



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:39 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

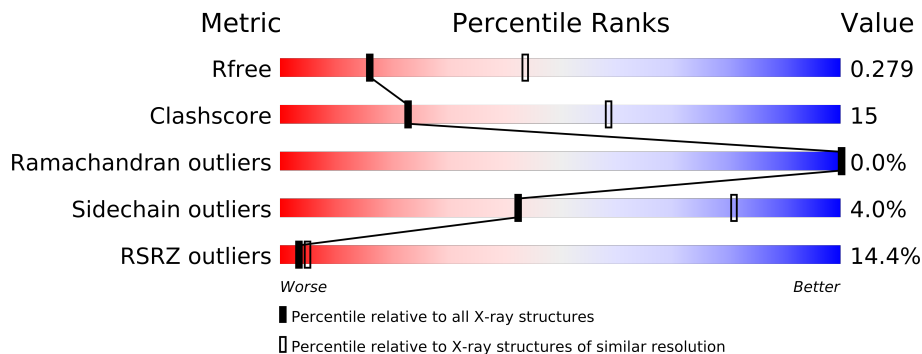
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	294	
1	B	294	
1	C	294	
1	D	294	
1	E	294	
1	F	294	
1	G	294	
1	H	294	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	291	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	D	291	-	X
2	SO4	E	292	-	X
2	SO4	G	292	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17519 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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: O₄S).



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

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

- Molecule 3 is water.

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

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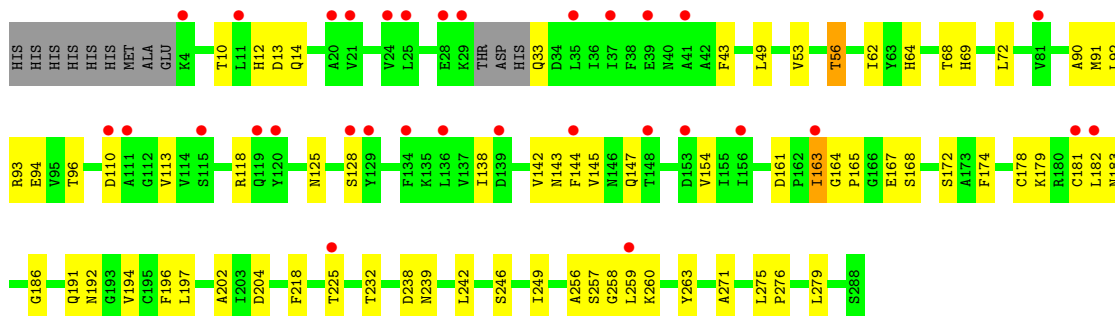
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 3	O 3	0	0
3	D	1	Total 1	O 1	0	0
3	E	3	Total 3	O 3	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

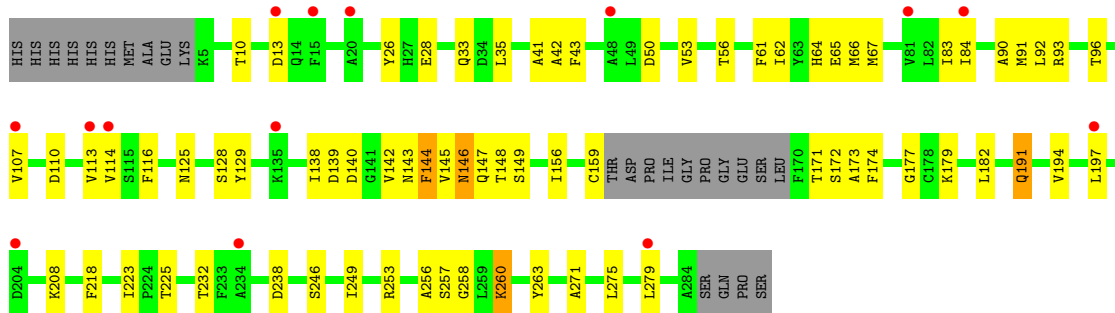
• Molecule 1: Spermidine synthase

Chain A: 



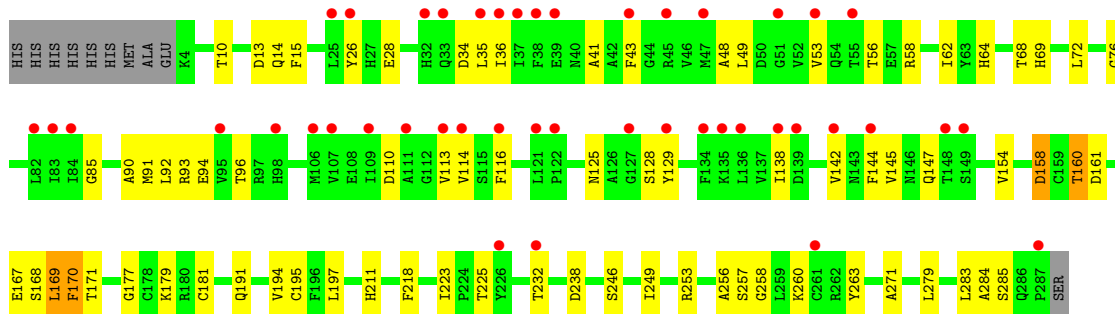
• Molecule 1: Spermidine synthase

Chain B: 



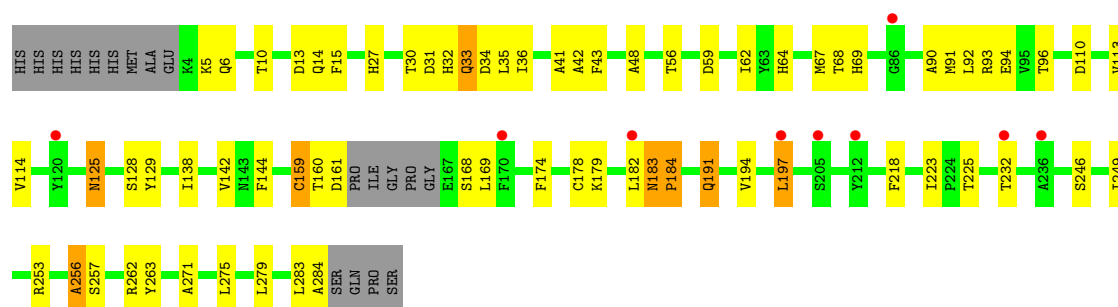
• Molecule 1: Spermidine synthase

Chain C: 



