Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:26 PM EDT

PDB ID	:	3O4F
Title	:	Crystal Structure of Spermidine Synthase from E. coli
Authors	:	Zhou, X.; Tkaczuk, K.L.; Chruszcz, M.; Chua, T.K.; Minor, W.; Sivaraman, J.
Deposited on	:	2010-07-27
Resolution	:	2.90 Å(reported)

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

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

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

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

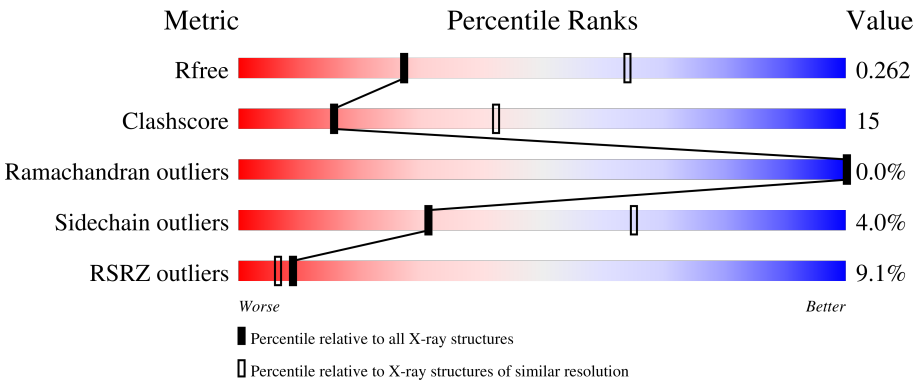
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	6%, 72%, 23%, • •
1	B	294	2%, 67%, 23%, • 8%
1	C	294	9%, 71%, 24%, • •
1	D	294	%, 70%, 21%, • 6%
1	E	294	17%, 68%, 25%, • •

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Mol	Chain	Length	Quality of chain
1	F	294	7% 75% 16% • 9%
1	G	294	15% 70% 23% • 5%
1	H	294	10% 71% 19% 10%

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	292	-	-	X	-
2	SO4	C	291	-	-	X	-
2	SO4	D	291	-	-	-	X
2	SO4	E	290	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17519 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 Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2212	1409	376	415	12	0	0	0
1	B	270	2135	1359	366	398	12	0	0	0
1	C	284	2228	1417	379	420	12	0	0	0
1	D	276	2176	1385	371	408	12	0	0	0
1	E	283	2208	1406	372	418	12	0	0	0
1	F	269	2116	1347	361	396	12	0	0	0
1	G	279	2189	1396	371	410	12	0	0	0
1	H	264	2087	1330	356	389	12	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P09158
A	-4	HIS	-	expression tag	UNP P09158
A	-3	HIS	-	expression tag	UNP P09158
A	-2	HIS	-	expression tag	UNP P09158
A	-1	HIS	-	expression tag	UNP P09158
A	0	HIS	-	expression tag	UNP P09158
B	-5	HIS	-	expression tag	UNP P09158
B	-4	HIS	-	expression tag	UNP P09158
B	-3	HIS	-	expression tag	UNP P09158
B	-2	HIS	-	expression tag	UNP P09158
B	-1	HIS	-	expression tag	UNP P09158
B	0	HIS	-	expression tag	UNP P09158
C	-5	HIS	-	expression tag	UNP P09158

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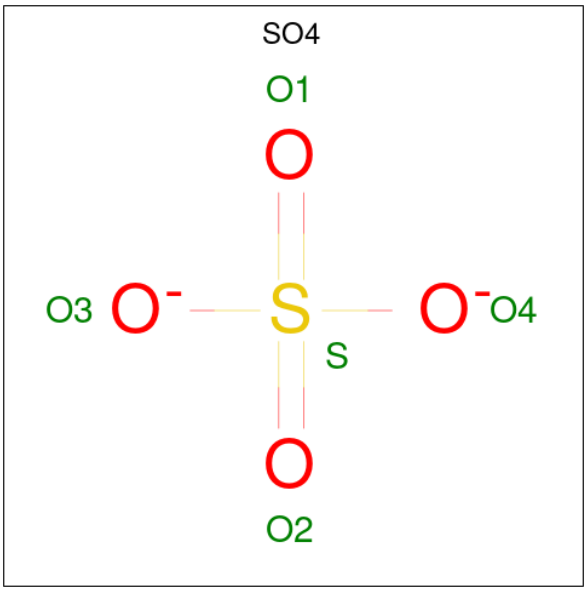
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P09158
C	-3	HIS	-	expression tag	UNP P09158
C	-2	HIS	-	expression tag	UNP P09158
C	-1	HIS	-	expression tag	UNP P09158
C	0	HIS	-	expression tag	UNP P09158
D	-5	HIS	-	expression tag	UNP P09158
D	-4	HIS	-	expression tag	UNP P09158
D	-3	HIS	-	expression tag	UNP P09158
D	-2	HIS	-	expression tag	UNP P09158
D	-1	HIS	-	expression tag	UNP P09158
D	0	HIS	-	expression tag	UNP P09158
E	-5	HIS	-	expression tag	UNP P09158
E	-4	HIS	-	expression tag	UNP P09158
E	-3	HIS	-	expression tag	UNP P09158
E	-2	HIS	-	expression tag	UNP P09158
E	-1	HIS	-	expression tag	UNP P09158
E	0	HIS	-	expression tag	UNP P09158
F	-5	HIS	-	expression tag	UNP P09158
F	-4	HIS	-	expression tag	UNP P09158
F	-3	HIS	-	expression tag	UNP P09158
F	-2	HIS	-	expression tag	UNP P09158
F	-1	HIS	-	expression tag	UNP P09158
F	0	HIS	-	expression tag	UNP P09158
G	-5	HIS	-	expression tag	UNP P09158
G	-4	HIS	-	expression tag	UNP P09158
G	-3	HIS	-	expression tag	UNP P09158
G	-2	HIS	-	expression tag	UNP P09158
G	-1	HIS	-	expression tag	UNP P09158
G	0	HIS	-	expression tag	UNP P09158
H	-5	HIS	-	expression tag	UNP P09158
H	-4	HIS	-	expression tag	UNP P09158
H	-3	HIS	-	expression tag	UNP P09158
H	-2	HIS	-	expression tag	UNP P09158
H	-1	HIS	-	expression tag	UNP P09158
H	0	HIS	-	expression tag	UNP P09158

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	1	Total O 1 1	0	0

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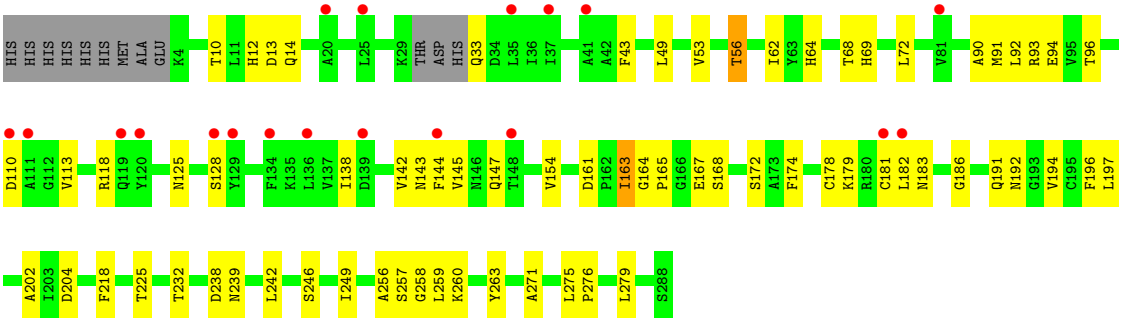
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	3	3	3	0	0
			Total	O		
3	D	1	1	1	0	0
			Total	O		
3	E	3	3	3	0	0
			Total	O		
3	F	1	1	1	0	0
			Total	O		
3	G	1	1	1	0	0
			Total	O		
3	H	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

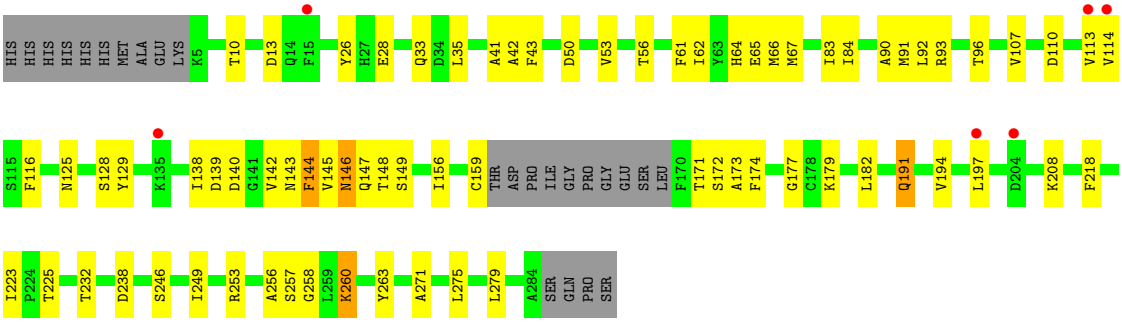
• Molecule 1: Spermidine synthase

Chain A:



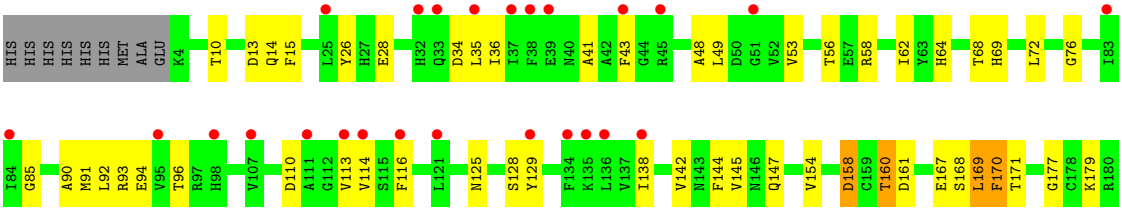
• Molecule 1: Spermidine synthase

Chain B:



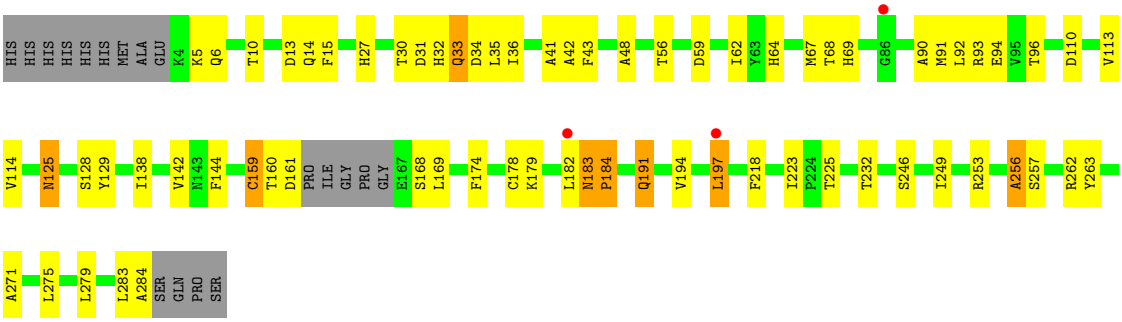
• Molecule 1: Spermidine synthase

Chain C:



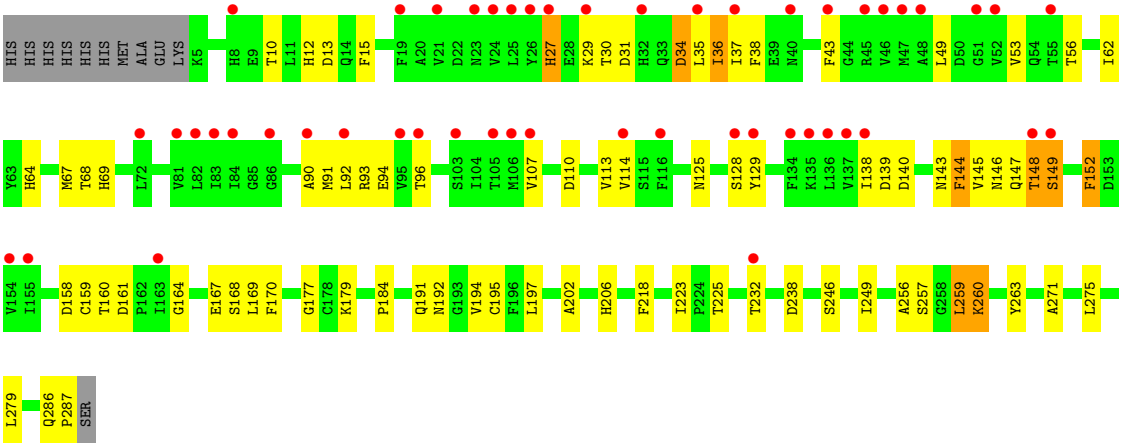
• Molecule 1: Spermidine synthase

Chain D:



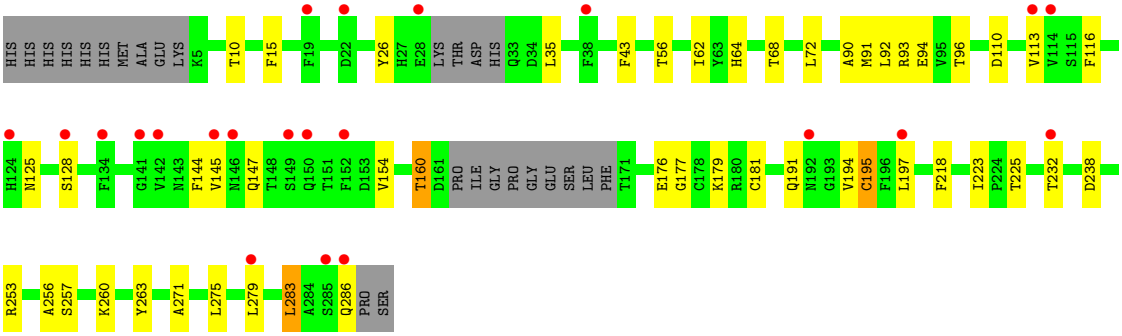
• Molecule 1: Spermidine synthase

Chain E:



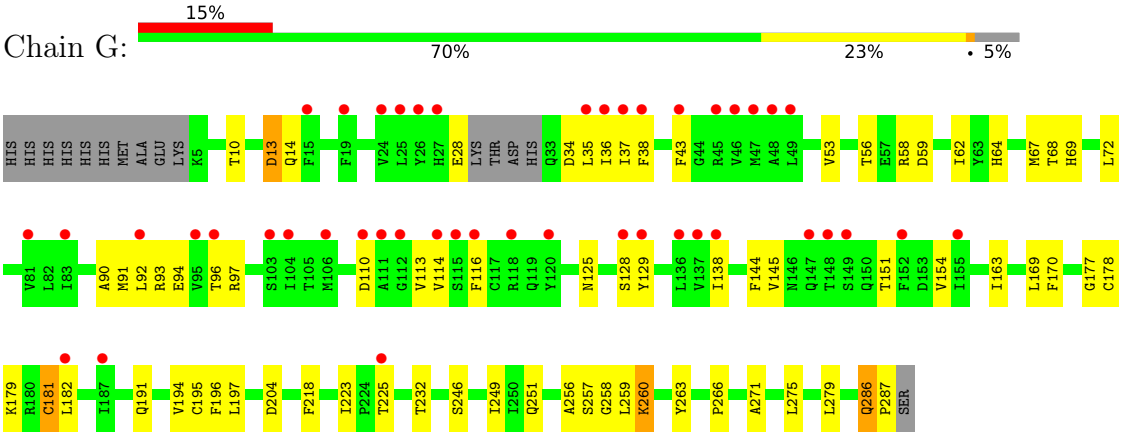
• Molecule 1: Spermidine synthase

Chain F:



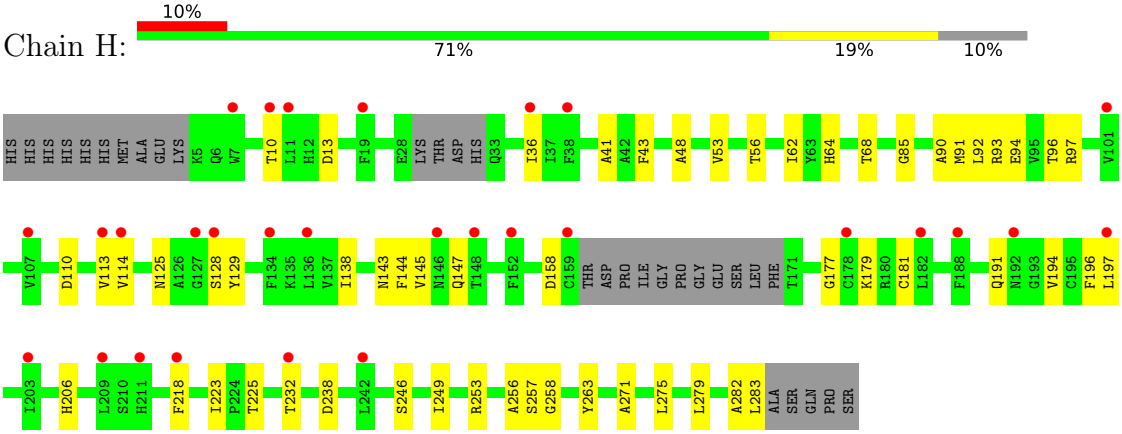
• Molecule 1: Spermidine synthase

Chain G:



• Molecule 1: Spermidine synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	123.11Å 123.11Å 210.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.90 48.29 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.29-2.90) 95.7 (48.29-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.208 , 0.241 0.248 , 0.262	Depositor DCC
R_{free} test set	3486 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 89.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17519	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 (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	0.79	0/2269	0.80	2/3083 (0.1%)
1	B	0.89	0/2189	0.79	0/2971
1	C	0.89	0/2287	0.81	2/3111 (0.1%)
1	D	0.86	0/2231	0.81	6/3030 (0.2%)
1	E	0.79	0/2266	0.77	2/3084 (0.1%)
1	F	0.72	2/2168 (0.1%)	0.74	1/2943 (0.0%)
1	G	0.83	1/2246 (0.0%)	0.77	2/3052 (0.1%)
1	H	0.71	1/2139 (0.0%)	0.74	0/2903
All	All	0.81	4/17795 (0.0%)	0.78	15/24177 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	178	CYS	CB-SG	-5.56	1.72	1.81
1	F	176	GLU	CG-CD	-5.18	1.44	1.51
1	F	195	CYS	CB-SG	5.12	1.91	1.82
1	H	143	ASN	CG-ND2	5.11	1.45	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	LEU	CA-CB-CG	-5.91	101.72	115.30
1	D	262	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	G	67	MET	CG-SD-CE	-5.62	91.21	100.20
1	A	260	LYS	N-CA-C	-5.39	96.43	111.00
1	F	283	LEU	CA-CB-CG	-5.34	103.02	115.30
1	E	260	LYS	N-CA-C	-5.30	96.69	111.00
1	D	262	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	118	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	197	LEU	CB-CG-CD1	-5.26	102.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	260	LYS	N-CA-C	-5.25	96.84	111.00
1	D	183	ASN	N-CA-C	-5.16	97.07	111.00
1	C	260	LYS	N-CA-C	-5.06	97.33	111.00
1	E	67	MET	CG-SD-CE	-5.03	92.15	100.20
1	D	67	MET	CG-SD-CE	-5.00	92.19	100.20
1	D	256	ALA	N-CA-C	-5.00	97.49	111.00

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	2212	0	2078	63	0
1	B	2135	0	2012	74	0
1	C	2228	0	2084	61	0
1	D	2176	0	2039	55	0
1	E	2208	0	2060	104	0
1	F	2116	0	1985	40	0
1	G	2189	0	2060	66	0
1	H	2087	0	1962	48	0
2	A	20	0	0	5	0
2	B	10	0	0	0	0
2	C	30	0	0	5	0
2	D	20	0	0	0	0
2	E	20	0	0	4	0
2	F	20	0	0	0	0
2	G	25	0	0	0	0
2	H	10	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
All	All	17519	0	16280	496	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 15.

