



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:14 PM GMT

PDB ID : 3IEK
Title : Crystal Structure of native TTHA0252 from *Thermus thermophilus* HB8
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.
Deposited on : 2009-07-22
Resolution : 2.05 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>

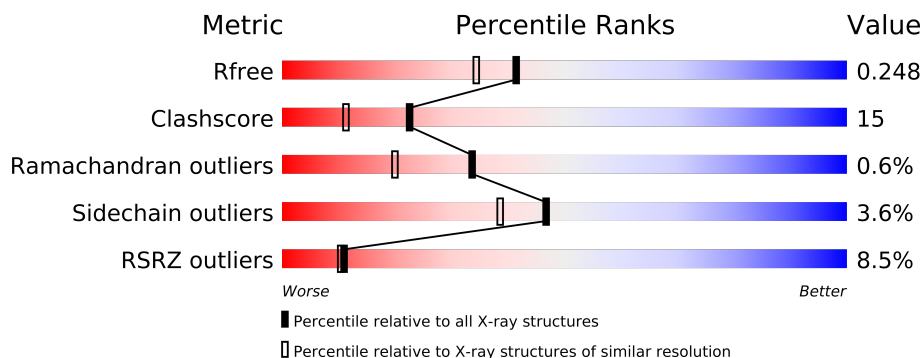
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.05 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	431	
1	B	431	
1	C	431	
1	D	431	

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	432	-	X
2	SO4	A	433	-	X
2	SO4	A	435	-	X
2	SO4	A	439	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	444	-	X
2	SO4	A	445	-	X
2	SO4	A	446	-	X
2	SO4	A	447	-	X
2	SO4	A	450	-	X
2	SO4	A	451	-	X
2	SO4	A	453	-	X
2	SO4	A	454	-	X
2	SO4	A	456	-	X
2	SO4	B	433	-	X
2	SO4	B	436	-	X
2	SO4	B	437	-	X
2	SO4	B	438	-	X
2	SO4	B	440	-	X
2	SO4	B	443	-	X
2	SO4	B	444	-	X
2	SO4	B	447	-	X
2	SO4	B	448	-	X
2	SO4	B	449	-	X
2	SO4	B	450	-	X
2	SO4	B	453	-	X
2	SO4	B	454	-	X
2	SO4	B	455	-	X
2	SO4	B	457	-	X
2	SO4	B	458	-	X
2	SO4	C	432	-	X
2	SO4	C	436	-	X
2	SO4	C	438	-	X
2	SO4	C	448	-	X
2	SO4	C	450	-	X
2	SO4	C	454	-	X
2	SO4	D	433	-	X
2	SO4	D	434	-	X
2	SO4	D	436	-	X
2	SO4	D	437	-	X
2	SO4	D	449	-	X
3	FLC	A	460	-	X
3	FLC	B	463	-	X

2 Entry composition

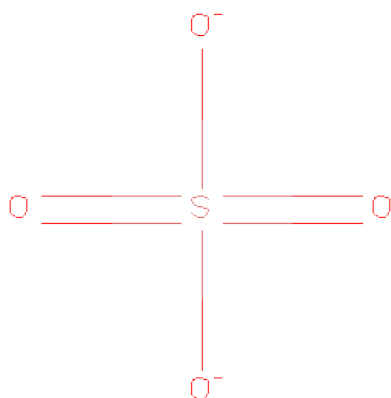
There are 5 unique types of molecules in this entry. The entry contains 14435 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			

- 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		

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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	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	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	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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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	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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

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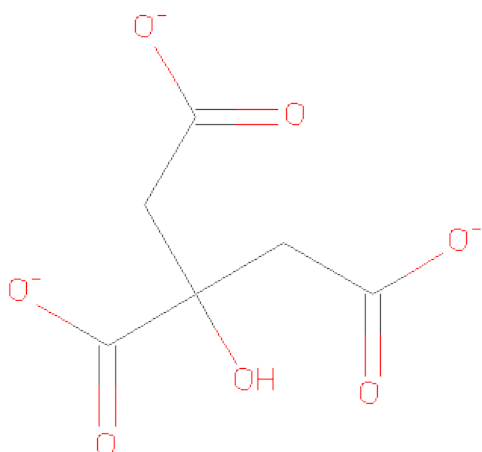
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

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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	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	196	Total	O	0	0
			196	196		
5	C	78	Total	O	0	0
			78	78		

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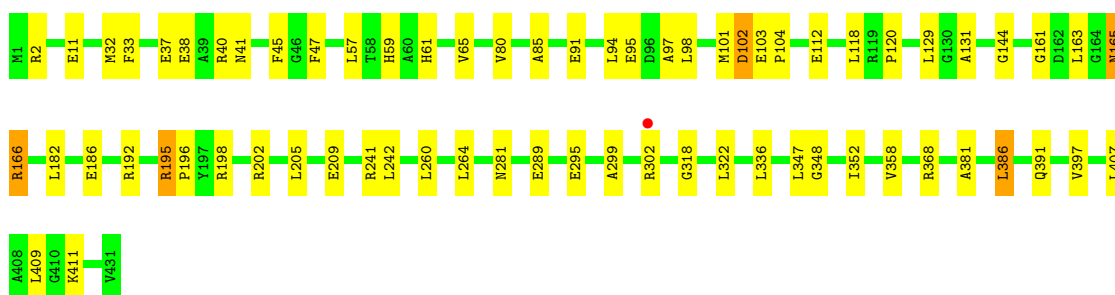
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	79	Total	O	0	0
			79	79		

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.