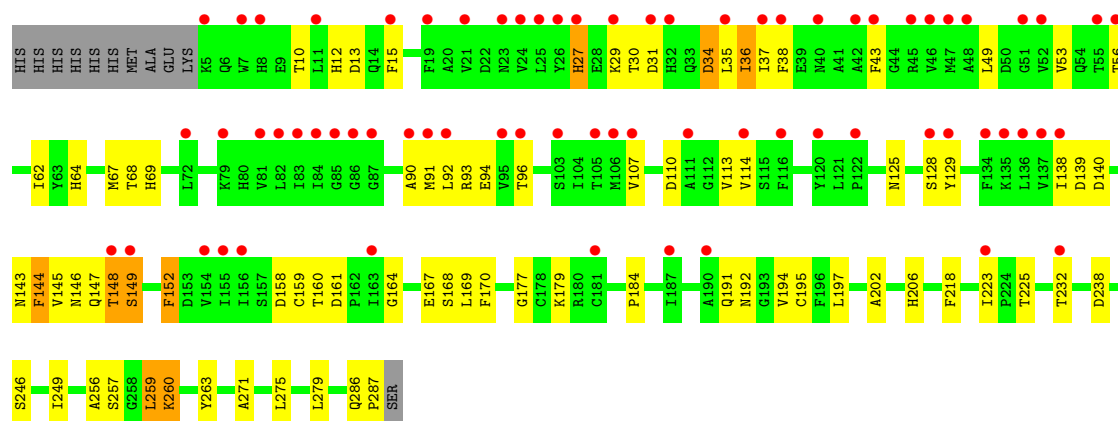
- Molecule 1: Spermidine synthase

Chain D:



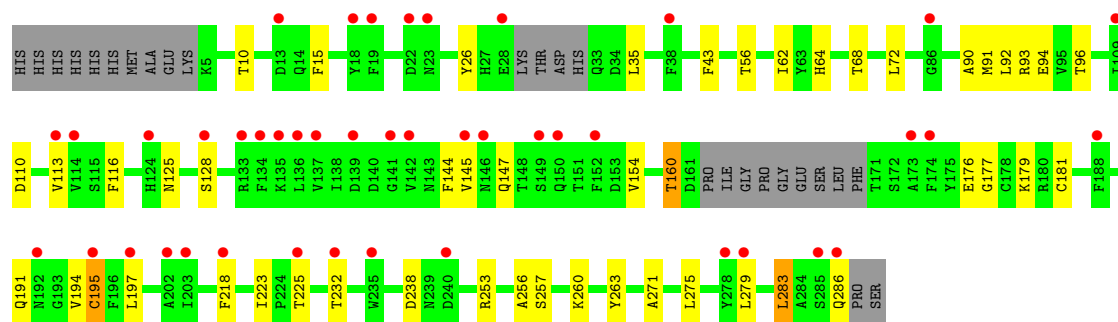
- Molecule 1: Spermidine synthase

Chain E:



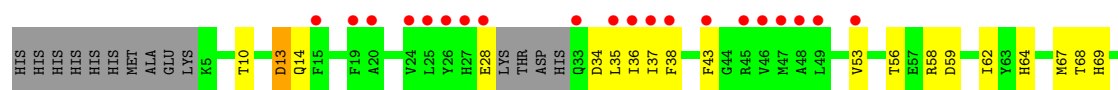
- Molecule 1: Spermidine synthase

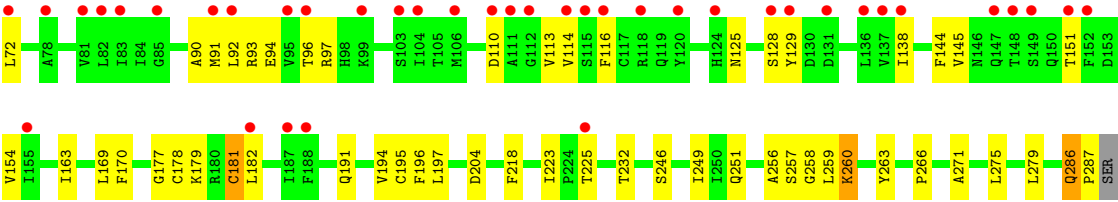
Chain F:



- Molecule 1: Spermidine synthase

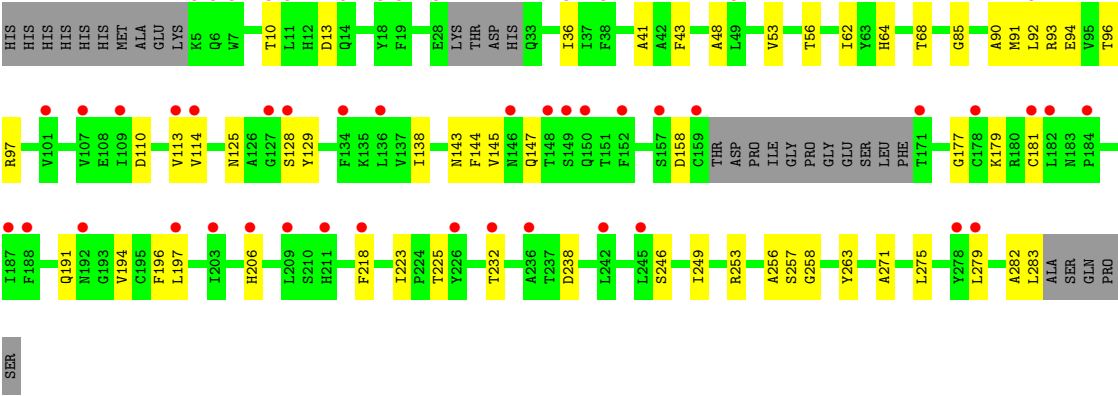
Chain G:





• Molecule 1: Spermidine synthase

Chain H:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.208 , 0.241 0.265 , 0.279	Depositor DCC
R_{free} test set	3484 reflections (5.03%)	DCC
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 , 95.5	EDS
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 69297 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.79	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(°)	Ideal(°)
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(°)	Ideal(°)
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 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (496) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:E:145:VAL:HG23	1:E:177:GLY:HA3	1.53	0.88
1:B:145:VAL:HG22	1:B:177:GLY:HA3	1.56	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:E:145:VAL:CG2	1:E:177:GLY:CA	2.52	0.87
1:B:148:THR:O	1:B:148:THR:HG22	1.75	0.87
1:C:271:ALA:HB1	1:D:271:ALA:HB1	1.57	0.87
1:G:286:GLN:HG3	1:G:287:PRO:HD2	1.58	0.85
1:E:144:PHE:CD1	1:E:144:PHE:O	2.30	0.85
1:D:68:THR:HB	1:D:91:MET:CE	2.07	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	Distance(Å)	Clash(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:H:275:LEU:HD13	1:H:279:LEU:HD23	1.65	0.77
1:C:168:SER:HB3	2:C:291:SO4:O1	1.85	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:O	1:E:148:THR:HG22	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:C	1:E:34:ASP:OD2	2.29	0.69
1:A:182:LEU:CD2	1:A:186:GLY:HA3	2.22	0.69
1:D:34:ASP:C	1:D:34:ASP:OD2	2.30	0.69
1:G:68:THR:HB	1:G:91:MET:CE	2.24	0.69
1:F:10:THR:O	1:F:10:THR:HG22	1.93	0.69
1:G:258:GLY:O	1:G:259:LEU:CD1	2.30	0.68
1:G:64:HIS:O	1:G:68:THR:HG22	1.93	0.68
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: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:HG22	1:D:160:THR:O	1.94	0.67
1:B:91:MET:HE3	1:B:156:ILE:HG21	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:139:ASP:OD1	1:E:140:ASP:N	2.29	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: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:C:170:PHE:N	1:C:170:PHE:CD1	2.65	0.63
1:B:43:PHE:HB3	1:B:56:THR:CG2	2.29	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:O	1:G:10:THR:HG22	1.99	0.62
1:E:35:LEU:C	1:E:36:ILE:HG22	2.20	0.61
1:A:165:PRO:HD2	1:A:167:GLU:OE2	2.00	0.61
1:C:34:ASP:OD2	1:C:35:LEU:N	2.33	0.61
1:H:68:THR:HG21	1:H:94:GLU:HB3	1.83	0.61
1:E:35:LEU:C	1:E:36:ILE:CG2	2.69	0.61
1:G:259:LEU:N	1:G:259:LEU:CD1	2.61	0.61
1:E:107:VAL:HG21	1:E:144:PHE:HD2	1.64	0.61
1:E:30:THR:CG2	1:E:31:ASP:H	2.13	0.61
1:D:10:THR:O	1:D:10:THR:HG22	2.01	0.61
1:D:68:THR:HB	1:D:91:MET:HE3	1.82	0.61
1:D:68:THR:HG21	1:D:94:GLU:HB3	1.83	0.60
1:C:76:GLY:CA	1:C:253:ARG:NH1	2.63	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:TYR:CE2	1:C:28:GLU:HB2	2.36	0.60
1:B:43:PHE:HB3	1:B:56:THR:HG21	1.83	0.60
1:H:10:THR:O	1:H:10:THR:HG22	2.01	0.60
1:H:68:THR:HB	1:H:91:MET:HE3	1.82	0.60
1:C:256:ALA:HA	1:C:258:GLY:N	2.17	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
2:C:291:SO4:O4	1:G:13:ASP:N	2.23	0.58
1:A:33:GLN:CG	1:A:49:LEU:HD11	2.33	0.58
1:H:196:PHE:CD2	1:H:197:LEU:HD12	2.38	0.58
1:A:275:LEU:HD13	1:A:279:LEU:HD23	1.85	0.58
1:F:286:GLN:HG3	1:F:286:GLN:O	2.02	0.58
1:D:183:ASN:HB3	1:D:184:PRO:CD	2.33	0.58
1:E:35:LEU:HD23	1:E:36:ILE:N	2.18	0.58
1:D:275:LEU:HD13	1:D:279:LEU:HD23	1.85	0.58
1:C:68:THR:HB	1:C:91:MET:HE3	1.86	0.58
1:C:26:TYR:CZ	1:C:28:GLU:HB2	2.38	0.58
1:G:256:ALA:CA	1:G:257:SER:C	2.62	0.58
1:E:144:PHE:C	1:E:144:PHE:CD1	2.73	0.58
1:F:68:THR:HG21	1:F:94:GLU:CB	2.34	0.58
2:A:292:SO4:O2	1:E:168:SER:HB2	2.03	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:160:THR:CG2	1:C:161:ASP:N	2.64	0.57
1:C:10:THR:HG22	1:C:10:THR:O	2.04	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:F:64:HIS:O	1:F:68:THR:HG22	2.03	0.57
1:E:10:THR:O	1:E:10:THR:HG22	2.04	0.57
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:G:34:ASP:O	1:G:34:ASP:CG	2.42	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:249:ILE:O	1:D:253:ARG:HG3	2.05	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:C:160:THR:HG23	1:C:161:ASP:N	2.19	0.56
1:B:10:THR:HG22	1:B:10:THR:O	2.06	0.56
1:E:144:PHE:HD1	1:E:144:PHE:O	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:68:THR:HB	1:E:91:MET:HE2	1.89	0.55
1:E:27:HIS:CE1	1:E:36:ILE:CG2	2.89	0.55
1:H:43:PHE:O	1:H:56:THR:HG23	2.06	0.55
1:B:197:LEU:H	1:B:197:LEU:HD22	1.73	0.55
1:G:68:THR:HG21	1:G:94:GLU:CB	2.36	0.54
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:A:163:ILE:O	1:A:163:ILE:HG23	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:O	1:G:225:THR:HG22	2.06	0.54
1:A:68:THR:HG21	1:A:94:GLU:CB	2.38	0.54
1:E:259:LEU:HD23	1:E:259:LEU:H	1.67	0.53
1:A:72:LEU:HD12	1:A:154:VAL:HG21	1.91	0.53
1:B:159:CYS:C	1:B:191:GLN:NE2	2.62	0.53
1:A:10:THR:O	1:A:10:THR:HG22	2.07	0.53
1:E:179:LYS:HZ1	1:E:238:ASP:CG	2.11	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:275:LEU:HD13	1:G:279:LEU:CD2	2.38	0.53
1:C:147:GLN:HG2	1:C:181:CYS:HB3	1.91	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:B:92:LEU:HG	1:B:128:SER:OG	2.09	0.53