All (496) 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:258:GLY:O	1:G:259:LEU:HD12	1.38	1.20
1:E:145:VAL:HG23	1:E:177:GLY:CA	1.80	1.12
1:B:171:THR:HG22	1:B:173:ALA:H	1.11	1.10
1:G:258:GLY:C	1:G:259:LEU:HD12	1.78	1.04
1:E:145:VAL:HG23	1:E:177:GLY:HA2	1.39	1.01
1:G:93:ARG:HG2	1:G:97:ARG:NH2	1.75	1.00
1:E:259:LEU:N	1:E:259:LEU:HD23	1.76	0.97
1:G:93:ARG:HG2	1:G:97:ARG:HH22	1.28	0.97
1:E:146:ASN:O	1:E:147:GLN:HB2	1.63	0.96
1:E:271:ALA:HB1	1:F:271:ALA:HB1	1.48	0.94
1:G:256:ALA:HA	1:G:257:SER:C	1.83	0.94
1:A:256:ALA:HA	1:A:257:SER:C	1.87	0.94
1:A:271:ALA:HB1	1:B:271:ALA:HB1	1.51	0.92
1:H:279:LEU:O	1:H:282:ALA:HB3	1.68	0.91
1:E:145:VAL:CG2	1:E:177:GLY:HA2	2.03	0.89
1:B:145:VAL:HG22	1:B:177:GLY:HA3	1.56	0.88
1:E:145:VAL:HG23	1:E:177:GLY:HA3	1.53	0.88
1:H:68:THR:HB	1:H:91:MET:CE	2.04	0.88
1:C:76:GLY:HA2	1:C:253:ARG:NH1	1.90	0.87
1:G:93:ARG:CG	1:G:97:ARG:HH22	1.87	0.87
1:B:148:THR:HG22	1:B:148:THR:O	1.75	0.87
1:E:145:VAL:CG2	1:E:177:GLY:CA	2.52	0.87
1:C:271:ALA:HB1	1:D:271:ALA:HB1	1.57	0.87
1:D:68:THR:HB	1:D:91:MET:CE	2.07	0.85
1:E:144:PHE:CD1	1:E:144:PHE:O	2.30	0.85
1:G:286:GLN:HG3	1:G:287:PRO:HD2	1.58	0.85
1:G:258:GLY:C	1:G:259:LEU:CD1	2.46	0.84
1:F:68:THR:HB	1:F:91:MET:CE	2.08	0.84
1:G:271:ALA:HB1	1:H:271:ALA:HB1	1.58	0.84
1:B:171:THR:HG22	1:B:173:ALA:N	1.93	0.83
1:C:168:SER:HB3	2:C:291:SO4:S	2.17	0.83
1:B:143:ASN:O	1:B:146:ASN:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD23	1:A:183:ASN:O	1.79	0.82
1:A:182:LEU:HD21	1:A:186:GLY:CA	2.09	0.81
1:C:68:THR:HB	1:C:91:MET:CE	2.10	0.81
1:B:140:ASP:HB3	1:B:143:ASN:HB2	1.62	0.80
1:E:68:THR:HB	1:E:91:MET:CE	2.11	0.80
1:D:33:GLN:HG3	1:D:34:ASP:N	1.98	0.79
1:E:35:LEU:O	1:E:36:ILE:HG22	1.83	0.79
1:E:30:THR:HG22	1:E:31:ASP:N	1.98	0.78
1:E:107:VAL:HG21	1:E:144:PHE:CD2	2.19	0.77
1:C:168:SER:HB3	2:C:291:SO4:O1	1.85	0.77
1:H:275:LEU:HD13	1:H:279:LEU:HD23	1.65	0.77
1:A:182:LEU:HD21	1:A:186:GLY:HA3	1.65	0.76
1:B:148:THR:O	1:B:149:SER:HB2	1.85	0.75
1:C:256:ALA:HA	1:C:257:SER:C	2.05	0.75
1:G:256:ALA:HA	1:G:258:GLY:N	2.00	0.74
1:B:84:ILE:HD13	1:B:174:PHE:CE1	2.23	0.74
1:E:147:GLN:HB3	1:E:149:SER:H	1.52	0.74
1:G:286:GLN:CG	1:G:287:PRO:HD2	2.18	0.74
1:E:145:VAL:CG2	1:E:177:GLY:HA3	2.17	0.73
1:A:68:THR:HB	1:A:91:MET:CE	2.18	0.73
1:E:30:THR:HG22	1:E:31:ASP:H	1.53	0.73
1:G:275:LEU:HB3	1:G:279:LEU:HD23	1.70	0.73
1:H:68:THR:HB	1:H:91:MET:HE2	1.72	0.71
1:E:148:THR:HG22	1:E:148:THR:O	1.90	0.70
1:A:164:GLY:HA3	1:A:167:GLU:CG	2.22	0.70
1:B:139:ASP:OD1	1:B:143:ASN:ND2	2.21	0.70
1:B:139:ASP:OD2	1:B:143:ASN:HB3	1.92	0.70
1:D:283:LEU:O	1:D:284:ALA:C	2.30	0.70
1:E:34:ASP:OD2	1:E:34:ASP:C	2.29	0.69
1:A:182:LEU:CD2	1:A:186:GLY:HA3	2.22	0.69
1:D:34:ASP:OD2	1:D:34:ASP:C	2.30	0.69
1:F:10:THR:HG22	1:F:10:THR:O	1.93	0.69
1:G:68:THR:HB	1:G:91:MET:CE	2.24	0.69
2:A:292:SO4:S	1:E:168:SER:HB2	2.33	0.68
1:D:160:THR:CG2	1:D:160:THR:O	2.41	0.68
1:G:64:HIS:O	1:G:68:THR:HG22	1.93	0.68
1:G:258:GLY:O	1:G:259:LEU:CD1	2.30	0.68
1:H:275:LEU:HD13	1:H:279:LEU:CD2	2.24	0.68
1:G:14:GLN:HG3	1:H:41:ALA:HB3	1.74	0.68
1:E:148:THR:O	1:E:148:THR:CG2	2.42	0.68
1:D:160:THR:O	1:D:160:THR:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:MET:HE3	1:B:156:ILE:HG21	1.76	0.67
1:B:148:THR:O	1:B:148:THR:CG2	2.42	0.67
1:F:43:PHE:HB3	1:F:56:THR:CG2	2.25	0.66
1:A:164:GLY:CA	1:A:167:GLU:HG2	2.25	0.66
1:C:64:HIS:O	1:C:68:THR:HG22	1.96	0.66
1:D:33:GLN:CG	1:D:34:ASP:N	2.58	0.66
1:C:167:GLU:OE1	1:C:167:GLU:N	2.29	0.66
1:A:256:ALA:HA	1:A:258:GLY:N	2.11	0.65
1:E:140:ASP:O	1:E:143:ASN:HB3	1.96	0.65
1:F:68:THR:HG21	1:F:94:GLU:HB3	1.79	0.65
1:B:84:ILE:HD13	1:B:174:PHE:HE1	1.59	0.65
1:A:164:GLY:HA3	1:A:167:GLU:HG2	1.77	0.65
1:B:256:ALA:HA	1:B:257:SER:C	2.16	0.65
1:E:139:ASP:OD1	1:E:140:ASP:N	2.29	0.65
1:H:196:PHE:HD2	1:H:197:LEU:HD12	1.62	0.65
1:B:172:SER:HB2	1:B:208:LYS:NZ	2.11	0.64
1:C:34:ASP:OD2	1:C:34:ASP:C	2.33	0.64
1:E:27:HIS:CE1	1:E:36:ILE:HG21	2.32	0.64
1:E:256:ALA:HA	1:E:257:SER:C	2.19	0.63
1:F:68:THR:HB	1:F:91:MET:HE3	1.80	0.63
1:E:64:HIS:O	1:E:68:THR:HG22	1.99	0.63
1:B:43:PHE:HB3	1:B:56:THR:CG2	2.29	0.63
1:C:170:PHE:N	1:C:170:PHE:CD1	2.65	0.63
1:H:64:HIS:O	1:H:68:THR:HG22	1.98	0.63
1:E:143:ASN:O	1:E:145:VAL:N	2.30	0.63
1:G:68:THR:HG21	1:G:94:GLU:HB3	1.81	0.63
1:A:68:THR:HG21	1:A:94:GLU:HB3	1.81	0.62
1:E:34:ASP:OD2	1:E:35:LEU:N	2.33	0.62
1:H:256:ALA:HA	1:H:257:SER:C	2.18	0.62
1:E:36:ILE:HD11	1:E:38:PHE:HD1	1.64	0.62
1:G:10:THR:HG22	1:G:10:THR:O	1.99	0.62
1:A:165:PRO:HD2	1:A:167:GLU:OE2	2.00	0.61
1:E:35:LEU:C	1:E:36:ILE:HG22	2.20	0.61
1:C:34:ASP:OD2	1:C:35:LEU:N	2.33	0.61
1:E:35:LEU:C	1:E:36:ILE:CG2	2.69	0.61
1:H:68:THR:HG21	1:H:94:GLU:HB3	1.83	0.61
1:G:259:LEU:CD1	1:G:259:LEU:N	2.61	0.61
1:D:10:THR:HG22	1:D:10:THR:O	2.01	0.61
1:E:30:THR:CG2	1:E:31:ASP:H	2.13	0.61
1:E:107:VAL:HG21	1:E:144:PHE:HD2	1.64	0.61
1:D:68:THR:HB	1:D:91:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:HG21	1:D:94:GLU:HB3	1.83	0.60
1:B:43:PHE:HB3	1:B:56:THR:HG21	1.83	0.60
1:C:26:TYR:CE2	1:C:28:GLU:HB2	2.36	0.60
1:C:76:GLY:CA	1:C:253:ARG:NH1	2.63	0.60
1:H:10:THR:O	1:H:10:THR:HG22	2.01	0.60
1:C:256:ALA:HA	1:C:258:GLY:N	2.17	0.60
1:H:68:THR:HB	1:H:91:MET:HE3	1.82	0.60
1:A:64:HIS:O	1:A:68:THR:HG22	2.02	0.60
1:F:145:VAL:HG23	1:F:177:GLY:HA2	1.84	0.60
1:A:164:GLY:C	1:A:167:GLU:HG2	2.22	0.60
1:F:43:PHE:HB3	1:F:56:THR:HG21	1.83	0.60
1:C:68:THR:HG21	1:C:94:GLU:HB3	1.85	0.59
1:A:196:PHE:HD2	1:A:197:LEU:HD22	1.66	0.59