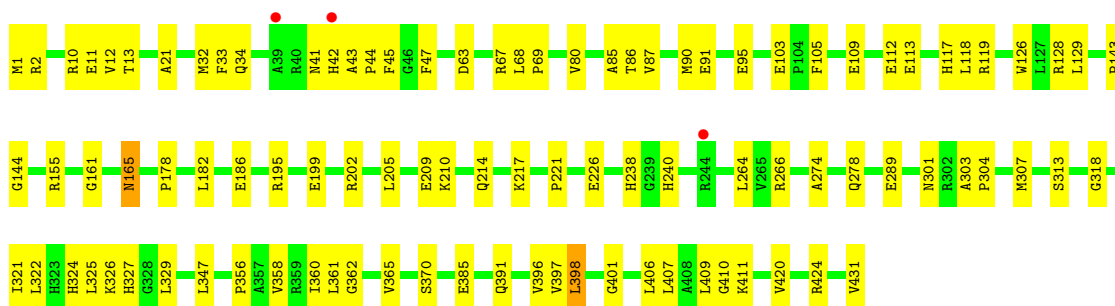
• Molecule 1: Ribonuclease TTHA0252

Chain A:



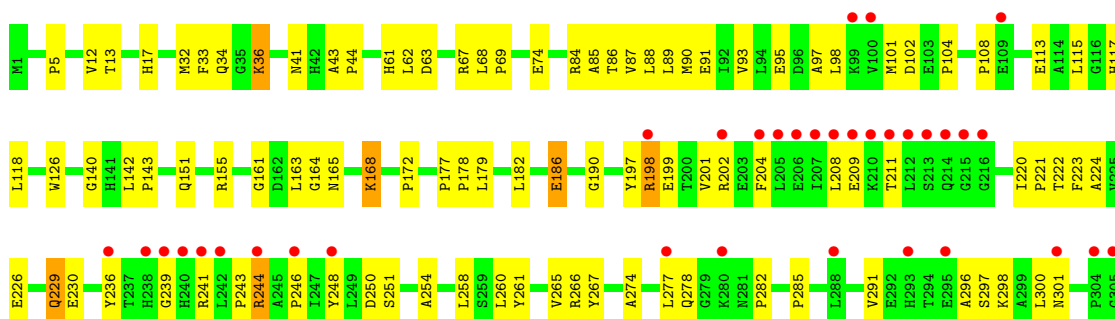
• Molecule 1: Ribonuclease TTHA0252

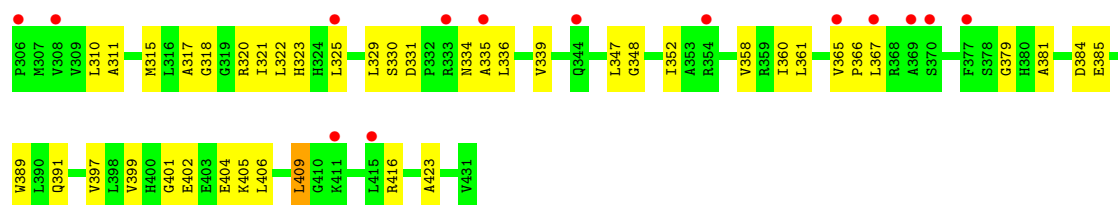
Chain B:



• Molecule 1: Ribonuclease TTHA0252

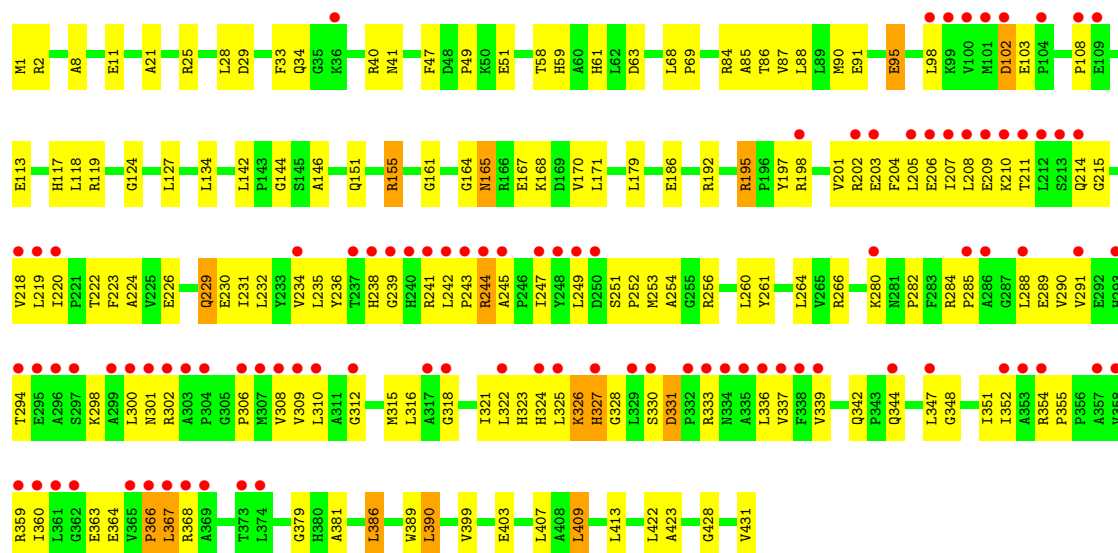
Chain C:





● Molecule 1: Ribonuclease TTHA0252

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.22Å 145.70Å 119.65Å 90.00° 110.52° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 49.71 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.05) 94.4 (49.71-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 2.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.250 0.217 , 0.248	Depositor DCC
R_{free} test set	13669 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 144351 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14435	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: FLC, ZN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/3407	0.65	1/4621 (0.0%)
1	B	0.33	0/3407	0.62	1/4621 (0.0%)
1	C	0.29	0/3407	0.57	1/4621 (0.0%)
1	D	0.28	0/3407	0.56	1/4621 (0.0%)
All	All	0.31	0/13628	0.60	4/18484 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLY	N-CA-C	-5.92	98.30	113.10
1	B	161	GLY	N-CA-C	-5.48	99.41	113.10
1	D	161	GLY	N-CA-C	-5.42	99.54	113.10
1	C	161	GLY	N-CA-C	-5.00	100.60	113.10