1:A:161:ASP:OD2	1:A:172:SER:HB2	2.09	0.53
1:D:34:ASP:OD2	1:D:35:LEU:N	2.42	0.52
1:C:246:SER:O	1:C:249:ILE:HG22	2.09	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:N	1:F:223:ILE:HD12	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:H:68:THR:HG21	1:H:94:GLU:CB	2.39	0.52
1:E:27:HIS:ND1	1:E:36:ILE:HG22	2.24	0.52
1:D:43:PHE:HB3	1:D:56:THR:HG23	1.91	0.52
1:E:43:PHE:HB3	1:E:56:THR:HG23	1.91	0.52
1:C:43:PHE:HB3	1:C:56:THR:CG2	2.39	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:HG22	1:E:145:VAL:O	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: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:A:182:LEU:HD21	1:A:186:GLY:C	2.31	0.51
1:E:27:HIS:ND1	1:E:36:ILE:CG2	2.73	0.51
1:D:159:CYS:SG	1:D:169:LEU:HD12	2.50	0.51
1:D:160:THR:H	1:D:191:GLN:NE2	2.09	0.51
1:C:85:GLY:HA3	1:C:158:ASP:HB2	1.93	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: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:A:259:LEU:HD12	1:A:259:LEU:H	1.75	0.51
1:C:110:ASP:O	1:C:113:VAL:HG12	2.11	0.51
1:D:93:ARG:O	1:D:96:THR:HB	2.10	0.51
1:H:179:LYS:HZ1	1:H:238:ASP:CG	2.13	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:142:VAL:HG21	1:D:168:SER:OG	2.10	0.51
1:B:83:ILE:HD13	1:B:91:MET:CG	2.41	0.50
1:B:28:GLU:HA	1:D:27:HIS:O	2.11	0.50
1:H:253:ARG:O	1:H:256:ALA:O	2.30	0.50
1:F:92:LEU:HG	1:F:128:SER:OG	2.11	0.50
1:C:283:LEU:O	1:C:284:ALA:C	2.49	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:E:148:THR:O	1:E:149:SER:OG	2.30	0.50
1:B:197:LEU:N	1:B:197:LEU:HD22	2.27	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:D:68:THR:HG21	1:D:94:GLU:CB	2.42	0.50
1:F:179:LYS:HZ1	1:F:238:ASP:CG	2.15	0.50
1:E:92:LEU:HG	1:E:128:SER:OG	2.12	0.50
1:H:145:VAL:HG23	1:H:177:GLY:HA2	1.94	0.50
1:C:92:LEU:HG	1:C:128:SER:OG	2.12	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:E:147:GLN:CB	1:E:149:SER:H	2.22	0.49
1:D:225:THR:O	1:D:225:THR:HG22	2.11	0.49
1:D:68:THR:HB	1:D:91:MET:HE2	1.88	0.49
1:C:35:LEU:HD21	1:C:116:PHE:CZ	2.48	0.49
1:G:34:ASP:C	1:G:34:ASP:OD2	2.51	0.49
1:C:62:ILE:HG12	1:C:263:TYR:CD1	2.47	0.49
1:G:68:THR:HB	1:G:91:MET:HE3	1.93	0.49
1:E:62:ILE:HG12	1:E:263:TYR:CD1	2.48	0.49
1:C:41:ALA:HB3	1:D:14:GLN:HG3	1.94	0.49
1:H:197:LEU:HD12	1:H:197:LEU:N	2.27	0.49
1:G:34:ASP:O	1:G:34:ASP:OD2	2.30	0.49
1:C:145:VAL:HG23	1:C:177:GLY:HA2	1.94	0.49
1:A:218:PHE:CD1	1:A:232:THR:HG22	2.47	0.49
1:F:218:PHE:CD1	1:F:232:THR:HG22	2.47	0.49
1:G:275:LEU:HD13	1:G:279:LEU:HD21	1.93	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:H:64:HIS:O	1:H:91:MET:HE1	2.13	0.49
1:C:283:LEU:O	1:C:285:SER:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:160:THR:O	1:F:160:THR:OG1	2.30	0.49
1:B:64:HIS:CE1	1:B:90:ALA:HB3	2.48	0.49
1:D:62:ILE:HG12	1:D:263:TYR:CD1	2.48	0.49
1:A:192:ASN:HD21	1:A:202:ALA:HA	1.77	0.49
2:A:292:SO4:O1	1:E:168:SER:HB2	2.14	0.48
1:D:43:PHE:O	1:D:56:THR:HG23	2.13	0.48
1:B:64:HIS:NE2	1:B:90:ALA:HB3	2.28	0.48
1:G:151:THR:HA	1:G:181:CYS:O	2.13	0.48
1:A:163:ILE:HD12	1:A:204:ASP:HB2	1.95	0.48
1:A:161:ASP:OD2	1:A:172:SER:CB	2.61	0.48
1:H:218:PHE:CD1	1:H:232:THR:HG22	2.48	0.48
1:E:29:LYS:HG2	1:E:29:LYS:O	2.13	0.48
1:E:223:ILE:N	1:E:223:ILE:HD12	2.27	0.48
1:E:147:GLN:HB3	1:E:149:SER:N	2.25	0.48
1:A:14:GLN:HG3	1:B:41:ALA:HB3	1.94	0.48
1:E:110:ASP:O	1:E:113:VAL:HG12	2.14	0.48
1:D:110:ASP:O	1:D:113:VAL:HG12	2.13	0.48
1:F:64:HIS:CD2	1:F:90:ALA:HB3	2.49	0.48
1:E:184:PRO:O	2:E:292:SO4:O1	2.32	0.48
1:C:76:GLY:HA2	1:C:253:ARG:HH11	1.75	0.48
1:B:107:VAL:HG21	1:B:144:PHE:CD2	2.49	0.48
1:B:67:MET:HG2	1:B:91:MET:HE3	1.96	0.48
1:F:145:VAL:HG23	1:F:177:GLY:CA	2.43	0.48
1:B:62:ILE:HG12	1:B:263:TYR:CD1	2.49	0.48
1:A:92:LEU:HG	1:A:128:SER:OG	2.14	0.48
1:C:114:VAL:HG13	1:C:129:TYR:OH	2.13	0.48
1:A:246:SER:O	1:A:249:ILE:HG22	2.14	0.48
1:C:68:THR:HG21	1:C:94:GLU:CB	2.43	0.48
1:B:53:VAL:HG11	1:B:225:THR:CG2	2.43	0.48
1:H:36:ILE:CG2	1:H:48:ALA:HB3	2.43	0.47
1:G:35:LEU:C	1:G:36:ILE:HG23	2.33	0.47
1:E:287:PRO:HG2	1:E:287:PRO:O	2.14	0.47
1:A:168:SER:HB3	2:E:290:SO4:O2	2.14	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
1:E:107:VAL:HG21	1:E:144:PHE:CE2	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:B:218:PHE:CD1	1:B:232:THR:HG22	2.49	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:E:31:ASP:C	1:E:31:ASP:OD1	2.53	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:218:PHE:CD1	1:D:232:THR:HG22	2.50	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:E:192:ASN:HD21	1:E:202:ALA:HA	1.79	0.46
1:D:114:VAL:HG13	1:D:129:TYR:OH	2.15	0.46
1:E:36:ILE:HG13	1:E:37:ILE:N	2.22	0.46
1:D:182:LEU:C	1:D:183:ASN:O	2.46	0.46
1:B:225:THR:HG22	1:B:225:THR:O	2.15	0.46
1:E:206:HIS:ND1	1:E:286:GLN:HG2	2.30	0.46
1:D:92:LEU:HG	1:D:128:SER:OG	2.16	0.46
1:A:62:ILE:HG12	1:A:263:TYR:CD1	2.50	0.46
1:F:225:THR:HG22	1:F:225:THR:O	2.15	0.46
1:C:15:PHE:CZ	1:C:197:LEU:HD11	2.50	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:110:ASP:O	1:G:113:VAL:HG12	2.16	0.46
1:G:58:ARG:O	1:G:58:ARG:HG3	2.15	0.46
1:E:107:VAL:CG2	1:E:144:PHE:CD2	2.96	0.46
1:B:246:SER:O	1:B:249:ILE:HG22	2.15	0.46
