
1:B:394:HIS:ND1	1:B:425:ARG:HD3	2.31	0.46
1:F:100:THR:HG21	1:F:242:GLN:HG2	1.98	0.46
1:E:553:PHE:CE2	1:E:583:ILE:HG12	2.51	0.46
1:C:166:HIS:CD2	4:C:2008:HOH:O	2.69	0.46
1:E:100:THR:HG21	1:E:242:GLN:HG2	1.98	0.46
1:D:86:MET:HE1	1:D:113:ASN:HA	1.97	0.45
1:B:207:PRO:HG3	1:B:296:MET:HG2	1.98	0.45
1:E:384:LEU:HD12	1:E:387:MET:HE2	1.97	0.45
1:F:322:PRO:HB3	1:F:520:MET:HE1	1.98	0.45
4:B:2163:HOH:O	1:F:520:MET:HE2	2.14	0.45
1:E:207:PRO:HG3	1:E:296:MET:HG2	1.98	0.45
1:E:661:LEU:CD2	1:E:661:LEU:N	2.53	0.45
1:B:505:MET:HE2	1:B:521:TYR:CA	2.38	0.45
1:C:100:THR:HG21	1:C:242:GLN:HG2	1.98	0.45
1:C:68:ILE:CD1	1:C:119:GLU:HB2	2.42	0.45
1:D:157[A]:ARG:HH21	1:D:160:LEU:HD23	1.82	0.45
1:E:394:HIS:ND1	1:E:425:ARG:HD3	2.32	0.45
1:F:314:PRO:HD3	1:F:353:GLN:OE1	2.17	0.45
1:E:314:PRO:HD3	1:E:353:GLN:OE1	2.17	0.45
1:C:207:PRO:HG3	1:C:296:MET:HG2	1.99	0.45
1:C:284:PHE:HD1	4:C:2060:HOH:O	1.98	0.45
1:E:583:ILE:HD13	1:E:594:GLN:HB2	1.97	0.45
1:B:528:LEU:HG	1:B:659:VAL:HG11	1.99	0.45
1:A:307:ASN:HA	1:A:352:ILE:O	2.17	0.45
1:F:65:ARG:HB3	1:F:360:TRP:CH2	2.52	0.45
1:B:307:ASN:HA	1:B:352:ILE:O	2.17	0.45
1:F:197:VAL:O	1:F:265[A]:ASN:ND2	2.50	0.45
1:F:534:THR:HG23	1:F:655:LYS:NZ	2.32	0.45
1:A:661:LEU:CD2	1:A:661:LEU:N	2.60	0.44
1:F:160:LEU:HD21	1:F:172:ILE:HD11	1.99	0.44
1:D:553:PHE:CE2	1:D:583:ILE:HG12	2.53	0.44
1:E:160:LEU:HD21	1:E:172:ILE:HD11	1.99	0.44
1:F:430:ARG:NE	4:F:2089:HOH:O	2.45	0.44
1:D:538:ARG:NH1	4:D:2058:HOH:O	2.46	0.44
1:D:661:LEU:N	1:D:661:LEU:CD2	2.56	0.44
1:F:394:HIS:ND1	1:F:425:ARG:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PRO:HG3	1:A:296:MET:HG2	2.00	0.44
1:B:68:ILE:CD1	1:B:119:GLU:HB2	2.46	0.44
1:D:100:THR:HG21	1:D:242:GLN:HG2	1.99	0.44
1:D:306:LEU:HB2	1:D:348:THR:HG21	1.99	0.44
1:B:435:TYR:HE2	1:F:520:MET:CE	2.30	0.44
1:F:62:ALA:CA	1:F:360:TRP:CZ3	3.00	0.44
1:D:583:ILE:HD13	1:D:594:GLN:HB2	1.99	0.43
1:F:562:THR:HG22	1:F:590:GLY:O	2.17	0.43
1:A:575:VAL:HG13	1:A:608:LYS:HG2	1.99	0.43
1:C:305:VAL:HG12	1:C:350:VAL:HG13	1.98	0.43
4:B:2137:HOH:O	1:F:446:PRO:HB2	2.17	0.43
1:A:394:HIS:ND1	1:A:425:ARG:HD3	2.33	0.43
1:B:160:LEU:HD21	1:B:172:ILE:HD11	2.00	0.43
1:D:68:ILE:CD1	1:D:119:GLU:HB2	2.44	0.43
1:D:160:LEU:HD21	1:D:172:ILE:HD11	2.00	0.43
1:D:394:HIS:ND1	1:D:425:ARG:HD3	2.33	0.43
1:E:371:ASP:HB3	1:E:413:LEU:HD21	2.01	0.43
1:E:95:LYS:NZ	4:E:2018:HOH:O	2.50	0.43