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	3326	0	3351	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3326	0	3351	81	0
1	C	3326	0	3351	127	0
1	D	3326	0	3351	144	0
2	A	140	0	0	5	0
2	B	155	0	0	9	0
2	C	115	0	0	6	0
2	D	90	0	0	3	0
3	A	13	0	5	4	0
3	B	13	0	5	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	244	0	0	7	0
5	B	196	0	0	6	0
5	C	78	0	0	1	0
5	D	79	0	0	3	0
All	All	14435	0	13414	404	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 (404) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:391:GLN:HG3	5:A:700:HOH:O	1.34	1.24
1:B:10:ARG:HH12	1:B:424:ARG:HG2	1.01	1.10
1:B:2:ARG:HG3	2:B:453:SO4:O1	1.55	1.06
1:A:120:PRO:HB2	2:A:451:SO4:O3	1.59	1.02
1:D:363:GLU:HG2	1:D:364:GLU:H	1.25	1.01
1:D:33:PHE:H	1:D:41:ASN:HD21	1.05	0.98
1:C:244:ARG:HD3	1:C:244:ARG:H	1.26	0.97
1:A:195:ARG:HB2	1:A:195:ARG:HH11	1.30	0.97
1:A:195:ARG:HB2	1:A:195:ARG:NH1	1.81	0.96
1:B:10:ARG:HH12	1:B:424:ARG:CG	1.80	0.94
1:C:33:PHE:H	1:C:41:ASN:HD21	1.14	0.94
1:B:10:ARG:NH1	1:B:424:ARG:HG2	1.83	0.92
1:A:302:ARG:NH2	1:B:303:ALA:HB1	1.84	0.92
1:A:33:PHE:H	1:A:41:ASN:HD21	1.12	0.90
1:B:33:PHE:H	1:B:41:ASN:HD21	0.89	0.88
1:B:33:PHE:N	1:B:41:ASN:HD21	1.71	0.86
1:B:33:PHE:H	1:B:41:ASN:ND2	1.72	0.86
1:C:44:PRO:CB	2:C:454:SO4:O4	2.24	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:302:ARG:HH22	1:B:303:ALA:HB1	1.40	0.85
1:B:411:LYS:HB2	3:B:463:FLC:HA2	1.56	0.85
1:C:97:ALA:O	1:C:101:MET:HB2	1.78	0.84
1:C:44:PRO:HB3	2:C:454:SO4:O4	1.78	0.84
1:D:209:GLU:HG2	1:D:243:PRO:HD3	1.60	0.82
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.62	0.81
1:D:168:LYS:HE3	1:D:230:GLU:OE1	1.80	0.81
1:D:231:ILE:O	1:D:234:VAL:HG22	1.81	0.79
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.65	0.78
1:B:391:GLN:HG3	5:B:655:HOH:O	1.82	0.77
1:B:313:SER:HA	2:B:457:SO4:O2	1.84	0.77
1:D:2:ARG:HG3	2:D:435:SO4:O1	1.87	0.75
1:A:129:LEU:HD21	5:A:470:HOH:O	1.87	0.74
1:D:91:GLU:O	1:D:95:GLU:HB2	1.86	0.74
1:D:331:ASP:N	1:D:368:ARG:HB2	2.03	0.74
1:C:198:ARG:HE	1:C:198:ARG:HA	1.53	0.74
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.70	0.74
1:A:120:PRO:CB	2:A:451:SO4:O3	2.35	0.73
1:C:209:GLU:HG2	1:C:243:PRO:HD3	1.69	0.72
1:C:229:GLN:CD	1:C:229:GLN:H	1.90	0.72
1:D:331:ASP:H	1:D:368:ARG:HB2	1.54	0.72
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.54	0.72
1:B:358:VAL:O	1:B:365:VAL:HG12	1.91	0.71
1:C:244:ARG:HD3	1:C:244:ARG:N	2.05	0.71
1:A:299:ALA:O	1:A:302:ARG:HD2	1.91	0.71
1:C:198:ARG:NE	1:C:198:ARG:HA	2.05	0.71
1:D:318:GLY:HA2	1:D:322:LEU:HD11	1.73	0.71
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.20	0.71
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.72	0.70
1:D:363:GLU:HG2	1:D:364:GLU:N	2.04	0.69
1:D:309:VAL:HG11	1:D:324:HIS:NE2	2.07	0.69
1:C:244:ARG:CD	1:C:244:ARG:H	2.05	0.69
1:A:131:ALA:HB1	2:A:450:SO4:O1	1.93	0.69
1:D:207:ILE:O	1:D:211:THR:HG22	1.91	0.69
1:A:368:ARG:NH2	2:A:435:SO4:O1	2.26	0.68
1:B:2:ARG:CG	2:B:453:SO4:O1	2.39	0.68
1:B:87:VAL:HA	1:B:90:MET:CE	2.24	0.68
1:C:199:GLU:HA	1:C:202:ARG:HD2	1.75	0.68
1:D:211:THR:HG21	1:D:218:VAL:HG22	1.74	0.68
1:D:33:PHE:H	1:D:41:ASN:ND2	1.87	0.67
1:B:411:LYS:N	3:B:463:FLC:HG2	2.09	0.67