1:H:43:PHE:HB3	1:H:56:THR:CG2	2.33	0.59
1:G:286:GLN:CB	1:G:287:PRO:HD2	2.32	0.59
1:E:30:THR:CG2	1:E:31:ASP:N	2.65	0.59
1:B:146:ASN:O	1:B:147:GLN:HB2	2.02	0.59
1:E:68:THR:HB	1:E:91:MET:HE3	1.85	0.59
1:E:68:THR:HG21	1:E:94:GLU:HB3	1.85	0.59
1:A:33:GLN:CG	1:A:49:LEU:HD11	2.33	0.58
2:C:291:SO4:O4	1:G:13:ASP:N	2.23	0.58
1:A:275:LEU:HD13	1:A:279:LEU:HD23	1.85	0.58
1:F:286:GLN:O	1:F:286:GLN:HG3	2.02	0.58
1:H:196:PHE:CD2	1:H:197:LEU:HD12	2.38	0.58
1:D:183:ASN:HB3	1:D:184:PRO:CD	2.33	0.58
1:D:275:LEU:HD13	1:D:279:LEU:HD23	1.85	0.58
1:E:35:LEU:HD23	1:E:36:ILE:N	2.18	0.58
1:C:26:TYR:CZ	1:C:28:GLU:HB2	2.38	0.58
1:C:68:THR:HB	1:C:91:MET:HE3	1.86	0.58
2:A:292:SO4:O2	1:E:168:SER:HB2	2.03	0.58
1:E:144:PHE:CD1	1:E:144:PHE:C	2.73	0.58
1:F:68:THR:HG21	1:F:94:GLU:CB	2.34	0.58
1:G:256:ALA:CA	1:G:257:SER:C	2.62	0.58
1:B:91:MET:CE	1:B:156:ILE:HG21	2.33	0.58
1:B:179:LYS:HZ1	1:B:238:ASP:CG	2.07	0.58
1:C:10:THR:O	1:C:10:THR:HG22	2.04	0.57
1:C:160:THR:CG2	1:C:161:ASP:N	2.64	0.57
1:E:143:ASN:C	1:E:145:VAL:H	2.06	0.57
1:E:275:LEU:HD13	1:E:279:LEU:HD23	1.87	0.57
1:E:10:THR:HG22	1:E:10:THR:O	2.04	0.57
1:F:64:HIS:O	1:F:68:THR:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:PHE:HB3	1:H:56:THR:HG21	1.85	0.57
1:D:43:PHE:HB3	1:D:56:THR:CG2	2.35	0.57
1:D:249:ILE:O	1:D:253:ARG:HG3	2.05	0.57
1:G:34:ASP:O	1:G:34:ASP:CG	2.42	0.57
1:G:114:VAL:HG13	1:G:129:TYR:OH	2.05	0.57
1:B:148:THR:O	1:B:149:SER:CB	2.53	0.56
1:E:43:PHE:HB3	1:E:56:THR:CG2	2.34	0.56
1:E:114:VAL:HG13	1:E:129:TYR:OH	2.04	0.56
1:E:152:PHE:N	1:E:152:PHE:CD2	2.71	0.56
1:G:72:LEU:HD12	1:G:154:VAL:HG21	1.87	0.56
1:F:15:PHE:HZ	1:F:197:LEU:HD11	1.69	0.56
1:F:64:HIS:NE2	1:F:90:ALA:HB3	2.20	0.56
1:C:171:THR:HB	2:C:291:SO4:O1	2.05	0.56
1:E:148:THR:O	1:E:149:SER:CB	2.53	0.56
1:G:36:ILE:O	1:G:37:ILE:HG12	2.05	0.56
1:C:179:LYS:HZ1	1:C:238:ASP:CG	2.09	0.56
1:B:10:THR:HG22	1:B:10:THR:O	2.06	0.56
1:C:160:THR:HG23	1:C:161:ASP:N	2.19	0.56
1:E:144:PHE:O	1:E:144:PHE:HD1	1.87	0.56
1:G:43:PHE:HB3	1:G:56:THR:CG2	2.36	0.55
1:E:144:PHE:C	1:E:144:PHE:HD1	2.09	0.55
1:D:64:HIS:O	1:D:68:THR:HG22	2.06	0.55
1:E:27:HIS:CE1	1:E:36:ILE:CG2	2.89	0.55
1:E:68:THR:HB	1:E:91:MET:HE2	1.89	0.55
1:B:197:LEU:HD22	1:B:197:LEU:H	1.73	0.55
1:H:43:PHE:O	1:H:56:THR:HG23	2.06	0.55
1:B:275:LEU:HD13	1:B:279:LEU:HD23	1.89	0.54
1:E:246:SER:O	1:E:249:ILE:HG22	2.07	0.54
1:G:68:THR:HG21	1:G:94:GLU:CB	2.36	0.54
1:A:163:ILE:HG23	1:A:163:ILE:O	2.07	0.54
1:E:15:PHE:CZ	1:E:197:LEU:HD11	2.41	0.54
1:F:15:PHE:CZ	1:F:197:LEU:HD11	2.42	0.54
1:G:246:SER:O	1:G:249:ILE:HG22	2.07	0.54
1:A:256:ALA:CA	1:A:257:SER:C	2.66	0.54
1:E:34:ASP:O	1:E:49:LEU:HD12	2.08	0.54
1:C:68:THR:HB	1:C:91:MET:HE2	1.87	0.54
1:E:145:VAL:O	1:E:147:GLN:NE2	2.41	0.54
1:E:36:ILE:HD11	1:E:38:PHE:CD1	2.43	0.54
1:G:225:THR:HG22	1:G:225:THR:O	2.06	0.54
1:A:68:THR:HG21	1:A:94:GLU:CB	2.38	0.54
1:A:72:LEU:HD12	1:A:154:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:HD23	1:E:259:LEU:H	1.67	0.53
1:A:10:THR:O	1:A:10:THR:HG22	2.07	0.53
1:B:159:CYS:C	1:B:191:GLN:NE2	2.62	0.53
1:E:179:LYS:HZ1	1:E:238:ASP:CG	2.11	0.53
1:C:147:GLN:HG2	1:C:181:CYS:HB3	1.91	0.53
1:G:275:LEU:HD13	1:G:279:LEU:CD2	2.38	0.53
1:B:249:ILE:O	1:B:253:ARG:HG3	2.09	0.53
1:B:42:ALA:HA	1:E:170:PHE:CZ	2.44	0.53
1:H:147:GLN:HG2	1:H:181:CYS:HB3	1.91	0.53
1:A:161:ASP:OD2	1:A:172:SER:HB2	2.09	0.53
1:B:92:LEU:HG	1:B:128:SER:OG	2.09	0.53
1:C:246:SER:O	1:C:249:ILE:HG22	2.09	0.52
1:D:34:ASP:OD2	1:D:35:LEU:N	2.42	0.52
1:B:67:MET:CG	1:B:91:MET:HE3	2.39	0.52
1:A:33:GLN:HG3	1:A:49:LEU:HD11	1.91	0.52
1:A:179:LYS:HZ1	1:A:238:ASP:CG	2.12	0.52
1:F:223:ILE:HD12	1:F:223:ILE:N	2.24	0.52
1:F:43:PHE:O	1:F:56:THR:HG23	2.09	0.52
1:F:275:LEU:HD13	1:F:279:LEU:HD23	1.91	0.52
1:D:43:PHE:HB3	1:D:56:THR:HG23	1.91	0.52
1:E:27:HIS:ND1	1:E:36:ILE:HG22	2.24	0.52
1:H:68:THR:HG21	1:H:94:GLU:CB	2.39	0.52
1:C:43:PHE:HB3	1:C:56:THR:CG2	2.39	0.52
1:E:43:PHE:HB3	1:E:56:THR:HG23	1.91	0.52
1:B:83:ILE:HD13	1:B:91:MET:HG3	1.91	0.52
1:B:91:MET:HE3	1:B:156:ILE:CG2	2.39	0.52
1:E:145:VAL:O	1:E:145:VAL:HG22	2.09	0.52
1:F:43:PHE:HB3	1:F:56:THR:HG23	1.91	0.52
1:F:253:ARG:O	1:F:256:ALA:O	2.28	0.52
1:B:146:ASN:O	1:B:147:GLN:CB	2.58	0.52
1:A:147:GLN:HG2	1:A:181:CYS:HB3	1.92	0.51
1:A:182:LEU:HD21	1:A:186:GLY:C	2.31	0.51
1:D:159:CYS:SG	1:D:169:LEU:HD12	2.50	0.51
1:E:27:HIS:ND1	1:E:36:ILE:CG2	2.73	0.51
1:E:147:GLN:C	1:E:149:SER:H	2.08	0.51
1:F:64:HIS:CE1	1:F:90:ALA:HB3	2.44	0.51
1:C:85:GLY:HA3	1:C:158:ASP:HB2	1.93	0.51
1:D:160:THR:H	1:D:191:GLN:NE2	2.09	0.51
1:A:68:THR:HB	1:A:91:MET:HE3	1.89	0.51
1:A:110:ASP:O	1:A:113:VAL:HG12	2.11	0.51
1:A:259:LEU:HD12	1:A:259:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:O	1:C:113:VAL:HG12	2.11	0.51
1:F:68:THR:HB	1:F:91:MET:HE2	1.90	0.51
1:G:43:PHE:HB3	1:G:56:THR:HG23	1.92	0.51
1:D:93:ARG:O	1:D:96:THR:HB	2.10	0.51
1:D:142:VAL:HG21	1:D:168:SER:OG	2.10	0.51
1:H:179:LYS:HZ1	1:H:238:ASP:CG	2.13	0.51
1:B:28:GLU:HA	1:D:27:HIS:O	2.11	0.50
1:B:83:ILE:HD13	1:B:91:MET:CG	2.41	0.50
1:C:283:LEU:O	1:C:284:ALA:C	2.49	0.50
1:F:92:LEU:HG	1:F:128:SER:OG	2.11	0.50
1:H:253:ARG:O	1:H:256:ALA:O	2.30	0.50
1:C:68:THR:HG23	1:C:69:HIS:N	2.25	0.50
1:G:53:VAL:HG11	1:G:225:THR:CG2	2.41	0.50
1:G:92:LEU:HG	1:G:128:SER:OG	2.12	0.50
1:B:43:PHE:O	1:B:56:THR:HG23	2.11	0.50
1:F:147:GLN:HG2	1:F:181:CYS:HB3	1.92	0.50
1:B:197:LEU:HD22	1:B:197:LEU:N	2.27	0.50
1:E:148:THR:O	1:E:149:SER:OG	2.30	0.50