1:F:86:MET:HE1	1:F:113:ASN:HA	2.00	0.43
1:A:344:TYR:O	1:A:348[A]:THR:HG22	2.19	0.43
1:B:213:HIS:CG	1:B:293:PRO:HB2	2.54	0.43
1:C:296:MET:CG	4:C:2060:HOH:O	2.52	0.43
4:E:2005:HOH:O	1:F:401:SER:HB3	2.18	0.43
1:A:160:LEU:HD21	1:A:172:ILE:HD11	2.00	0.43
1:E:305:VAL:HG12	1:E:350:VAL:HG13	2.00	0.43
1:C:237:VAL:HG11	1:C:522:MET:HB3	2.01	0.43
1:E:86:MET:HE1	1:E:113:ASN:HA	2.01	0.43
1:F:31:SER:HB3	1:F:35:LYS:HE3	2.00	0.43
1:B:100:THR:HG21	1:B:242:GLN:HG2	2.00	0.43
1:C:314:PRO:HD3	1:C:353:GLN:OE1	2.19	0.43
1:A:68:ILE:CD1	1:A:119:GLU:HB2	2.44	0.42
1:A:536:ASP:OD1	1:A:539:GLY:HA2	2.16	0.42
1:B:514:ASN:HB3	1:B:517:TRP:HB2	2.01	0.42
1:D:237:VAL:HG12	1:D:243:ALA:HB1	2.01	0.42
1:C:126:GLN:HB2	4:C:2021:HOH:O	2.18	0.42
1:C:132:PRO:O	1:C:250:PHE:HB3	2.19	0.42
1:C:160:LEU:HD21	1:C:172:ILE:HD11	2.01	0.42
1:C:213:HIS:CG	1:C:293:PRO:HB2	2.54	0.42
1:F:384:LEU:HD12	1:F:387:MET:HE2	2.01	0.42
1:B:322:PRO:HB3	1:B:520:MET:HE1	2.01	0.42
1:B:95:LYS:NZ	4:B:2016:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:LEU:HD12	1:E:305:VAL:CG2	2.50	0.42
1:C:169:LYS:HB2	1:C:169:LYS:HE3	1.84	0.42
1:E:320:LEU:HD13	1:E:327:VAL:HG13	2.02	0.42
1:A:348[A]:THR:HG23	1:A:365:VAL:HG21	2.02	0.42
1:D:575:VAL:HG13	1:D:608:LYS:HG2	2.01	0.42
1:A:170[A]:LYS:HD3	4:A:2060:HOH:O	2.20	0.42
1:A:305:VAL:HG12	1:A:350:VAL:HG13	2.01	0.42
1:F:300:LEU:HB2	1:F:305:VAL:HG22	2.02	0.42
1:C:575:VAL:HG13	1:C:608:LYS:HG2	2.01	0.42
1:D:586:THR:CG2	4:D:2166:HOH:O	2.67	0.42
1:D:610:THR:HB	1:D:612:PRO:HD2	2.01	0.42
1:A:514:ASN:HB3	1:A:517:TRP:HB2	2.01	0.42
1:F:40:ILE:CD1	1:F:40:ILE:H	2.31	0.42
1:F:575:VAL:HG13	1:F:608:LYS:HG2	2.02	0.42
1:C:31:SER:HB3	1:C:35:LYS:HE3	2.01	0.41
4:C:2098:HOH:O	1:E:448:VAL:HG13	2.18	0.41
1:F:207:PRO:HG3	1:F:296:MET:HG2	2.01	0.41
1:A:517:TRP:HA	1:A:520:MET:HE3	2.02	0.41
1:D:307:ASN:HA	1:D:352:ILE:O	2.20	0.41
1:E:306:LEU:HB2	1:E:348:THR:HG21	2.03	0.41
1:C:306:LEU:HB2	1:C:348:THR:HG21	2.03	0.41
1:C:514:ASN:HB3	1:C:517:TRP:HB2	2.01	0.41
1:E:182[A]:ILE:H	1:E:182[A]:ILE:HG13	1.72	0.41
1:F:68:ILE:CD1	1:F:119:GLU:HB2	2.46	0.41
1:B:30:GLU:N	4:B:2001:HOH:O	2.53	0.41
1:B:610:THR:HB	1:B:612:PRO:HD2	2.02	0.41
1:E:237:VAL:CG2	1:E:244:GLN:CB	2.87	0.41
1:E:213:HIS:CG	1:E:293:PRO:HB2	2.56	0.41
1:E:60:PHE:HD2	1:E:107:ARG:NH2	2.18	0.41
1:A:430:ARG:NE	4:A:2132:HOH:O	2.50	0.41
1:B:258:THR:HG23	1:B:540:LYS:O	2.19	0.41
1:C:307:ASN:HA	1:C:352:ILE:O	2.20	0.41