1:C:168:LYS:HE3	1:C:230:GLU:OE1	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:289:GLU:HG3	5:B:527:HOH:O	1.93	0.67
1:D:239:GLY:HA2	1:D:242:LEU:HG	1.76	0.67
1:D:336:LEU:HD23	1:D:337:VAL:N	2.10	0.66
1:B:347:LEU:HD11	1:B:358:VAL:HG11	1.78	0.66
1:B:87:VAL:HA	1:B:90:MET:HE3	1.78	0.65
1:D:229:GLN:H	1:D:229:GLN:CD	1.99	0.65
1:D:34:GLN:NE2	1:D:63:ASP:HB3	2.11	0.65
1:D:205:LEU:HD13	1:D:241:ARG:HD2	1.77	0.64
1:C:329:LEU:HD23	1:C:367:LEU:HD13	1.77	0.64
1:D:33:PHE:N	1:D:41:ASN:HD21	1.87	0.64
1:D:195:ARG:HD2	1:D:195:ARG:H	1.62	0.64
1:D:316:LEU:HD13	1:D:347:LEU:HD12	1.78	0.64
1:A:381:ALA:HB3	1:A:386:LEU:HD13	1.79	0.64
1:A:59:HIS:HD2	1:A:61:HIS:H	1.46	0.63
1:C:331:ASP:HB3	1:C:334:ASN:ND2	2.14	0.63
1:D:294:THR:HG22	1:D:298:LYS:NZ	2.14	0.63
1:D:61:HIS:CE1	1:D:142:LEU:HD11	2.34	0.62
1:B:90:MET:HE3	1:B:118:LEU:HD13	1.82	0.62
1:B:411:LYS:HA	3:B:463:FLC:OB2	1.98	0.62
1:D:326:LYS:O	1:D:326:LYS:HG2	2.00	0.62
1:C:229:GLN:HG3	1:C:261:TYR:CZ	2.35	0.62
1:A:33:PHE:H	1:A:41:ASN:ND2	1.93	0.61
1:D:215:GLY:HA2	1:D:306:PRO:HD3	1.81	0.61
1:D:34:GLN:HE21	1:D:63:ASP:HB3	1.65	0.61
1:A:102:ASP:CG	1:A:103:GLU:H	2.03	0.61
1:C:86:THR:HG22	1:C:90:MET:CE	2.29	0.61
1:C:33:PHE:H	1:C:41:ASN:ND2	1.93	0.61
1:A:295:GLU:HG3	5:A:693:HOH:O	1.99	0.61
1:D:291:VAL:HG21	1:D:300:LEU:HD11	1.83	0.61
1:D:348:GLY:O	1:D:352:ILE:HG13	2.00	0.61
1:C:250:ASP:HA	1:C:291:VAL:HB	1.83	0.61
1:A:318:GLY:HA2	1:A:322:LEU:HD11	1.83	0.61
1:C:34:GLN:NE2	1:C:63:ASP:HB3	2.15	0.61
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.82	0.60
1:C:220:ILE:HG22	1:C:222:THR:HG23	1.84	0.60
1:D:170:VAL:HG12	1:D:171:LEU:HD12	1.83	0.60
1:C:91:GLU:OE2	1:C:115:LEU:HD13	2.01	0.60
1:A:11:GLU:OE2	1:A:40:ARG:NH1	2.34	0.60
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.36	0.60
1:B:356:PRO:HG2	5:B:536:HOH:O	2.02	0.60
1:D:229:GLN:H	1:D:229:GLN:NE2	1.99	0.59
1:B:34:GLN:HE21	1:B:63:ASP:HB3	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:274:ALA:O	1:C:277:LEU:HB3	2.02	0.59
1:D:204:PHE:O	1:D:208:LEU:HG	2.03	0.59
1:C:74:GLU:OE2	2:C:454:SO4:O1	2.21	0.59
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.18	0.59
1:D:389:TRP:HE3	1:D:390:LEU:HD13	1.67	0.58
1:C:197:TYR:O	1:C:201:VAL:HG23	2.03	0.58
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.39	0.58
1:C:33:PHE:N	1:C:41:ASN:HD21	1.93	0.58
1:C:44:PRO:HB2	2:C:454:SO4:O4	2.03	0.58
1:A:318:GLY:HA2	1:A:322:LEU:CD1	2.33	0.58
1:D:309:VAL:C	1:D:310:LEU:HD12	2.24	0.58
1:D:155:ARG:NH2	2:D:449:SO4:O1	2.33	0.57
1:B:326:LYS:HD2	1:B:361:LEU:HB2	1.86	0.57
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.87	0.57
1:D:309:VAL:HG11	1:D:324:HIS:CD2	2.39	0.57
1:D:239:GLY:HA2	1:D:242:LEU:CG	2.34	0.57
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.86	0.57
1:D:155:ARG:HD3	1:D:431:VAL:O	2.05	0.57
1:A:281:ASN:HB2	3:A:460:FLC:OB2	2.05	0.56
1:A:260:LEU:HD22	1:A:264:LEU:HD11	1.85	0.56
1:D:98:LEU:HD21	1:D:108:PRO:HB3	1.85	0.56
1:B:86:THR:O	1:B:90:MET:HG3	2.05	0.56
1:D:202:ARG:O	1:D:206:GLU:HG3	2.05	0.56
1:C:404:GLU:CD	1:C:404:GLU:H	2.08	0.56
1:D:223:PHE:HZ	1:D:315:MET:HG3	1.71	0.56
1:A:205:LEU:O	1:A:209:GLU:HG3	2.04	0.56
1:C:61:HIS:NE2	1:C:142:LEU:HD11	2.21	0.56
1:B:80:VAL:HB	1:B:118:LEU:HD23	1.87	0.55