1:F:93:ARG:O	1:F:96:THR:HB	2.12	0.50
1:H:64:HIS:NE2	1:H:90:ALA:HB3	2.27	0.50
1:C:92:LEU:HG	1:C:128:SER:OG	2.12	0.50
1:D:68:THR:HG21	1:D:94:GLU:CB	2.42	0.50
1:E:92:LEU:HG	1:E:128:SER:OG	2.12	0.50
1:F:179:LYS:HZ1	1:F:238:ASP:CG	2.15	0.50
1:H:145:VAL:HG23	1:H:177:GLY:HA2	1.94	0.50
1:A:143:ASN:C	1:A:145:VAL:H	2.15	0.49
1:H:93:ARG:O	1:H:96:THR:HB	2.11	0.49
1:F:110:ASP:O	1:F:113:VAL:HG12	2.11	0.49
1:D:225:THR:O	1:D:225:THR:HG22	2.11	0.49
1:E:147:GLN:CB	1:E:149:SER:H	2.22	0.49
1:C:35:LEU:HD21	1:C:116:PHE:CZ	2.48	0.49
1:C:62:ILE:HG12	1:C:263:TYR:CD1	2.47	0.49
1:D:68:THR:HB	1:D:91:MET:HE2	1.88	0.49
1:G:34:ASP:C	1:G:34:ASP:OD2	2.51	0.49
1:G:68:THR:HB	1:G:91:MET:HE3	1.93	0.49
1:C:41:ALA:HB3	1:D:14:GLN:HG3	1.94	0.49
1:E:62:ILE:HG12	1:E:263:TYR:CD1	2.48	0.49
1:A:218:PHE:CD1	1:A:232:THR:HG22	2.47	0.49
1:C:145:VAL:HG23	1:C:177:GLY:HA2	1.94	0.49
1:F:218:PHE:CD1	1:F:232:THR:HG22	2.47	0.49
1:G:34:ASP:O	1:G:34:ASP:OD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LEU:HD12	1:H:197:LEU:N	2.27	0.49
1:C:14:GLN:HG3	1:D:41:ALA:HB3	1.94	0.49
1:D:5:LYS:CG	1:D:6:GLN:N	2.76	0.49
1:G:275:LEU:HD13	1:G:279:LEU:HD21	1.93	0.49
1:B:64:HIS:CE1	1:B:90:ALA:HB3	2.48	0.49
1:C:283:LEU:O	1:C:285:SER:N	2.45	0.49
1:F:160:THR:O	1:F:160:THR:OG1	2.30	0.49
1:H:64:HIS:O	1:H:91:MET:HE1	2.13	0.49
1:A:192:ASN:HD21	1:A:202:ALA:HA	1.77	0.49
1:D:62:ILE:HG12	1:D:263:TYR:CD1	2.48	0.49
2:A:292:SO4:O1	1:E:168:SER:HB2	2.14	0.48
1:B:64:HIS:NE2	1:B:90:ALA:HB3	2.28	0.48
1:D:43:PHE:O	1:D:56:THR:HG23	2.13	0.48
1:G:151:THR:HA	1:G:181:CYS:O	2.13	0.48
1:A:161:ASP:OD2	1:A:172:SER:CB	2.61	0.48
1:A:163:ILE:HD12	1:A:204:ASP:HB2	1.95	0.48
1:H:218:PHE:CD1	1:H:232:THR:HG22	2.48	0.48
1:E:29:LYS:O	1:E:29:LYS:HG2	2.13	0.48
1:E:223:ILE:N	1:E:223:ILE:HD12	2.27	0.48
1:A:14:GLN:HG3	1:B:41:ALA:HB3	1.94	0.48
1:E:147:GLN:HB3	1:E:149:SER:N	2.25	0.48
1:D:110:ASP:O	1:D:113:VAL:HG12	2.13	0.48
1:E:110:ASP:O	1:E:113:VAL:HG12	2.14	0.48
1:E:184:PRO:O	2:E:292:SO4:O1	2.32	0.48
1:F:64:HIS:CD2	1:F:90:ALA:HB3	2.49	0.48
1:C:76:GLY:HA2	1:C:253:ARG:HH11	1.75	0.48
1:A:92:LEU:HG	1:A:128:SER:OG	2.14	0.48
1:A:246:SER:O	1:A:249:ILE:HG22	2.14	0.48
1:B:62:ILE:HG12	1:B:263:TYR:CD1	2.49	0.48
1:B:67:MET:HG2	1:B:91:MET:HE3	1.96	0.48
1:B:107:VAL:HG21	1:B:144:PHE:CD2	2.49	0.48
1:C:114:VAL:HG13	1:C:129:TYR:OH	2.13	0.48
1:F:145:VAL:HG23	1:F:177:GLY:CA	2.43	0.48
1:B:53:VAL:HG11	1:B:225:THR:CG2	2.43	0.48
1:C:68:THR:HG21	1:C:94:GLU:CB	2.43	0.48
1:H:36:ILE:CG2	1:H:48:ALA:HB3	2.43	0.47
1:A:168:SER:HB3	2:E:290:SO4:O2	2.14	0.47
1:E:287:PRO:O	1:E:287:PRO:HG2	2.14	0.47
1:G:35:LEU:C	1:G:36:ILE:HG23	2.33	0.47
1:B:172:SER:HB2	1:B:208:LYS:HZ1	1.79	0.47
1:C:34:ASP:O	1:C:49:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PHE:CD1	1:B:232:THR:HG22	2.49	0.47
1:C:171:THR:CB	2:C:291:SO4:O1	2.63	0.47
1:E:31:ASP:OD1	1:E:31:ASP:O	2.32	0.47
1:E:107:VAL:HG21	1:E:144:PHE:CE2	2.49	0.47
1:D:218:PHE:CD1	1:D:232:THR:HG22	2.50	0.47
1:E:31:ASP:OD1	1:E:31:ASP:C	2.53	0.47
1:E:143:ASN:C	1:E:145:VAL:N	2.67	0.47
1:H:64:HIS:CE1	1:H:90:ALA:HB3	2.49	0.47
1:H:206:HIS:CG	1:H:283:LEU:HD21	2.50	0.47
1:A:43:PHE:HB3	1:A:56:THR:CG2	2.44	0.47
1:C:43:PHE:HB3	1:C:56:THR:HG23	1.97	0.46
1:D:114:VAL:HG13	1:D:129:TYR:OH	2.15	0.46
1:E:192:ASN:HD21	1:E:202:ALA:HA	1.79	0.46
1:A:62:ILE:HG12	1:A:263:TYR:CD1	2.50	0.46
1:B:225:THR:HG22	1:B:225:THR:O	2.15	0.46
1:C:15:PHE:CZ	1:C:197:LEU:HD11	2.50	0.46
1:D:92:LEU:HG	1:D:128:SER:OG	2.16	0.46
1:D:182:LEU:C	1:D:183:ASN:O	2.46	0.46
1:E:36:ILE:HG13	1:E:37:ILE:N	2.22	0.46
1:E:206:HIS:ND1	1:E:286:GLN:HG2	2.30	0.46
1:F:225:THR:HG22	1:F:225:THR:O	2.15	0.46
1:E:68:THR:HG21	1:E:94:GLU:CB	2.43	0.46
1:B:84:ILE:HD13	1:B:174:PHE:CZ	2.49	0.46
1:E:161:ASP:C	1:E:161:ASP:OD2	2.53	0.46
1:H:53:VAL:HG11	1:H:225:THR:CG2	2.46	0.46
1:D:183:ASN:HB3	1:D:184:PRO:HD2	1.96	0.46
1:F:256:ALA:HA	1:F:257:SER:C	2.35	0.46
1:G:58:ARG:O	1:G:58:ARG:HG3	2.15	0.46
1:G:110:ASP:O	1:G:113:VAL:HG12	2.16	0.46
1:A:174:PHE:CE1	1:A:178:CYS:SG	3.09	0.46
1:B:246:SER:O	1:B:249:ILE:HG22	2.15	0.46
1:E:107:VAL:CG2	1:E:144:PHE:CD2	2.96	0.46
1:B:256:ALA:HA	1:B:258:GLY:N	2.30	0.46
1:F:62:ILE:HG12	1:F:263:TYR:CD1	2.51	0.46
1:G:163:ILE:HD12	1:G:204:ASP:HB2	1.98	0.46
1:B:159:CYS:C	1:B:191:GLN:HE21	2.20	0.46
1:E:195:CYS:SG	1:E:232:THR:OG1	2.59	0.45
1:G:218:PHE:CD1	1:G:232:THR:HG22	2.51	0.45
1:H:62:ILE:HG12	1:H:263:TYR:CD1	2.51	0.45
1:B:93:ARG:O	1:B:96:THR:HB	2.15	0.45
1:D:68:THR:HG23	1:D:69:HIS:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:VAL:HG23	1:G:177:GLY:CA	2.46	0.45
1:B:43:PHE:HB3	1:B:56:THR:HG23	1.97	0.45
1:B:114:VAL:HG13	1:B:129:TYR:OH	2.17	0.45
1:G:28:GLU:O	1:G:34:ASP:OD2	2.34	0.45
1:A:142:VAL:O	1:A:145:VAL:HB	2.17	0.45
1:G:225:THR:O	1:G:225:THR:CG2	2.64	0.45
1:B:142:VAL:O	1:B:145:VAL:HG23	2.17	0.45
1:A:163:ILE:O	1:A:163:ILE:CG2	2.65	0.45
1:B:33:GLN:HA	1:B:50:ASP:OD1	2.17	0.45
1:C:218:PHE:CD1	1:C:232:THR:HG22	2.52	0.45
1:G:196:PHE:CD2	1:G:197:LEU:HD13	2.52	0.45
1:H:114:VAL:HG13	1:H:129:TYR:OH	2.17	0.45
1:A:68:THR:HB	1:A:91:MET:HE2	1.98	0.45
1:E:68:THR:HG23	1:E:69:HIS:N	2.31	0.45
1:F:26:TYR:CE2	1:F:35:LEU:HD23	2.51	0.45
1:H:92:LEU:HG	1:H:128:SER:OG	2.17	0.45
1:D:174:PHE:CZ	1:D:178:CYS:SG	3.10	0.45
1:A:43:PHE:O	1:A:56:THR:HG23	2.16	0.44
1:D:256:ALA:HA	1:D:257:SER:C	2.38	0.44
1:A:197:LEU:HB3	1:E:169:LEU:HD13	1.99	0.44
1:E:43:PHE:HB3	1:E:56:THR:HG21	1.99	0.44
1:H:246:SER:O	1:H:249:ILE:HG22	2.16	0.44