1:D:611:LYS:HB3	1:D:612:PRO:HD3	2.03	0.41
1:E:31:SER:HB3	1:E:35:LYS:HE3	2.03	0.41
1:E:536:ASP:OD1	1:E:539:GLY:HA2	2.18	0.41
1:A:300:LEU:HB2	1:A:305:VAL:HG22	2.02	0.41
1:D:65:ARG:HB3	1:D:360:TRP:CH2	2.55	0.41
1:F:661:LEU:N	1:F:661:LEU:CD2	2.55	0.41
1:B:31:SER:HB3	1:B:35:LYS:HE3	2.02	0.41
1:D:320:LEU:HD13	1:D:327:VAL:HG13	2.03	0.41
1:E:387:MET:HE3	1:E:432:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:609:LEU:HD23	1:E:633:VAL:HG22	2.02	0.41
1:A:100:THR:HG21	1:A:242:GLN:HG2	2.03	0.41
1:A:371:ASP:HB3	1:A:413:LEU:HD21	2.03	0.41
1:D:213:HIS:CG	1:D:293:PRO:HB2	2.56	0.41
1:F:307:ASN:HA	1:F:352:ILE:O	2.21	0.41
1:C:528:LEU:HG	1:C:659:VAL:HG11	2.03	0.41
1:D:514:ASN:HB3	1:D:517:TRP:HB2	2.03	0.41
1:A:414:ARG:HD2	4:A:2165:HOH:O	2.22	0.41
1:A:611:LYS:HB3	1:A:612:PRO:HD3	2.03	0.41
1:B:549:PRO:HB2	1:B:583:ILE:HD12	2.03	0.41
1:E:307:ASN:HA	1:E:352:ILE:O	2.21	0.41
1:F:213:HIS:CG	1:F:293:PRO:HB2	2.56	0.41
1:E:97:ALA:HA	1:E:106:TRP:CD2	2.56	0.40
1:E:514:ASN:HB3	1:E:517:TRP:HB2	2.04	0.40
1:C:97:ALA:HA	1:C:106:TRP:CD2	2.56	0.40
1:C:351:LEU:HD11	1:C:369:LEU:HD21	2.02	0.40
1:C:611:LYS:HB3	1:C:612:PRO:HD3	2.02	0.40
1:F:97:ALA:HA	1:F:106:TRP:CD2	2.56	0.40
1:A:610:THR:HB	1:A:612:PRO:HD2	2.02	0.40
1:D:314:PRO:HD3	1:D:353:GLN:OE1	2.20	0.40
1:A:75:ILE:O	1:A:83:VAL:HG22	2.21	0.40
1:C:430:ARG:NE	4:C:2072:HOH:O	2.53	0.40
1:A:435:TYR:HE2	1:D:520:MET:CE	2.35	0.40
1:D:573:ASN:HB3	1:D:599:LEU:HD22	2.04	0.40
1:F:306:LEU:HB2	1:F:348:THR:HG21	2.03	0.40
1:F:611:LYS:HB3	1:F:612:PRO:HD3	2.04	0.40
1:A:500:LEU:HD12	1:A:500:LEU:HA	1.94	0.40
1:F:514:ASN:HB3	1:F:517:TRP:HB2	2.03	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	647/668 (97%)	626 (97%)	18 (3%)	3 (0%)	29	54
1	B	636/668 (95%)	615 (97%)	19 (3%)	2 (0%)	41	66
1	C	634/668 (95%)	613 (97%)	19 (3%)	2 (0%)	41	66
1	D	636/668 (95%)	614 (96%)	20 (3%)	2 (0%)	41	66
1	E	637/668 (95%)	618 (97%)	17 (3%)	2 (0%)	41	66
1	F	635/668 (95%)	613 (96%)	18 (3%)	4 (1%)	25	50
All	All	3825/4008 (95%)	3699 (97%)	111 (3%)	15 (0%)	34	60

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	665	HIS
1	B	57	ARG
1	C	57	ARG
1	D	56	ASP
1	E	57	ARG
1	F	57	ARG
1	A	56	ASP
1	B	56	ASP
1	C	56	ASP
1	D	57	ARG
1	E	56	ASP
1	F	56	ASP
1	F	539	GLY
1	F	540	LYS

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	527/539 (98%)	485 (92%)	42 (8%)	12	27
1	B	516/539 (96%)	476 (92%)	40 (8%)	12	29