1:A:174:PHE:CE1	1:A:178:CYS:SG	3.09	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:H:62:ILE:HG12	1:H:263:TYR:CD1	2.51	0.45
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:D:68:THR:HG23	1:D:69:HIS:N	2.30	0.45
1:G:145:VAL:HG23	1:G:177:GLY:CA	2.46	0.45
1:B:93:ARG:O	1:B:96:THR:HB	2.15	0.45
1:B:43:PHE:HB3	1:B:56:THR:HG23	1.97	0.45
1:G:28:GLU:O	1:G:34:ASP:OD2	2.34	0.45
1:B:114:VAL:HG13	1:B:129:TYR:OH	2.17	0.45
1:A:142:VAL:O	1:A:145:VAL:HB	2.17	0.45
1:G:225:THR:CG2	1:G:225:THR:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:33:GLN:HA	1:B:50:ASP:OD1	2.17	0.45
1:H:114:VAL:HG13	1:H:129:TYR:OH	2.17	0.45
1:E:68:THR:HG23	1:E:69:HIS:N	2.31	0.45
1:A:68:THR:HB	1:A:91:MET:HE2	1.98	0.45
1:H:92:LEU:HG	1:H:128:SER:OG	2.17	0.45
1:F:26:TYR:CE2	1:F:35:LEU:HD23	2.51	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:B:223:ILE:N	1:B:223:ILE:HD12	2.33	0.44
1:A:93:ARG:O	1:A:96:THR:HB	2.16	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: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:225:THR:O	1:A:225:THR:HG22	2.17	0.44
1:A:53:VAL:HG11	1:A:225:THR:CG2	2.48	0.44
1:C:53:VAL:HG11	1:C:225:THR:CG2	2.48	0.44
1:A:68:THR:HG23	1:A:69:HIS:N	2.33	0.44
1:G:68:THR:HB	1:G:91:MET:HE2	1.98	0.44
1:C:142:VAL:O	1:C:145:VAL:HG12	2.18	0.44
1:H:223:ILE:HD12	1:H:223:ILE:N	2.33	0.44
1:H:110:ASP:O	1:H:113:VAL:HG12	2.17	0.44
1:C:64:HIS:O	1:C:91:MET:HE1	2.18	0.44
1:E:64:HIS:NE2	1:E:90:ALA:HB3	2.32	0.44
1:B:256:ALA:CA	1:B:257:SER:C	2.85	0.44
1:D:56:THR:HB	1:D:59:ASP:OD2	2.18	0.44
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:B:26:TYR:CE2	1:B:35:LEU:HD23	2.53	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:D:160:THR:H	1:D:191:GLN:HE21	1.64	0.43
1:B:67:MET:HG3	1:B:91:MET:HE3	2.00	0.43
1:A:43:PHE:HB3	1:A:56:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:64:HIS:NE2	1:D:90:ALA:HB3	2.34	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:H:279:LEU:O	1:H:282:ALA:CB	2.53	0.43
1:F:35:LEU:HD21	1:F:116:PHE:CZ	2.53	0.43
1:B:182:LEU:HA	1:B:182:LEU:HD23	1.78	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:E:53:VAL:HG11	1:E:225:THR:CG2	2.48	0.43
1:G:258:GLY:C	1:G:259:LEU:HD13	2.35	0.43
1:D:15:PHE:HZ	1:D:197:LEU:HD11	1.83	0.43
1:B:110:ASP:O	1:B:113:VAL:HG12	2.18	0.43
1:G:56:THR:HB	1:G:59:ASP:OD2	2.19	0.43
1:C:36:ILE:CG2	1:C:48:ALA:HB3	2.48	0.43
1:E:29:LYS:CG	1:E:29:LYS:O	2.66	0.43
1:B:260:LYS:HA	1:B:260:LYS:HD2	1.73	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:F:72:LEU:HD12	1:F:154:VAL:HG21	2.01	0.42
1:E:93:ARG:O	1:E:96:THR:HB	2.19	0.42
1:H:275:LEU:HB3	1:H:279:LEU:HD23	2.01	0.42
1:G:195:CYS:SG	1:G:232:THR:OG1	2.63	0.42
1:C:26:TYR:OH	1:C:28:GLU:HB2	2.20	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:110:ASP:HA	1:A:138:ILE:HG23	2.01	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:A:64:HIS:CE1	1:A:90:ALA:HB3	2.54	0.42
1:A:12:HIS:HB3	2:A:292:SO4:O3	2.20	0.42
1:E:286:GLN:O	1:E:287:PRO:C	2.58	0.42
1:B:35:LEU:HD21	1:B:116:PHE:CZ	2.54	0.42
1:E:164:GLY:HA3	1:E:167:GLU:HG3	2.01	0.42
1:A:168:SER:CB	2:E:290:SO4:O4	2.68	0.42
1:G:64:HIS:NE2	1:G:90:ALA:HB3	2.35	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:C:43:PHE:O	1:C:56:THR:HG23	2.20	0.42
1:H:225:THR:HG22	1:H:225:THR:O	2.20	0.42
1:G:93:ARG:HG2	1:G:97:ARG:HH21	1.76	0.42
1:G:43:PHE:HB3	1:G:56:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:ASN:ND2	1:A:242:LEU:HG	2.34	0.42
1:A:13:ASP:HB2	2:A:292:SO4:O1	2.20	0.41
1:D:223:ILE:N	1:D:223:ILE:HD12	2.35	0.41
1:H:85:GLY:HA3	1:H:158:ASP:O	2.20	0.41
1:B:66:MET:HB3	1:B:66:MET:HE2	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:172:SER:HB2	1:B:208:LYS:HZ2	1.84	0.41
1:B:110:ASP:HA	1:B:138:ILE:HG23	2.02	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:H:196:PHE:HD2	1:H:197:LEU:CD1	2.30	0.41
1:E:110:ASP:HA	1:E:138:ILE:HG23	2.02	0.41
1:G:93:ARG:O	1:G:96:THR:HB	2.20	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:E:144:PHE:CG	1:E:144:PHE:O	2.70	0.41
1:E:35:LEU:O	1:E:36:ILE:CG2	2.63	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:B:61:PHE:O	1:B:65:GLU:HB2	2.21	0.41
1:G:93:ARG:CD	1:G:97:ARG:HH22	2.31	0.41
1:A:164:GLY:CA	1:A:167:GLU:CG	2.91	0.41
1:H:110:ASP:HA	1:H:138:ILE:HG23	2.03	0.41
1:D:36:ILE:CG2	1:D:48:ALA:HB3	2.51	0.41
1:H:94:GLU:HA	1:H:97:ARG:HD3	2.03	0.40
1:C:64:HIS:NE2	1:C:90:ALA:HB3	2.36	0.40
1:B:146:ASN:C	1:B:147:GLN:HG3	2.41	0.40
1:E:43:PHE:O	1:E:56:THR:HG23	2.22	0.40
1:D:110:ASP:HA	1:D:138:ILE:HG23	2.03	0.40
1:A:276:PRO:HB3	1:B:263:TYR:CE1	2.56	0.40
1:B:83:ILE:CD1	1:B:91:MET:HG3	2.51	0.40
1:E:160:THR:O	1:E:161:ASP:C	2.56	0.40
1:C:93:ARG:O	1:C:96:THR:HB	2.21	0.40
1:D:125:ASN:O	1:D:128:SER:CB	2.70	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:B:144:PHE:C	1:B:146:ASN:N	2.73	0.40
1:H:64:HIS:CD2	1:H:90:ALA:HB3	2.56	0.40
1:A:196:PHE:CD2	1:A:197:LEU:HD22	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:PHE:HD1	1:A:232:THR:HG22	1.85	0.40
1:G:169:LEU:HA	1:G:169:LEU:HD23	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	43	82
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 ⓘ