1:A:93:ARG:O	1:A:96:THR:HB	2.16	0.44
1:B:223:ILE:N	1:B:223:ILE:HD12	2.33	0.44
1:D:246:SER:O	1:D:249:ILE:HG22	2.17	0.44
1:C:211:HIS:NE2	1:H:41:ALA:HB2	2.33	0.44
1:E:218:PHE:CD1	1:E:232:THR:HG22	2.52	0.44
1:E:15:PHE:CZ	1:E:197:LEU:CD1	3.01	0.44
1:A:53:VAL:HG11	1:A:225:THR:CG2	2.48	0.44
1:A:225:THR:HG22	1:A:225:THR:O	2.17	0.44
1:C:53:VAL:HG11	1:C:225:THR:CG2	2.48	0.44
1:F:64:HIS:CE1	1:F:90:ALA:CB	3.01	0.44
1:G:35:LEU:HD23	1:G:36:ILE:N	2.31	0.44
1:A:68:THR:HG23	1:A:69:HIS:N	2.33	0.44
1:C:142:VAL:O	1:C:145:VAL:HG12	2.18	0.44
1:G:68:THR:HB	1:G:91:MET:HE2	1.98	0.44
1:H:110:ASP:O	1:H:113:VAL:HG12	2.17	0.44
1:H:223:ILE:N	1:H:223:ILE:HD12	2.33	0.44
1:B:256:ALA:CA	1:B:257:SER:C	2.85	0.44
1:C:64:HIS:O	1:C:91:MET:HE1	2.18	0.44
1:D:56:THR:HB	1:D:59:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:HIS:NE2	1:E:90:ALA:HB3	2.32	0.44
1:B:26:TYR:CE2	1:B:35:LEU:HD23	2.53	0.43
1:B:145:VAL:O	1:B:147:GLN:HG3	2.18	0.43
1:E:12:HIS:HB3	2:E:290:SO4:O1	2.17	0.43
1:G:37:ILE:HG22	1:G:38:PHE:N	2.33	0.43
1:G:110:ASP:HA	1:G:138:ILE:HG23	2.00	0.43
1:A:43:PHE:HB3	1:A:56:THR:HG23	2.00	0.43
1:B:67:MET:HG3	1:B:91:MET:HE3	2.00	0.43
1:D:160:THR:H	1:D:191:GLN:HE21	1.64	0.43
1:C:169:LEU:HB2	1:C:170:PHE:CE1	2.53	0.43
1:D:30:THR:O	1:D:31:ASP:C	2.55	0.43
1:D:64:HIS:NE2	1:D:90:ALA:HB3	2.34	0.43
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.78	0.43
1:F:35:LEU:HD21	1:F:116:PHE:CZ	2.53	0.43
1:H:279:LEU:O	1:H:282:ALA:CB	2.53	0.43
1:E:53:VAL:HG11	1:E:225:THR:CG2	2.48	0.43
1:F:15:PHE:HZ	1:F:197:LEU:CD1	2.31	0.43
1:G:62:ILE:HG12	1:G:263:TYR:CD1	2.54	0.43
1:B:110:ASP:O	1:B:113:VAL:HG12	2.18	0.43
1:D:15:PHE:HZ	1:D:197:LEU:HD11	1.83	0.43
1:G:258:GLY:C	1:G:259:LEU:HD13	2.35	0.43
1:C:36:ILE:CG2	1:C:48:ALA:HB3	2.48	0.43
1:G:56:THR:HB	1:G:59:ASP:OD2	2.19	0.43
1:B:260:LYS:HD2	1:B:260:LYS:HA	1.73	0.43
1:E:29:LYS:O	1:E:29:LYS:CG	2.66	0.43
1:D:64:HIS:CE1	1:D:90:ALA:HB3	2.54	0.43
1:C:72:LEU:HD12	1:C:154:VAL:HG21	2.01	0.42
1:G:68:THR:HG23	1:G:69:HIS:N	2.34	0.42
1:E:93:ARG:O	1:E:96:THR:HB	2.19	0.42
1:F:72:LEU:HD12	1:F:154:VAL:HG21	2.01	0.42
1:G:195:CYS:SG	1:G:232:THR:OG1	2.63	0.42
1:H:275:LEU:HB3	1:H:279:LEU:HD23	2.01	0.42
1:A:110:ASP:HA	1:A:138:ILE:HG23	2.01	0.42
1:C:26:TYR:OH	1:C:28:GLU:HB2	2.20	0.42
1:D:5:LYS:HG3	1:D:6:GLN:H	1.84	0.42
1:G:223:ILE:N	1:G:223:ILE:HD12	2.34	0.42
1:H:256:ALA:HA	1:H:258:GLY:N	2.34	0.42
1:H:256:ALA:CA	1:H:257:SER:C	2.86	0.42
1:A:12:HIS:HB3	2:A:292:SO4:O3	2.20	0.42
1:A:64:HIS:CE1	1:A:90:ALA:HB3	2.54	0.42
1:B:35:LEU:HD21	1:B:116:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:GLY:HA3	1:E:167:GLU:HG3	2.01	0.42
1:E:286:GLN:O	1:E:287:PRO:C	2.58	0.42
1:A:168:SER:CB	2:E:290:SO4:O4	2.68	0.42
1:C:43:PHE:O	1:C:56:THR:HG23	2.20	0.42
1:D:43:PHE:HB3	1:D:56:THR:HG21	2.00	0.42
1:E:15:PHE:HZ	1:E:197:LEU:CD1	2.32	0.42
1:G:64:HIS:NE2	1:G:90:ALA:HB3	2.35	0.42
1:H:225:THR:HG22	1:H:225:THR:O	2.20	0.42
1:A:239:ASN:ND2	1:A:242:LEU:HG	2.34	0.42
1:G:43:PHE:HB3	1:G:56:THR:HG21	2.01	0.42
1:G:93:ARG:HG2	1:G:97:ARG:HH21	1.76	0.42
1:A:13:ASP:HB2	2:A:292:SO4:O1	2.20	0.41
1:D:223:ILE:HD12	1:D:223:ILE:N	2.35	0.41
1:H:85:GLY:HA3	1:H:158:ASP:O	2.20	0.41
1:B:66:MET:HE2	1:B:66:MET:HB3	1.82	0.41
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.63	0.41
1:G:251:GLN:OE1	1:G:266:PRO:HG2	2.20	0.41
1:B:110:ASP:HA	1:B:138:ILE:HG23	2.02	0.41
1:B:172:SER:HB2	1:B:208:LYS:HZ2	1.84	0.41
1:B:225:THR:CG2	1:B:225:THR:O	2.68	0.41
1:C:64:HIS:CE1	1:C:90:ALA:HB3	2.55	0.41
1:E:110:ASP:HA	1:E:138:ILE:HG23	2.02	0.41
1:H:196:PHE:HD2	1:H:197:LEU:CD1	2.30	0.41
1:C:223:ILE:N	1:C:223:ILE:HD12	2.35	0.41
1:D:42:ALA:HA	1:G:170:PHE:CZ	2.55	0.41
1:G:93:ARG:O	1:G:96:THR:HB	2.20	0.41
1:E:35:LEU:O	1:E:36:ILE:CG2	2.63	0.41
1:E:144:PHE:O	1:E:144:PHE:CG	2.70	0.41
1:B:61:PHE:O	1:B:65:GLU:HB2	2.21	0.41
1:C:26:TYR:CE2	1:C:35:LEU:HD23	2.56	0.41
1:C:26:TYR:CE2	1:C:28:GLU:CB	3.03	0.41
1:C:110:ASP:HA	1:C:138:ILE:HG23	2.03	0.41
1:D:225:THR:O	1:D:225:THR:CG2	2.68	0.41
1:A:164:GLY:CA	1:A:167:GLU:CG	2.91	0.41
1:D:36:ILE:CG2	1:D:48:ALA:HB3	2.51	0.41
1:G:93:ARG:CD	1:G:97:ARG:HH22	2.31	0.41
1:H:110:ASP:HA	1:H:138:ILE:HG23	2.03	0.41
1:C:64:HIS:NE2	1:C:90:ALA:HB3	2.36	0.40
1:H:94:GLU:HA	1:H:97:ARG:HD3	2.03	0.40
1:A:276:PRO:HB3	1:B:263:TYR:CE1	2.56	0.40
1:B:146:ASN:C	1:B:147:GLN:HG3	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:HA	1:D:138:ILE:HG23	2.03	0.40
1:E:43:PHE:O	1:E:56:THR:HG23	2.22	0.40
1:B:83:ILE:CD1	1:B:91:MET:HG3	2.51	0.40
1:C:93:ARG:O	1:C:96:THR:HB	2.21	0.40
1:E:160:THR:O	1:E:161:ASP:C	2.56	0.40
1:D:125:ASN:O	1:D:128:SER:CB	2.70	0.40
1:A:196:PHE:CD2	1:A:197:LEU:HD22	2.50	0.40
1:A:218:PHE:HD1	1:A:232:THR:HG22	1.85	0.40
1:B:144:PHE:C	1:B:146:ASN:N	2.73	0.40
1:E:146:ASN:C	1:E:147:GLN:O	2.58	0.40
1:E:271:ALA:HB1	1:F:271:ALA:CB	2.34	0.40
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.88	0.40
1:H:64:HIS:CD2	1:H:90:ALA:HB3	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	278/294 (95%)	269 (97%)	9 (3%)	0	100	100
1	B	266/294 (90%)	255 (96%)	11 (4%)	0	100	100
1	C	282/294 (96%)	272 (96%)	10 (4%)	0	100	100
1	D	272/294 (92%)	263 (97%)	9 (3%)	0	100	100
1	E	281/294 (96%)	272 (97%)	8 (3%)	1 (0%)	34	66
1	F	263/294 (90%)	254 (97%)	9 (3%)	0	100	100
1	G	275/294 (94%)	264 (96%)	11 (4%)	0	100	100
1	H	258/294 (88%)	248 (96%)	10 (4%)	0	100	100
All	All	2175/2352 (92%)	2097 (96%)	77 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	149	SER