1	C	514/539 (95%)	464 (90%)	50 (10%)	8	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	516/539 (96%)	472 (92%)	44 (8%)	10 24
1	E	516/539 (96%)	470 (91%)	46 (9%)	9 22
1	F	515/539 (96%)	471 (92%)	44 (8%)	10 24
All	All	3104/3234 (96%)	2838 (91%)	266 (9%)	10 24

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	56	ASP
1	A	72	SER
1	A	95	LYS
1	A	101	VAL
1	A	151	THR
1	A	198	LYS
1	A	215	VAL
1	A	223	THR
1	A	235	VAL
1	A	261	LEU
1	A	266	VAL
1	A	267	LEU
1	A	276	THR
1	A	282	LEU
1	A	327	VAL
1	A	359	VAL
1	A	363[A]	ASP
1	A	363[B]	ASP
1	A	365	VAL
1	A	384	LEU
1	A	396	ILE
1	A	402	LYS
1	A	413	LEU
1	A	483	LEU
1	A	500	LEU
1	A	536	ASP
1	A	538	ARG
1	A	555	LEU
1	A	560	LEU
1	A	575	VAL
1	A	586	THR
1	A	609	LEU

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Mol	Chain	Res	Type
1	A	614	LEU
1	A	616	GLN
1	A	624	LEU
1	A	629	LYS
1	A	635	LEU
1	A	641	LYS
1	A	651	SER
1	A	655	LYS
1	A	661	LEU
1	B	49	LEU
1	B	56	ASP
1	B	72	SER
1	B	79	GLU
1	B	95	LYS
1	B	101	VAL
1	B	147	ILE
1	B	198	LYS
1	B	201	LYS
1	B	215	VAL
1	B	235	VAL
1	B	261	LEU
1	B	266	VAL
1	B	267	LEU
1	B	276	THR
1	B	282	LEU
1	B	327	VAL
1	B	353	GLN
1	B	359	VAL
1	B	365	VAL
1	B	382	ARG
1	B	384	LEU
1	B	402	LYS
1	B	409	ARG
1	B	483	LEU
1	B	500	LEU
1	B	538	ARG
1	B	555	LEU
1	B	586	THR
1	B	600	ASN
1	B	609	LEU
1	B	614	LEU
1	B	616	GLN

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Mol	Chain	Res	Type
1	B	624	LEU
1	B	629	LYS
1	B	635	LEU
1	B	649	LEU
1	B	651	SER
1	B	655	LYS
1	B	661	LEU
1	C	49	LEU
1	C	56	ASP
1	C	79	GLU
1	C	90	GLN
1	C	101	VAL
1	C	189	ARG
1	C	198	LYS
1	C	201	LYS
1	C	215	VAL
1	C	225	MET
1	C	235	VAL
1	C	261	LEU
1	C	266	VAL
1	C	267	LEU
1	C	327	VAL
1	C	353	GLN
1	C	359	VAL
1	C	363	ASP
1	C	365	VAL
1	C	382	ARG
1	C	384	LEU
1	C	396	ILE
1	C	399	GLU
1	C	402	LYS
1	C	409	ARG
1	C	413	LEU
1	C	449	GLU
1	C	482	GLN
1	C	483	LEU
1	C	500	LEU
1	C	534	THR
1	C	538	ARG
1	C	550	ASP
1	C	555	LEU
1	C	560	LEU

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Mol	Chain	Res	Type
1	C	575	VAL
1	C	580	LYS
1	C	586	THR
1	C	609	LEU
1	C	611	LYS
1	C	614	LEU
1	C	616	GLN
1	C	624	LEU
1	C	629	LYS
1	C	635	LEU
1	C	649	LEU
1	C	651	SER
1	C	655	LYS
1	C	661	LEU
1	C	662	GLU
1	D	49	LEU
1	D	54	PHE
1	D	79	GLU
1	D	90[A]	GLN
1	D	90[B]	GLN
1	D	99	ASP
1	D	147[A]	ILE
1	D	147[B]	ILE
1	D	151	THR
1	D	189	ARG
1	D	198	LYS
1	D	215	VAL
1	D	235	VAL
1	D	261	LEU
1	D	267	LEU
1	D	282	LEU