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%)	59	90
1	B	222/247 (90%)	215 (97%)	7 (3%)	51	88
1	C	232/247 (94%)	221 (95%)	11 (5%)	36	75
1	D	226/247 (92%)	215 (95%)	11 (5%)	35	73
1	E	229/247 (93%)	215 (94%)	14 (6%)	26	62
1	F	219/247 (89%)	212 (97%)	7 (3%)	51	88
1	G	228/247 (92%)	217 (95%)	11 (5%)	35	74
1	H	217/247 (88%)	212 (98%)	5 (2%)	63	92
All	All	1803/1976 (91%)	1731 (96%)	72 (4%)	42	81

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	H	144	PHE
1	H	191	GLN
1	H	194	VAL

Some 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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.25	0	6,6,6	0.30	0
2	SO4	A	290	-	4,4,4	0.94	0	6,6,6	0.33	0
2	SO4	A	291	-	4,4,4	0.81	0	6,6,6	0.50	0
2	SO4	A	292	-	4,4,4	0.20	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	289	-	4,4,4	1.29	0	6,6,6	0.21	0
2	SO4	B	290	-	4,4,4	1.07	0	6,6,6	0.17	0
2	SO4	C	289	-	4,4,4	1.29	0	6,6,6	0.49	0
2	SO4	C	290	-	4,4,4	0.89	0	6,6,6	0.24	0
2	SO4	C	291	-	4,4,4	0.31	0	6,6,6	0.77	0
2	SO4	C	292	-	4,4,4	0.64	0	6,6,6	0.26	0
2	SO4	C	293	-	4,4,4	0.73	0	6,6,6	0.46	0
2	SO4	C	294	-	4,4,4	0.29	0	6,6,6	0.55	0
2	SO4	D	289	-	4,4,4	1.05	0	6,6,6	0.11	0
2	SO4	D	290	-	4,4,4	1.50	0	6,6,6	0.54	0
2	SO4	D	291	-	4,4,4	0.10	0	6,6,6	0.19	0
2	SO4	D	292	-	4,4,4	0.71	0	6,6,6	0.29	0
2	SO4	E	289	-	4,4,4	1.25	0	6,6,6	0.27	0
2	SO4	E	290	-	4,4,4	2.01	1 (25%)	6,6,6	0.82	0
2	SO4	E	291	-	4,4,4	0.93	0	6,6,6	0.19	0
2	SO4	E	292	-	4,4,4	0.64	0	6,6,6	0.26	0
2	SO4	F	289	-	4,4,4	0.97	0	6,6,6	0.18	0
2	SO4	F	290	-	4,4,4	0.96	0	6,6,6	0.18	0
2	SO4	F	291	-	4,4,4	0.73	0	6,6,6	0.18	0
2	SO4	F	292	-	4,4,4	0.76	0	6,6,6	0.54	0
2	SO4	G	289	-	4,4,4	1.31	0	6,6,6	0.46	0
2	SO4	G	290	-	4,4,4	0.93	0	6,6,6	0.26	0
2	SO4	G	291	-	4,4,4	0.87	0	6,6,6	0.26	0
2	SO4	G	292	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	G	293	-	4,4,4	0.74	0	6,6,6	0.13	0
2	SO4	H	289	-	4,4,4	1.11	0	6,6,6	0.28	0
2	SO4	H	290	-	4,4,4	0.50	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	289	-	-	0/0/0/0	0/0/0/0
2	SO4	A	290	-	-	0/0/0/0	0/0/0/0
2	SO4	A	291	-	-	0/0/0/0	0/0/0/0
2	SO4	A	292	-	-	0/0/0/0	0/0/0/0
2	SO4	B	289	-	-	0/0/0/0	0/0/0/0
2	SO4	B	290	-	-	0/0/0/0	0/0/0/0
2	SO4	C	289	-	-	0/0/0/0	0/0/0/0
2	SO4	C	290	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	291	-	-	0/0/0/0	0/0/0/0
2	SO4	C	292	-	-	0/0/0/0	0/0/0/0
2	SO4	C	293	-	-	0/0/0/0	0/0/0/0
2	SO4	C	294	-	-	0/0/0/0	0/0/0/0
2	SO4	D	289	-	-	0/0/0/0	0/0/0/0
2	SO4	D	290	-	-	0/0/0/0	0/0/0/0
2	SO4	D	291	-	-	0/0/0/0	0/0/0/0
2	SO4	D	292	-	-	0/0/0/0	0/0/0/0
2	SO4	E	289	-	-	0/0/0/0	0/0/0/0
2	SO4	E	290	-	-	0/0/0/0	0/0/0/0
2	SO4	E	291	-	-	0/0/0/0	0/0/0/0
2	SO4	E	292	-	-	0/0/0/0	0/0/0/0
2	SO4	F	289	-	-	0/0/0/0	0/0/0/0
2	SO4	F	290	-	-	0/0/0/0	0/0/0/0
2	SO4	F	291	-	-	0/0/0/0	0/0/0/0
2	SO4	F	292	-	-	0/0/0/0	0/0/0/0
2	SO4	G	289	-	-	0/0/0/0	0/0/0/0
2	SO4	G	290	-	-	0/0/0/0	0/0/0/0
2	SO4	G	291	-	-	0/0/0/0	0/0/0/0
2	SO4	G	292	-	-	0/0/0/0	0/0/0/0
2	SO4	G	293	-	-	0/0/0/0	0/0/0/0
2	SO4	H	289	-	-	0/0/0/0	0/0/0/0
2	SO4	H	290	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	290	SO4	O2-S	-2.26	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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	282/294 (95%)	0.91	32 (11%) 6 7	42, 108, 189, 247	0
1	B	270/294 (91%)	0.56	14 (5%) 26 32	35, 85, 146, 177	0
1	C	284/294 (96%)	0.96	44 (15%) 3 4	36, 104, 186, 242	0
1	D	276/294 (93%)	0.57	9 (3%) 44 53	36, 85, 145, 197	0
1	E	283/294 (96%)	1.18	70 (24%) 1 2	44, 128, 218, 271	0
1	F	269/294 (91%)	0.99	43 (15%) 3 3	35, 107, 186, 241	0
1	G	279/294 (94%)	1.15	59 (21%) 1 2	42, 107, 200, 319	0
1	H	264/294 (89%)	1.11	50 (18%) 2 2	39, 121, 231, 276	0
All	All	2207/2352 (93%)	0.93	321 (14%) 3 5	35, 103, 198, 319	0