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	230/247 (93%)	224 (97%)	6 (3%)	46	77
1	B	222/247 (90%)	215 (97%)	7 (3%)	39	73
1	C	232/247 (94%)	221 (95%)	11 (5%)	26	59
1	D	226/247 (92%)	215 (95%)	11 (5%)	25	57
1	E	229/247 (93%)	215 (94%)	14 (6%)	18	48
1	F	219/247 (89%)	212 (97%)	7 (3%)	39	73
1	G	228/247 (92%)	217 (95%)	11 (5%)	25	58
1	H	217/247 (88%)	212 (98%)	5 (2%)	50	80
All	All	1803/1976 (91%)	1731 (96%)	72 (4%)	31	65

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	125	ASN
1	A	144	PHE
1	A	163	ILE
1	A	191	GLN
1	A	194	VAL
1	B	13	ASP
1	B	125	ASN
1	B	144	PHE
1	B	146	ASN
1	B	191	GLN
1	B	194	VAL
1	B	260	LYS

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Mol	Chain	Res	Type
1	C	13	ASP
1	C	58	ARG
1	C	125	ASN
1	C	144	PHE
1	C	158	ASP
1	C	160	THR
1	C	170	PHE
1	C	191	GLN
1	C	194	VAL
1	C	195	CYS
1	C	279	LEU
1	D	13	ASP
1	D	32	HIS
1	D	33	GLN
1	D	125	ASN
1	D	144	PHE
1	D	159	CYS
1	D	161	ASP
1	D	179	LYS
1	D	184	PRO
1	D	191	GLN
1	D	194	VAL
1	E	13	ASP
1	E	27	HIS
1	E	34	ASP
1	E	36	ILE
1	E	125	ASN
1	E	144	PHE
1	E	148	THR
1	E	152	PHE
1	E	158	ASP
1	E	159	CYS
1	E	191	GLN
1	E	194	VAL
1	E	259	LEU
1	E	260	LYS
1	F	125	ASN
1	F	144	PHE
1	F	160	THR
1	F	191	GLN
1	F	194	VAL
1	F	195	CYS