1:D:223:PHE:CZ	1:D:315:MET:HG3	2.41	0.55
1:D:90:MET:HE3	1:D:118:LEU:HD13	1.88	0.55
1:B:266:ARG:HG2	5:B:573:HOH:O	2.06	0.55
1:D:236:TYR:OH	1:D:280:LYS:HD3	2.05	0.55
1:B:396:VAL:HG12	1:B:398:LEU:HD13	1.88	0.55
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.88	0.55
1:B:91:GLU:O	1:B:95:GLU:HG2	2.07	0.55
1:C:322:LEU:HB3	1:C:361:LEU:HD11	1.87	0.55
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.88	0.55
1:C:211:THR:HG21	1:C:335:ALA:HB2	1.87	0.55
1:A:289:GLU:HG3	5:A:603:HOH:O	2.07	0.55
1:B:401:GLY:HA3	1:B:406:LEU:HD13	1.88	0.55
1:B:205:LEU:O	1:B:209:GLU:HG3	2.07	0.55
1:B:202:ARG:NE	2:B:458:SO4:O3	2.35	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:302:ARG:HG2	1:D:302:ARG:HH21	1.70	0.54
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.90	0.54
1:D:407:LEU:HD22	1:D:422:LEU:HD21	1.88	0.54
1:D:224:ALA:HB3	1:D:253:MET:CE	2.38	0.54
1:C:236:TYR:HD1	1:C:285:PRO:HA	1.73	0.54
1:B:362:GLY:N	2:B:451:SO4:O1	2.41	0.54
1:D:325:LEU:C	1:D:327:HIS:H	2.11	0.53
1:D:244:ARG:HD2	1:D:244:ARG:N	2.24	0.53
1:D:84:ARG:HD2	1:D:266:ARG:HH12	1.73	0.53
1:B:128:ARG:O	1:B:129:LEU:HD23	2.07	0.53
1:C:321:ILE:O	1:C:325:LEU:HD13	2.09	0.53
1:B:385:GLU:CD	5:B:551:HOH:O	2.47	0.53
1:D:381:ALA:HB3	1:D:386:LEU:HD13	1.91	0.53
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.90	0.53
1:D:229:GLN:HG3	1:D:261:TYR:CE1	2.43	0.53
1:C:325:LEU:HG	1:C:329:LEU:HD11	1.91	0.53
1:D:88:LEU:HB3	1:D:260:LEU:HD21	1.91	0.53
1:B:238:HIS:HA	1:B:240:HIS:CE1	2.43	0.53
1:C:199:GLU:HA	1:C:202:ARG:CD	2.40	0.53
1:D:359:ARG:HA	1:D:363:GLU:O	2.09	0.52
1:C:86:THR:O	1:C:90:MET:HB2	2.10	0.52
1:D:87:VAL:HA	1:D:90:MET:CE	2.40	0.52
1:C:211:THR:HG21	1:C:335:ALA:CB	2.39	0.52
1:B:155:ARG:HD2	1:B:431:VAL:O	2.09	0.52
1:C:358:VAL:O	1:C:365:VAL:HG22	2.09	0.52
2:A:450:SO4:O2	1:D:179:LEU:HD21	2.09	0.52
1:C:318:GLY:HA2	1:C:322:LEU:HD11	1.92	0.52
1:A:195:ARG:HG3	1:A:196:PRO:HD2	1.92	0.52
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.90	0.52
1:D:219:LEU:N	1:D:219:LEU:HD12	2.24	0.52
1:D:218:VAL:HB	1:D:308:VAL:HG22	1.92	0.52
1:C:86:THR:HG22	1:C:90:MET:HE3	1.91	0.52
1:C:402:GLU:HB2	1:C:405:LYS:HG2	1.92	0.52
1:B:327:HIS:O	2:B:438:SO4:O4	2.28	0.52
1:D:321:ILE:O	1:D:325:LEU:HD13	2.11	0.51
1:C:236:TYR:CA	1:C:285:PRO:HB3	2.40	0.51
1:D:285:PRO:HD2	1:D:288:LEU:HD22	1.92	0.51
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.93	0.51
1:B:128:ARG:HH11	1:C:179:LEU:HA	1.76	0.51
1:A:166:ARG:HB2	1:A:166:ARG:NH2	2.25	0.51
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.46	0.51
1:D:119:ARG:HD2	5:D:585:HOH:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:236:TYR:HA	1:C:285:PRO:HB3	1.91	0.51
1:D:68:LEU:HB3	1:D:69:PRO:HD3	1.93	0.51
1:B:370:SER:HA	2:B:455:SO4:O2	2.10	0.51
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.93	0.51
1:C:204:PHE:O	1:C:208:LEU:HG	2.12	0.50
1:C:297:SER:OG	1:C:320:ARG:HD3	2.11	0.50
1:D:85:ALA:HB3	1:D:144:GLY:HA3	1.94	0.50
1:B:68:LEU:HB3	1:B:69:PRO:HD3	1.93	0.50
1:D:1:MET:HG3	1:D:21:ALA:CB	2.41	0.50
1:D:47:PHE:O	1:D:49:PRO:HD3	2.12	0.50
1:D:326:LYS:HB2	1:D:360:ILE:HG21	1.93	0.50
1:C:391:GLN:HA	1:C:416:ARG:NH2	2.26	0.50
1:D:171:LEU:HD11	1:D:226:GLU:OE1	2.11	0.50