All (321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	111	ALA	15.9
1	F	141	GLY	10.0
1	A	111	ALA	9.3
1	E	92	LEU	7.2
1	F	142	VAL	7.0
1	F	285	SER	6.9
1	E	19	PHE	5.6
1	H	218	PHE	5.4
1	G	115	SER	5.0
1	C	134	PHE	4.9
1	E	43	PHE	4.8
1	E	137	VAL	4.8
1	E	148	THR	4.8
1	H	188	PHE	4.4
1	C	114	VAL	4.4
1	G	25	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	146	ASN	4.4
1	C	43	PHE	4.3
1	G	118	ARG	4.3
1	H	232	THR	4.2
1	G	110	ASP	4.2
1	E	55	THR	4.1
1	H	7	TRP	4.1
1	F	114	VAL	4.1
1	C	116	PHE	4.1
1	G	46	VAL	4.0
1	C	25	LEU	4.0
1	C	33	GLN	4.0
1	F	113	VAL	3.9
1	C	35	LEU	3.9
1	C	38	PHE	3.9
1	E	83	ILE	3.9
1	A	134	PHE	3.9
1	E	37	ILE	3.8
1	G	103	SER	3.8
1	B	113	VAL	3.8
1	H	209	LEU	3.8
1	E	135	LYS	3.8
1	E	8	HIS	3.8
1	A	81	VAL	3.7
1	C	37	ILE	3.7
1	F	149	SER	3.7
1	F	150	GLN	3.6
1	H	152	PHE	3.6
1	G	96	THR	3.6
1	E	95	VAL	3.6
1	C	95	VAL	3.6
1	C	111	ALA	3.6
1	G	114	VAL	3.6
1	G	149	SER	3.5
1	A	35	LEU	3.5
1	A	110	ASP	3.5
1	A	119	GLN	3.5
1	H	10	THR	3.5
1	F	124	HIS	3.5
1	H	19	PHE	3.5
1	E	52	VAL	3.5
1	H	203	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	29	LYS	3.4
1	H	128	SER	3.4
1	E	35	LEU	3.4
1	E	107	VAL	3.4
1	C	113	VAL	3.4
1	A	128	SER	3.4
1	E	149	SER	3.3
1	E	25	LEU	3.3
1	G	37	ILE	3.3
1	E	86	GLY	3.3
1	F	197	LEU	3.3
1	A	139	ASP	3.3
1	G	120	TYR	3.3
1	E	81	VAL	3.3
1	C	138	ILE	3.3
1	H	136	LEU	3.2
1	G	129	TYR	3.2
1	E	84	ILE	3.2
1	A	41	ALA	3.2
1	D	86	GLY	3.2
1	E	45	ARG	3.2
1	E	116	PHE	3.2
1	F	286	GLN	3.2
1	C	287	PRO	3.2
1	A	181	CYS	3.1
1	D	182	LEU	3.1
1	G	106	MET	3.1
1	D	197	LEU	3.1
1	H	101	VAL	3.1
1	G	81	VAL	3.1
1	G	137	VAL	3.1
1	C	121	LEU	3.1
1	A	129	TYR	3.1
1	G	19	PHE	3.1
1	G	27	HIS	3.1
1	G	128	SER	3.1
1	A	136	LEU	3.1
1	G	24	VAL	3.1
1	F	134	PHE	3.1
1	E	32	HIS	3.1
1	G	35	LEU	3.1
1	E	154	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	105	THR	3.0
1	G	152	PHE	3.0
1	E	134	PHE	3.0
1	H	148	THR	3.0
1	G	112	GLY	3.0
1	E	40	ASN	3.0
1	F	19	PHE	3.0
1	E	155	ILE	2.9
1	F	145	VAL	2.9
1	B	135	LYS	2.9
1	E	47	MET	2.9
1	B	15	PHE	2.9
1	C	84	ILE	2.9
1	F	139	ASP	2.9
1	C	129	TYR	2.8
1	E	129	TYR	2.8
1	E	106	MET	2.8
1	E	27	HIS	2.8
1	H	11	LEU	2.8
1	A	20	ALA	2.8
1	E	48	ALA	2.8
1	E	90	ALA	2.8
1	F	279	LEU	2.8
1	G	26	TYR	2.8
1	C	98	HIS	2.8
1	H	127	GLY	2.8
1	E	232	THR	2.8
1	E	82	LEU	2.8
1	C	45	ARG	2.8
1	F	128	SER	2.8
1	H	159	CYS	2.8
1	E	26	TYR	2.8
1	G	15	PHE	2.7
1	A	25	LEU	2.7
1	A	37	ILE	2.7
1	A	144	PHE	2.7
1	B	197	LEU	2.7
1	G	43	PHE	2.7
1	G	45	ARG	2.7
1	A	182	LEU	2.7
1	C	136	LEU	2.7
1	E	190	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	2.7
1	G	187	ILE	2.7
1	G	225	THR	2.7
1	H	242	LEU	2.7
1	G	48	ALA	2.7
1	H	192	ASN	2.7
1	G	155	ILE	2.7
1	E	38	PHE	2.7
1	C	226	TYR	2.7
1	C	32	HIS	2.7
1	G	83	ILE	2.6
1	F	152	PHE	2.6
1	C	51	GLY	2.6
1	D	212	TYR	2.6
1	H	211	HIS	2.6
1	E	21	VAL	2.6
1	E	85	GLY	2.6
1	G	136	LEU	2.6
1	C	83	ILE	2.6
1	F	192	ASN	2.6
1	H	107	VAL	2.6
1	F	23	ASN	2.6
1	F	137	VAL	2.6
1	H	38	PHE	2.6
1	H	134	PHE	2.6
1	A	120	TYR	2.6
1	F	109	ILE	2.5
1	G	78	ALA	2.5
1	F	28	GLU	2.5
1	H	146	ASN	2.5
1	G	95	VAL	2.5
1	E	51	GLY	2.5
1	H	182	LEU	2.5
1	F	218	PHE	2.5
1	E	138	ILE	2.5
1	B	114	VAL	2.5
1	E	46	VAL	2.5
1	E	42	ALA	2.5
1	G	47	MET	2.5
1	G	148	THR	2.5
1	B	81	VAL	2.5
1	E	120	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	56	THR	2.5
1	C	39	GLU	2.5
1	E	103	SER	2.5
1	H	36	ILE	2.5
1	C	47	MET	2.5
1	E	91	MET	2.5
1	G	38	PHE	2.5
1	H	197	LEU	2.5
1	G	138	ILE	2.4
1	F	22	ASP	2.4
1	C	107	VAL	2.4
1	E	7	TRP	2.4
1	H	178	CYS	2.4
1	F	38	PHE	2.4
1	E	163	ILE	2.4
1	G	104	ILE	2.4
1	A	24	VAL	2.4
1	G	53	VAL	2.4
1	F	232	THR	2.4
1	F	203	ILE	2.4