1	D	327	VAL
1	D	359	VAL
1	D	365	VAL
1	D	384	LEU
1	D	399	GLU
1	D	402	LYS
1	D	409	ARG
1	D	482	GLN
1	D	483	LEU
1	D	495	LYS
1	D	500	LEU

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Mol	Chain	Res	Type
1	D	555	LEU
1	D	560	LEU
1	D	575	VAL
1	D	580	LYS
1	D	583	ILE
1	D	586	THR
1	D	609	LEU
1	D	614	LEU
1	D	616	GLN
1	D	624	LEU
1	D	629	LYS
1	D	635	LEU
1	D	649	LEU
1	D	651	SER
1	D	655	LYS
1	D	661	LEU
1	D	662	GLU
1	E	49	LEU
1	E	52	LEU
1	E	56	ASP
1	E	59	GLU
1	E	79	GLU
1	E	95	LYS
1	E	99	ASP
1	E	101	VAL
1	E	145	VAL
1	E	182[A]	ILE
1	E	182[B]	ILE
1	E	189	ARG
1	E	194	GLU
1	E	198	LYS
1	E	215	VAL
1	E	225	MET
1	E	235	VAL
1	E	261	LEU
1	E	266	VAL
1	E	267	LEU
1	E	276	THR
1	E	282	LEU
1	E	327	VAL
1	E	359	VAL
1	E	382	ARG

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Mol	Chain	Res	Type
1	E	384	LEU
1	E	402	LYS
1	E	409	ARG
1	E	413	LEU
1	E	466	LYS
1	E	482	GLN
1	E	483	LEU
1	E	500	LEU
1	E	536	ASP
1	E	538	ARG
1	E	550	ASP
1	E	555	LEU
1	E	560	LEU
1	E	575	VAL
1	E	583	ILE
1	E	586	THR
1	E	609	LEU
1	E	624	LEU
1	E	635	LEU
1	E	649	LEU
1	E	661	LEU
1	F	56	ASP
1	F	79	GLU
1	F	90	GLN
1	F	95	LYS
1	F	99	ASP
1	F	101	VAL
1	F	145	VAL
1	F	189	ARG
1	F	193	ASP
1	F	215	VAL
1	F	235	VAL
1	F	261	LEU
1	F	266	VAL
1	F	267	LEU
1	F	274	ARG
1	F	282	LEU
1	F	327	VAL
1	F	353	GLN
1	F	359	VAL
1	F	365	VAL
1	F	382	ARG

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Mol	Chain	Res	Type
1	F	384	LEU
1	F	399[A]	GLU
1	F	399[B]	GLU
1	F	402	LYS
1	F	413	LEU
1	F	483	LEU
1	F	500	LEU
1	F	538	ARG
1	F	555	LEU
1	F	560	LEU
1	F	575	VAL
1	F	585	LEU
1	F	586	THR
1	F	609	LEU
1	F	614	LEU
1	F	616	GLN
1	F	624	LEU
1	F	629	LYS
1	F	635	LEU
1	F	649	LEU
1	F	651	SER
1	F	661	LEU
1	F	662	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	665	HIS
1	A	667	HIS
1	B	259	ASN
1	B	311	ASN
1	D	213	HIS
1	E	311	ASN
1	E	616	GLN
1	F	259	ASN
1	F	311	ASN

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 18 ligands modelled in this entry, 12 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	C	801	-	4,4,4	0.38	0	6,6,6	0.35	0
3	SO4	B	801	-	4,4,4	0.28	0	6,6,6	0.45	0
3	SO4	D	801	-	4,4,4	0.74	0	6,6,6	0.33	0
3	SO4	F	801	-	4,4,4	0.35	0	6,6,6	0.29	0
3	SO4	A	801	-	4,4,4	0.42	0	6,6,6	0.21	0
3	SO4	E	801	-	4,4,4	0.54	0	6,6,6	0.28	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	639/668 (95%)	-0.60	5 (0%)	86	87	21, 41, 78, 135	0
1	B	634/668 (94%)	-0.51	13 (2%)	63	65	25, 42, 86, 133	0