1:D:102:ASP:CG	1:D:103:GLU:H	2.14	0.50
1:D:325:LEU:HD12	1:D:325:LEU:N	2.26	0.50
1:B:401:GLY:HA3	1:B:406:LEU:CD1	2.42	0.49
1:D:164:GLY:HA2	1:D:379:GLY:O	2.12	0.49
1:C:34:GLN:HE21	1:C:63:ASP:HB3	1.78	0.49
1:B:87:VAL:HA	1:B:90:MET:HE2	1.94	0.49
1:D:234:VAL:O	1:D:238:HIS:HB2	2.12	0.49
1:D:224:ALA:HB3	1:D:253:MET:HE2	1.94	0.49
1:B:210:LYS:O	1:B:214:GLN:HG2	2.13	0.49
1:D:409:LEU:HD22	1:D:413:LEU:HG	1.93	0.49
1:C:360:ILE:CG2	1:C:361:LEU:HD13	2.41	0.49
1:C:402:GLU:HB3	1:C:404:GLU:OE2	2.12	0.49
1:D:88:LEU:HD13	1:D:260:LEU:HD11	1.95	0.49
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.48	0.48
1:D:61:HIS:CD2	1:D:142:LEU:HD11	2.48	0.48
1:A:260:LEU:HD22	1:A:264:LEU:CD1	2.43	0.48
1:A:281:ASN:HD22	3:A:460:FLC:HA2	1.78	0.48
1:C:236:TYR:CE2	1:C:282:PRO:HA	2.48	0.48
1:C:399:VAL:HG12	1:C:423:ALA:CB	2.44	0.48
1:C:61:HIS:CE1	1:C:142:LEU:HD11	2.49	0.48
1:C:164:GLY:HA2	1:C:379:GLY:O	2.12	0.48
1:C:318:GLY:HA2	1:C:322:LEU:CD1	2.43	0.48
1:C:348:GLY:O	1:C:352:ILE:HG13	2.13	0.48
1:D:171:LEU:N	1:D:171:LEU:HD12	2.28	0.48
1:B:398:LEU:HB3	1:B:406:LEU:HG	1.95	0.48
1:B:113:GLU:OE2	1:B:117:HIS:HE1	1.97	0.48
1:C:68:LEU:HB3	1:C:69:PRO:HD3	1.96	0.48
1:B:318:GLY:HA2	1:B:322:LEU:CD1	2.43	0.48
1:C:190:GLY:HA3	1:C:409:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:PHE:N	1:A:41:ASN:HD21	1.94	0.48
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.17	0.48
1:A:101:MET:HE2	1:A:104:PRO:HA	1.96	0.48
1:B:360:ILE:HD12	1:B:365:VAL:HG11	1.96	0.47
1:D:203:GLU:O	1:D:207:ILE:HG13	2.13	0.47
1:C:298:LYS:HA	1:C:301:ASN:ND2	2.29	0.47
1:A:97:ALA:O	1:A:101:MET:HB2	2.14	0.47
1:D:102:ASP:OD2	1:D:103:GLU:HG2	2.14	0.47
1:B:165:ASN:C	1:B:165:ASN:HD22	2.16	0.47
1:D:253:MET:HA	1:D:256:ARG:NH1	2.29	0.47
1:C:246:PRO:HG2	1:C:248:TYR:HE1	1.80	0.47
1:C:36:LYS:NZ	1:C:36:LYS:HB2	2.29	0.47
1:D:33:PHE:CD2	1:D:40:ARG:HB2	2.50	0.47
1:D:249:LEU:HD23	1:D:290:VAL:HG22	1.96	0.47
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.15	0.47
1:A:209:GLU:HG2	1:A:242:LEU:HD23	1.96	0.47
1:D:165:ASN:HD22	1:D:165:ASN:C	2.18	0.47
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.96	0.47
1:B:411:LYS:CB	3:B:463:FLC:HA2	2.37	0.47
1:C:91:GLU:O	1:C:95:GLU:HG2	2.15	0.47
1:C:402:GLU:HB2	1:C:405:LYS:CG	2.45	0.47
1:D:354:ARG:N	1:D:355:PRO:CD	2.78	0.47
1:D:428:GLY:HA3	2:D:446:SO4:O1	2.14	0.46
1:C:140:GLY:O	1:C:164:GLY:HA3	2.15	0.46
1:D:1:MET:HB3	1:D:431:VAL:HB	1.97	0.46
1:C:88:LEU:HD13	1:C:260:LEU:HD11	1.96	0.46
1:D:315:MET:HA	1:D:342:GLN:HE22	1.80	0.46
1:D:252:PRO:HD2	5:D:495:HOH:O	2.16	0.46
1:C:163:LEU:HD11	1:C:389:TRP:CE3	2.51	0.46
1:C:221:PRO:HA	1:C:311:ALA:O	2.15	0.46
1:D:403:GLU:O	1:D:407:LEU:HD23	2.15	0.46
1:A:198:ARG:HG3	1:A:198:ARG:HH21	1.80	0.46
1:B:85:ALA:HB3	1:B:144:GLY:HA3	1.98	0.46
1:C:265:VAL:HG23	1:C:266:ARG:N	2.31	0.46
1:A:209:GLU:OE2	1:A:241:ARG:NH2	2.48	0.46
1:A:198:ARG:NH2	1:A:198:ARG:HG3	2.31	0.46
1:D:321:ILE:C	1:D:323:HIS:H	2.19	0.45
1:B:143:PRO:HD3	1:B:226:GLU:HG3	1.99	0.45
1:A:59:HIS:NE2	1:A:61:HIS:HB2	2.30	0.45
1:C:62:LEU:HD13	1:C:93:VAL:HG12	1.99	0.45
1:D:363:GLU:CG	1:D:364:GLU:H	2.09	0.45
1:C:222:THR:HG22	1:C:339:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:89:LEU:O	1:C:93:VAL:HG23	2.16	0.45