1	C	53	VAL	2.4
1	E	114	VAL	2.4
1	H	5	LYS	2.4
1	H	245	LEU	2.4
1	H	28	GLU	2.4
1	A	148	THR	2.4
1	H	149	SER	2.4
1	H	184	PRO	2.4
1	E	111	ALA	2.4
1	B	107	VAL	2.4
1	G	182	LEU	2.4
1	C	122	PRO	2.4
1	F	278	TYR	2.4
1	G	85	GLY	2.4
1	D	236	ALA	2.4
1	E	136	LEU	2.3
1	E	24	VAL	2.3
1	E	96	THR	2.3
1	H	206	HIS	2.3
1	G	36	ILE	2.3
1	B	234	ALA	2.3
1	H	114	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	49	LEU	2.3
1	C	142	VAL	2.3
1	G	33	GLN	2.3
1	D	170	PHE	2.3
1	A	153	ASP	2.3
1	A	163	ILE	2.3
1	A	11	LEU	2.3
1	A	29	LYS	2.3
1	G	91	MET	2.3
1	F	18	TYR	2.3
1	G	151	THR	2.3
1	C	109	ILE	2.3
1	E	72	LEU	2.3
1	B	20	ALA	2.3
1	G	20	ALA	2.3
1	H	236	ALA	2.3
1	G	116	PHE	2.3
1	G	72	LEU	2.2
1	H	171	THR	2.2
1	B	13	ASP	2.2
1	H	109	ILE	2.2
1	A	115	SER	2.2
1	G	188	PHE	2.2
1	A	259	LEU	2.2
1	C	261	CYS	2.2
1	E	156	ILE	2.2
1	G	99	LYS	2.2
1	E	87	GLY	2.2
1	F	86	GLY	2.2
1	E	23	ASN	2.2
1	H	6	GLN	2.2
1	A	4	LYS	2.2
1	F	173	ALA	2.2
1	G	147	GLN	2.2
1	F	136	LEU	2.2
1	C	232	THR	2.2
1	A	28	GLU	2.2
1	C	82	LEU	2.2
1	H	157	SER	2.2
1	E	122	PRO	2.2
1	C	26	TYR	2.2
1	H	49	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	131	ASP	2.2
1	A	225	THR	2.2
1	F	225	THR	2.2
1	C	106	MET	2.2
1	G	28	GLU	2.2
1	C	135	LYS	2.2
1	E	181	CYS	2.2
1	B	279	LEU	2.1
1	F	202	ALA	2.1
1	C	127	GLY	2.1
1	D	120	TYR	2.1
1	H	187	ILE	2.1
1	F	133	ARG	2.1
1	G	124	HIS	2.1
1	C	139	ASP	2.1
1	H	18	TYR	2.1
1	D	205	SER	2.1
1	F	13	ASP	2.1
1	F	240	ASP	2.1
1	E	187	ILE	2.1
1	H	278	TYR	2.1
1	C	36	ILE	2.1
1	E	223	ILE	2.1
1	G	82	LEU	2.1
1	H	113	VAL	2.1
1	H	150	GLN	2.1
1	E	11	LEU	2.1
1	C	148	THR	2.1
1	D	232	THR	2.1
1	E	128	SER	2.1
1	A	21	VAL	2.1
1	A	156	ILE	2.1
1	C	144	PHE	2.1
1	E	5	LYS	2.1
1	F	135	LYS	2.1
1	F	174	PHE	2.1
1	F	188	PHE	2.0
1	A	39	GLU	2.0
1	H	92	LEU	2.0
1	C	149	SER	2.0
1	E	31	ASP	2.0
1	C	55	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.0
1	F	195	CYS	2.0
1	H	181	CYS	2.0
1	H	226	TYR	2.0
1	H	279	LEU	2.0
1	E	15	PHE	2.0
1	F	235	TRP	2.0
1	G	92	LEU	2.0
1	E	79	LYS	2.0
1	H	14	GLN	2.0
1	B	84	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q < 0.9
2	SO4	G	292	5/5	0.54	11.21	128,131,159,164	0
2	SO4	E	292	5/5	0.36	4.05	122,147,162,174	0
2	SO4	A	291	5/5	0.28	2.76	84,119,163,185	0
2	SO4	D	291	5/5	0.40	2.71	115,117,151,165	0
2	SO4	C	293	5/5	0.41	1.57	99,119,140,150	0
2	SO4	F	292	5/5	0.30	1.32	96,117,146,154	0
2	SO4	C	290	5/5	0.23	0.58	90,90,125,125	0
2	SO4	G	291	5/5	0.26	0.05	99,108,132,153	0
2	SO4	C	292	5/5	0.21	-0.63	122,128,153,158	0
2	SO4	H	290	5/5	0.23	-0.82	101,113,139,153	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	H	289	5/5	0.18	-0.95	76,96,100,113	0
2	SO4	G	290	5/5	0.14	-1.20	96,108,126,139	0
2	SO4	C	291	5/5	0.21	-1.28	59,60,82,87	0
2	SO4	A	292	5/5	0.14	-1.72	47,64,68,70	0
2	SO4	A	290	5/5	0.23	-1.78	107,109,125,146	0
2	SO4	D	290	5/5	0.15	-2.09	58,91,94,98	0
2	SO4	G	293	5/5	0.16	-2.25	122,127,140,171	0
2	SO4	D	289	5/5	0.10	-2.36	88,108,116,119	0
2	SO4	E	290	5/5	0.11	-2.56	63,65,74,79	0
2	SO4	B	290	5/5	0.11	-2.62	85,86,110,114	0
2	SO4	E	289	5/5	0.09	-2.87	74,79,94,102	0
2	SO4	C	294	5/5	0.14	-3.39	56,66,73,74	0
2	SO4	F	289	5/5	0.16	-3.81	76,108,119,121	0
2	SO4	F	291	5/5	0.10	-4.02	109,109,138,141	0
2	SO4	B	289	5/5	0.09	-4.41	78,93,103,115	0
2	SO4	C	289	5/5	0.13	-4.71	79,87,92,98	0
2	SO4	F	290	5/5	0.14	-5.43	87,92,101,111	0
2	SO4	G	289	5/5	0.13	-18.43	70,77,93,105	0
2	SO4	E	291	5/5	0.07	-19.22	92,107,125,142	0
2	SO4	A	289	5/5	0.10	-29.22	79,87,101,108	0
2	SO4	D	292	5/5	0.24	-	99,129,147,159	0

6.5 Other polymers ⓘ

There are no such residues in this entry.