1	C	634/668 (94%)	-0.28	11 (1%)	70	72	25, 49, 85, 120	0
1	D	634/668 (94%)	-0.50	10 (1%)	72	74	25, 42, 76, 127	0
1	E	634/668 (94%)	-0.44	18 (2%)	53	54	24, 42, 80, 135	0
1	F	634/668 (94%)	-0.50	10 (1%)	72	74	22, 44, 76, 134	0
All	All	3809/4008 (95%)	-0.47	67 (1%)	68	70	21, 43, 82, 135	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	54	PHE	6.7
1	F	55	ALA	5.5
1	B	54	PHE	5.4
1	A	54	PHE	5.1
1	C	54	PHE	4.9
1	E	54	PHE	4.9
1	B	618	ALA	4.8
1	C	142	SER	4.7
1	E	53	PRO	4.4
1	E	55	ALA	4.4
1	E	620	ARG	4.3
1	A	620	ARG	4.1
1	D	54	PHE	4.1
1	B	620	ARG	4.0
1	E	56	ASP	3.9
1	F	619	ALA	3.7
1	B	57	ARG	3.6
1	E	616	GLN	3.2
1	F	56	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	3.1
1	E	622	LEU	3.1
1	C	56	ASP	3.0
1	F	57	ARG	3.0
1	B	629	LYS	2.9
1	B	53	PRO	2.9
1	E	655	LYS	2.8
1	C	619	ALA	2.8
1	F	53	PRO	2.8
1	E	618	ALA	2.7
1	B	621	LYS	2.7
1	D	622	LEU	2.7
1	C	68	ILE	2.7
1	D	626	THR	2.7
1	F	620	ARG	2.7
1	B	663	HIS	2.6
1	F	621	LYS	2.6
1	D	602	LYS	2.6
1	D	619	ALA	2.5
1	C	198	LYS	2.5
1	B	574	TRP	2.5
1	D	630	GLN	2.5
1	E	57	ARG	2.5
1	C	52	LEU	2.4
1	D	56	ASP	2.4
1	A	618	ALA	2.4
1	B	55	ALA	2.3
1	D	55	ALA	2.3
1	D	620	ARG	2.3
1	E	50	LYS	2.3
1	A	668	HIS	2.3
1	B	625	PRO	2.2
1	C	57	ARG	2.2
1	E	539	GLY	2.2
1	E	617	ILE	2.2
1	C	602	LYS	2.2
1	E	601	PRO	2.2
1	D	621	LYS	2.2
1	F	622	LEU	2.1
1	F	663	HIS	2.1
1	E	621	LYS	2.1
1	E	602	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	563	ASP	2.1
1	A	621	LYS	2.1
1	E	535	TYR	2.1
1	C	165	GLN	2.0
1	E	619	ALA	2.0
1	B	363	ASP	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	700	1/1	0.98	0.03	46,46,46,46	0
2	ZN	B	701	1/1	0.99	0.07	40,40,40,40	0
3	SO4	B	801	5/5	0.99	0.07	36,38,41,42	0
3	SO4	C	801	5/5	0.99	0.11	45,49,50,52	0
3	SO4	E	801	5/5	0.99	0.09	30,34,35,36	0
2	ZN	D	701	1/1	0.99	0.07	34,34,34,34	0
2	ZN	B	700	1/1	0.99	0.05	44,44,44,44	0
2	ZN	A	700	1/1	0.99	0.04	39,39,39,39	0
2	ZN	F	700	1/1	0.99	0.03	43,43,43,43	0
2	ZN	A	701	1/1	0.99	0.07	38,38,38,38	0
2	ZN	E	700	1/1	0.99	0.03	43,43,43,43	0
2	ZN	C	701	1/1	0.99	0.06	45,45,45,45	0
2	ZN	E	701	1/1	0.99	0.06	37,37,37,37	0
3	SO4	D	801	5/5	0.99	0.08	28,31,34,37	0
2	ZN	D	700	1/1	1.00	0.05	45,45,45,45	0
2	ZN	F	701	1/1	1.00	0.09	46,46,46,46	0
3	SO4	F	801	5/5	1.00	0.06	30,32,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	801	5/5	1.00	0.10	34,35,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.