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Mol	Chain	Res	Type
1	F	260	LYS
1	G	13	ASP
1	G	116	PHE
1	G	125	ASN
1	G	144	PHE
1	G	179	LYS
1	G	181	CYS
1	G	182	LEU
1	G	191	GLN
1	G	194	VAL
1	G	260	LYS
1	G	286	GLN
1	H	13	ASP
1	H	125	ASN
1	H	144	PHE
1	H	191	GLN
1	H	194	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	191	GLN
1	E	147	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	A	289	-	4,4,4	0.58	0	6,6,6	0.30	0
2	SO4	D	291	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	A	292	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	E	292	-	4,4,4	0.28	0	6,6,6	0.35	0
2	SO4	G	290	-	4,4,4	0.41	0	6,6,6	0.33	0
2	SO4	E	291	-	4,4,4	0.42	0	6,6,6	0.28	0
2	SO4	D	289	-	4,4,4	0.48	0	6,6,6	0.13	0
2	SO4	F	290	-	4,4,4	0.43	0	6,6,6	0.20	0
2	SO4	E	290	-	4,4,4	0.98	0	6,6,6	0.77	0
2	SO4	A	291	-	4,4,4	0.36	0	6,6,6	0.55	0
2	SO4	D	290	-	4,4,4	0.71	0	6,6,6	0.55	0
2	SO4	C	290	-	4,4,4	0.40	0	6,6,6	0.39	0
2	SO4	A	290	-	4,4,4	0.42	0	6,6,6	0.23	0
2	SO4	B	289	-	4,4,4	0.60	0	6,6,6	0.31	0
2	SO4	G	292	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	F	291	-	4,4,4	0.32	0	6,6,6	0.20	0
2	SO4	C	292	-	4,4,4	0.28	0	6,6,6	0.33	0
2	SO4	C	289	-	4,4,4	0.59	0	6,6,6	0.29	0
2	SO4	C	291	-	4,4,4	0.30	0	6,6,6	0.75	0
2	SO4	C	294	-	4,4,4	0.14	0	6,6,6	0.66	0
2	SO4	H	290	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	G	289	-	4,4,4	0.61	0	6,6,6	0.49	0
2	SO4	G	293	-	4,4,4	0.33	0	6,6,6	0.16	0
2	SO4	D	292	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	B	290	-	4,4,4	0.49	0	6,6,6	0.26	0
2	SO4	H	289	-	4,4,4	0.51	0	6,6,6	0.28	0
2	SO4	F	292	-	4,4,4	0.33	0	6,6,6	0.65	0
2	SO4	F	289	-	4,4,4	0.44	0	6,6,6	0.26	0
2	SO4	E	289	-	4,4,4	0.57	0	6,6,6	0.27	0
2	SO4	G	291	-	4,4,4	0.39	0	6,6,6	0.26	0
2	SO4	C	293	-	4,4,4	0.32	0	6,6,6	0.39	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.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	292	SO4	5	0
2	E	292	SO4	1	0
2	E	290	SO4	3	0
2	C	291	SO4	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	282/294 (95%)	0.63	19 (6%)	17	13	42, 108, 189, 247	0
1	B	270/294 (91%)	0.28	6 (2%)	62	59	34, 85, 146, 177	0
1	C	284/294 (96%)	0.64	26 (9%)	9	6	36, 104, 186, 242	0
1	D	276/294 (93%)	0.28	3 (1%)	80	80	36, 85, 145, 197	0
1	E	283/294 (96%)	0.87	50 (17%)	1	1	44, 128, 218, 271	0
1	F	269/294 (91%)	0.67	22 (8%)	11	9	35, 107, 186, 241	0
1	G	279/294 (94%)	0.84	45 (16%)	1	1	42, 107, 200, 319	0
1	H	264/294 (89%)	0.81	29 (10%)	5	4	39, 121, 231, 276	0
All	All	2207/2352 (93%)	0.63	200 (9%)	9	6	34, 103, 198, 319	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	111	ALA	13.9
1	A	111	ALA	8.0
1	F	141	GLY	7.9
1	F	285	SER	6.4
1	E	92	LEU	5.8
1	F	142	VAL	5.2
1	E	19	PHE	4.8
1	H	218	PHE	4.7
1	G	115	SER	4.5
1	C	134	PHE	4.2
1	E	137	VAL	4.1
1	H	188	PHE	4.0
1	E	43	PHE	3.9
1	E	148	THR	3.9
1	G	110	ASP	3.8
1	C	25	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	25	LEU	3.7
1	F	146	ASN	3.6
1	H	7	TRP	3.6
1	F	114	VAL	3.5
1	G	114	VAL	3.5
1	E	8	HIS	3.5
1	G	118	ARG	3.4
1	E	37	ILE	3.4
1	G	103	SER	3.4
1	E	29	LYS	3.4
1	E	55	THR	3.4
1	A	134	PHE	3.4
1	C	43	PHE	3.3
1	C	35	LEU	3.3
1	E	83	ILE	3.3
1	E	135	LYS	3.3
1	H	209	LEU	3.3
1	C	116	PHE	3.3
1	A	35	LEU	3.3
1	E	35	LEU	3.2
1	E	32	HIS	3.2
1	C	33	GLN	3.2
1	C	37	ILE	3.2
1	G	37	ILE	3.2
1	E	52	VAL	3.2
1	C	38	PHE	3.2
1	H	232	THR	3.1
1	H	203	ILE	3.1
1	F	149	SER	3.1
1	E	25	LEU	3.1
1	C	114	VAL	3.1
1	H	152	PHE	3.0
1	H	10	THR	3.0
1	F	197	LEU	3.0
1	A	119	GLN	3.0
1	F	150	GLN	3.0
1	A	128	SER	3.0
1	A	139	ASP	3.0
1	C	95	VAL	3.0
1	H	128	SER	3.0
1	E	81	VAL	3.0
1	G	149	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	3.0
1	H	136	LEU	3.0
1	G	120	TYR	2.9
1	G	35	LEU	2.9
1	E	107	VAL	2.9
1	E	45	ARG	2.9
1	G	46	VAL	2.9
1	F	113	VAL	2.8
1	A	20	ALA	2.8
1	G	129	TYR	2.8
1	A	110	ASP	2.8
1	H	19	PHE	2.8
1	B	113	VAL	2.8
1	C	111	ALA	2.8
1	C	138	ILE	2.8
1	D	182	LEU	2.7
1	G	96	THR	2.7
1	C	113	VAL	2.7
1	G	19	PHE	2.7
1	G	27	HIS	2.7
1	E	105	THR	2.7
1	E	95	VAL	2.7
1	G	24	VAL	2.7
1	A	136	LEU	2.7
1	H	101	VAL	2.7
1	F	19	PHE	2.7
1	H	11	LEU	2.7
1	E	84	ILE	2.7
1	E	86	GLY	2.7
1	A	81	VAL	2.6
1	E	27	HIS	2.6
1	G	128	SER	2.6
1	F	286	GLN	2.6
1	F	124	HIS	2.6
1	A	25	LEU	2.6
1	H	148	THR	2.6
1	A	41	ALA	2.6
1	F	279	LEU	2.6
1	G	137	VAL	2.6
1	E	154	VAL	2.5
1	G	81	VAL	2.5
1	G	106	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	120	TYR	2.5
1	C	129	TYR	2.5
1	E	232	THR	2.5
1	E	96	THR	2.5
1	E	155	ILE	2.5
1	C	121	LEU	2.5
1	E	116	PHE	2.5
1	B	135	LYS	2.5
1	H	211	HIS	2.5
1	E	134	PHE	2.5
1	E	90	ALA	2.4
1	E	26	TYR	2.4
1	E	82	LEU	2.4
1	F	134	PHE	2.4
1	G	15	PHE	2.4
1	H	36	ILE	2.4
1	F	145	VAL	2.4
1	G	152	PHE	2.4
1	H	146	ASN	2.4
1	D	86	GLY	2.4
1	A	181	CYS	2.4
1	A	129	TYR	2.4
1	E	21	VAL	2.4
1	G	26	TYR	2.4
1	E	106	MET	2.4
1	G	138	ILE	2.4
1	G	112	GLY	2.3
1	E	47	MET	2.3
1	F	128	SER	2.3
1	A	144	PHE	2.3
1	H	127	GLY	2.3
1	A	37	ILE	2.3
1	A	182	LEU	2.3
1	C	84	ILE	2.3
1	E	149	SER	2.3
1	G	43	PHE	2.3
1	E	129	TYR	2.3
1	C	287	PRO	2.3
1	H	178	CYS	2.3
1	B	197	LEU	2.3
1	E	40	ASN	2.3
1	G	225	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	159	CYS	2.3
1	B	15	PHE	2.3
1	G	95	VAL	2.2
1	G	45	ARG	2.2
1	F	22	ASP	2.2
1	H	197	LEU	2.2
1	F	152	PHE	2.2
1	E	163	ILE	2.2
1	E	103	SER	2.2
1	C	32	HIS	2.2
1	H	38	PHE	2.2
1	B	204	ASP	2.2
1	E	51	GLY	2.2
1	F	192	ASN	2.2
1	H	182	LEU	2.2
1	C	136	LEU	2.2
1	E	48	ALA	2.2
1	G	116	PHE	2.2
1	G	187	ILE	2.2
1	H	107	VAL	2.2
1	E	128	SER	2.2
1	H	113	VAL	2.2
1	C	45	ARG	2.2
1	C	51	GLY	2.1
1	F	38	PHE	2.1
1	G	92	LEU	2.1
1	G	48	ALA	2.1
1	G	104	ILE	2.1
1	E	46	VAL	2.1
1	G	136	LEU	2.1
1	H	134	PHE	2.1
1	C	39	GLU	2.1
1	B	114	VAL	2.1
1	G	148	THR	2.1
1	G	38	PHE	2.1
1	H	242	LEU	2.1
1	C	83	ILE	2.1
1	G	83	ILE	2.1
1	G	47	MET	2.1
1	C	135	LYS	2.1
1	F	28	GLU	2.1
1	A	148	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	155	ILE	2.1
1	H	192	ASN	2.1
1	E	114	VAL	2.1
1	G	36	ILE	2.1
1	C	98	HIS	2.0
1	E	136	LEU	2.0
1	G	182	LEU	2.0
1	E	138	ILE	2.0
1	E	72	LEU	2.0
1	C	107	VAL	2.0
1	H	114	VAL	2.0
1	E	24	VAL	2.0
1	F	232	THR	2.0
1	G	49	LEU	2.0
1	G	147	GLN	2.0
1	E	23	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	292	5/5	0.68	0.33	122,147,162,174	0
2	SO4	F	292	5/5	0.72	0.28	96,117,146,154	0
2	SO4	C	293	5/5	0.73	0.37	99,119,140,150	0
2	SO4	C	292	5/5	0.74	0.18	122,128,153,158	0
2	SO4	A	291	5/5	0.75	0.31	84,119,163,185	0
2	SO4	D	291	5/5	0.77	0.43	115,117,151,165	0
2	SO4	H	290	5/5	0.77	0.20	101,113,139,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	291	5/5	0.88	0.19	59,60,82,87	0
2	SO4	C	290	5/5	0.88	0.18	90,90,125,125	0
2	SO4	D	292	5/5	0.88	0.25	99,129,147,159	0
2	SO4	G	291	5/5	0.90	0.23	99,108,132,153	0
2	SO4	G	293	5/5	0.90	0.16	122,127,140,171	0
2	SO4	H	289	5/5	0.90	0.15	76,96,100,113	0
2	SO4	A	290	5/5	0.90	0.22	107,109,125,146	0
2	SO4	C	289	5/5	0.92	0.11	79,87,92,98	0
2	SO4	G	289	5/5	0.92	0.11	70,77,93,105	0
2	SO4	F	289	5/5	0.93	0.14	76,108,119,121	0
2	SO4	G	292	5/5	0.93	0.50	128,131,159,164	0
2	SO4	F	290	5/5	0.93	0.13	87,92,101,111	0
2	SO4	E	289	5/5	0.93	0.09	74,79,94,102	0
2	SO4	A	289	5/5	0.93	0.09	79,87,101,108	0
2	SO4	B	290	5/5	0.94	0.11	85,86,110,114	0
2	SO4	A	292	5/5	0.95	0.13	47,64,68,70	0
2	SO4	D	289	5/5	0.95	0.10	88,108,116,119	0
2	SO4	G	290	5/5	0.95	0.12	96,108,126,139	0
2	SO4	D	290	5/5	0.95	0.12	58,91,94,98	0
2	SO4	E	291	5/5	0.96	0.08	92,107,125,142	0
2	SO4	F	291	5/5	0.96	0.09	109,109,138,141	0
2	SO4	B	289	5/5	0.98	0.08	78,93,103,115	0
2	SO4	E	290	5/5	0.98	0.10	63,65,74,79	0
2	SO4	C	294	5/5	0.98	0.12	56,66,73,74	0

6.5 Other polymers (i)

There are no such residues in this entry.