1:B:12:VAL:HG23	1:B:13:THR:HG23	1.98	0.45
1:B:410:GLY:C	3:B:463:FLC:HG2	2.36	0.45
1:C:325:LEU:O	1:C:329:LEU:HD13	2.16	0.45
1:B:396:VAL:O	1:B:420:VAL:HA	2.17	0.45
1:C:320:ARG:HA	1:C:323:HIS:HD2	1.81	0.45
1:D:58:THR:HB	1:D:146:ALA:O	2.17	0.45
1:D:211:THR:CG2	1:D:218:VAL:HG22	2.44	0.45
1:D:244:ARG:O	1:D:245:ALA:HB2	2.17	0.45
1:D:288:LEU:HD12	1:D:289:GLU:H	1.81	0.45
1:C:204:PHE:CE1	1:C:208:LEU:HD11	2.51	0.45
1:B:109:GLU:O	1:B:112:GLU:HG2	2.17	0.45
1:D:310:LEU:N	1:D:310:LEU:HD12	2.32	0.45
1:D:336:LEU:C	1:D:336:LEU:HD23	2.36	0.45
1:A:59:HIS:CD2	1:A:61:HIS:H	2.30	0.45
1:D:61:HIS:NE2	1:D:142:LEU:HD11	2.31	0.45
1:A:281:ASN:HB3	3:A:460:FLC:HG2	1.99	0.45
1:D:347:LEU:HD13	1:D:347:LEU:O	2.17	0.45
1:D:280:LYS:O	1:D:282:PRO:HD3	2.17	0.45
1:A:102:ASP:CG	1:A:103:GLU:N	2.70	0.45
1:B:128:ARG:NH2	1:C:391:GLN:O	2.50	0.45
1:D:165:ASN:ND2	1:D:167:GLU:H	2.15	0.45
1:B:109:GLU:HA	1:B:112:GLU:HG2	1.99	0.45
1:D:197:TYR:O	1:D:201:VAL:HG23	2.17	0.45
1:B:34:GLN:NE2	1:B:63:ASP:HB3	2.30	0.44
1:C:32:MET:HA	1:C:67:ARG:HG3	1.98	0.44
1:C:172:PRO:HA	2:C:442:SO4:O3	2.17	0.44
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.98	0.44
1:C:98:LEU:HD23	1:C:98:LEU:O	2.16	0.44
1:C:209:GLU:HG2	1:C:243:PRO:CD	2.42	0.44
1:C:32:MET:SD	1:C:62:LEU:HG	2.56	0.44
1:C:143:PRO:HD3	1:C:226:GLU:HG3	1.98	0.44
1:D:381:ALA:HB3	1:D:386:LEU:CD1	2.47	0.44
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.53	0.44
1:C:296:ALA:O	1:C:300:LEU:HD13	2.17	0.44
1:C:88:LEU:O	1:C:91:GLU:HB3	2.18	0.44
1:D:86:THR:O	1:D:90:MET:HG3	2.18	0.44
1:B:195:ARG:CZ	1:B:199:GLU:HG2	2.48	0.44
1:B:217:LYS:HG2	1:B:307:MET:HG2	1.99	0.44
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.99	0.44
1:D:28:LEU:O	1:D:29:ASP:HB2	2.17	0.44
1:C:98:LEU:HD23	1:C:98:LEU:C	2.37	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:301:ASN:OD1	1:B:324:HIS:HA	2.18	0.44
1:C:223:PHE:CZ	1:C:315:MET:HG3	2.53	0.44
1:C:248:TYR:CD2	1:C:300:LEU:HD21	2.52	0.44
1:D:312:GLY:O	1:D:321:ILE:HB	2.18	0.44
1:A:101:MET:CE	1:A:104:PRO:HA	2.48	0.44
1:A:2:ARG:NH2	5:A:618:HOH:O	2.49	0.44
1:A:91:GLU:O	1:A:95:GLU:HG2	2.17	0.44
1:D:399:VAL:HG12	1:D:423:ALA:HB3	2.00	0.44
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.53	0.44
1:A:80:VAL:HB	1:A:118:LEU:HD23	2.00	0.44
1:D:220:ILE:HG23	1:D:339:VAL:HG13	2.00	0.43
1:D:318:GLY:HA2	1:D:322:LEU:CD1	2.46	0.43
1:D:88:LEU:HD12	1:D:264:LEU:HD21	2.01	0.43
1:C:229:GLN:CD	1:C:229:GLN:N	2.66	0.43
1:A:281:ASN:CB	3:A:460:FLC:HG2	2.48	0.43
1:D:327:HIS:O	1:D:327:HIS:ND1	2.50	0.43
1:B:32:MET:HA	1:B:67:ARG:HG3	1.99	0.43
1:B:42:HIS:ND1	1:B:105:PHE:HB3	2.33	0.43
1:D:86:THR:HG22	1:D:90:MET:HE2	1.99	0.43
1:C:163:LEU:HD11	1:C:389:TRP:CD2	2.53	0.43
1:C:381:ALA:HB1	1:C:385:GLU:HB2	1.99	0.43
1:B:424:ARG:HA	2:B:454:SO4:O3	2.18	0.43
1:C:399:VAL:HG12	1:C:423:ALA:HB3	2.01	0.43
1:D:251:SER:HB3	1:D:254:ALA:HB3	2.01	0.43
1:C:365:VAL:O	1:C:365:VAL:HG23	2.18	0.43
1:A:37:GLU:HG3	1:A:40:ARG:HH11	1.83	0.43
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.54	0.43
1:D:210:LYS:HG3	1:D:210:LYS:O	2.19	0.43
1:C:5:PRO:HA	1:C:17:HIS:HD2	1.83	0.43
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.53	0.43
1:D:239:GLY:HA2	1:D:242:LEU:CD1	2.49	0.42
1:C:224:ALA:HB1	1:C:254:ALA:HA	2.02	0.42
1:C:310:LEU:N	1:C:310:LEU:HD12	2.33	0.42
1:B:1:MET:N	2:B:453:SO4:O3	2.43	0.42
1:D:214:GLN:NE2	1:D:333:ARG:HA	2.34	0.42
1:A:411:LYS:NZ	5:A:488:HOH:O	2.51	0.42
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.54	0.42
1:C:317:ALA:HB2	5:C:494:HOH:O	2.18	0.42
1:D:326:LYS:HD2	1:D:360:ILE:HG22	2.01	0.42
1:C:186:GLU:HA	1:C:399:VAL:O	2.19	0.42
1:B:318:GLY:HA2	1:B:322:LEU:HD11	2.01	0.42
1:C:98:LEU:HD11	1:C:108:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:113:GLU:OE2	1:C:117:HIS:HE1	2.03	0.42
1:D:124:GLY:C	5:D:526:HOH:O	2.57	0.42
1:A:32:MET:HE2	1:A:32:MET:HB3	1.93	0.42
1:B:365:VAL:HG13	1:B:365:VAL:O	2.19	0.42
1:D:244:ARG:CD	1:D:244:ARG:N	2.83	0.42
1:B:109:GLU:HA	1:B:112:GLU:OE2	2.20	0.42
1:B:10:ARG:NH1	1:B:424:ARG:HA	2.34	0.42
1:A:166:ARG:HH21	1:A:166:ARG:CB	2.33	0.42
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.55	0.42
1:B:274:ALA:O	1:B:278:GLN:HG3	2.19	0.42
1:D:87:VAL:HA	1:D:90:MET:HE2	2.00	0.41
1:A:202:ARG:NH2	5:A:479:HOH:O	2.53	0.41
1:C:384:ASP:N	1:C:384:ASP:OD2	2.53	0.41
1:A:348:GLY:O	1:A:352:ILE:HG13	2.19	0.41
1:B:266:ARG:NE	5:B:622:HOH:O	2.34	0.41
1:D:198:ARG:HB3	1:D:202:ARG:NH2	2.36	0.41
1:D:253:MET:HA	1:D:256:ARG:CZ	2.50	0.41
1:D:366:PRO:O	1:D:367:LEU:HB2	2.20	0.41
1:D:389:TRP:CE3	1:D:390:LEU:HD13	2.52	0.41
1:C:12:VAL:HG23	1:C:13:THR:HG23	2.01	0.41
1:C:347:LEU:HD11	1:C:358:VAL:HG11	2.03	0.41
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.50	0.41
1:C:322:LEU:HB3	1:C:361:LEU:CD1	2.51	0.41
1:C:224:ALA:HB1	1:C:254:ALA:CA	2.50	0.41
1:C:101:MET:HE2	1:C:104:PRO:HB3	2.01	0.41
1:C:251:SER:HB3	1:C:254:ALA:HB3	2.02	0.41
1:C:330:SER:HA	1:C:366:PRO:O	2.20	0.41
1:C:151:GLN:HB2	2:C:448:SO4:O3	2.21	0.41
1:D:316:LEU:CD1	1:D:347:LEU:HD12	2.49	0.41
1:D:284:ARG:HD3	1:D:288:LEU:HD23	2.03	0.41
1:D:232:LEU:HB3	1:D:285:PRO:HD3	2.03	0.41
1:D:285:PRO:HG2	1:D:288:LEU:HB2	2.03	0.41
1:D:25:ARG:NH1	1:D:51:GLU:HB3	2.36	0.41
1:D:8:ALA:HA	1:D:11:GLU:HG3	2.03	0.41
1:D:330:SER:O	1:D:331:ASP:HB2	2.21	0.41
1:C:274:ALA:O	1:C:278:GLN:HG3	2.21	0.41
1:D:302:ARG:HG2	1:D:302:ARG:NH2	2.35	0.41
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	0.41
1:A:165:ASN:C	1:A:165:ASN:HD22	2.24	0.41
1:C:236:TYR:CD2	1:C:282:PRO:HA	2.56	0.40
1:D:209:GLU:HG2	1:D:243:PRO:CD	2.41	0.40
1:C:360:ILE:HD12	1:C:365:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:347:LEU:CD1	1:D:351:ILE:HD11	2.51	0.40
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.55	0.40
1:A:302:ARG:HD3	1:B:304:PRO:HD2	2.02	0.40
1:D:87:VAL:HA	1:D:90:MET:HE3	2.03	0.40
1:C:229:GLN:HG3	1:C:261:TYR:CE1	2.56	0.40
1:A:57:LEU:HD13	1:A:65:VAL:HG12	2.03	0.40
1:D:113:GLU:OE2	1:D:117:HIS:HE1	2.04	0.40
1:C:239:GLY:C	1:C:241:ARG:H	2.23	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	429/431 (100%)	418 (97%)	10 (2%)	1 (0%)	56	47
1	B	429/431 (100%)	416 (97%)	13 (3%)	0	100	100
1	C	429/431 (100%)	400 (93%)	26 (6%)	3 (1%)	30	16
1	D	429/431 (100%)	394 (92%)	28 (6%)	7 (2%)	14	4
All	All	1716/1724 (100%)	1628 (95%)	77 (4%)	11 (1%)	33	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	D	102	ASP
1	D	366	PRO
1	C	102	ASP
1	D	327	HIS
1	D	367	LEU
1	C	198	ARG
1	D	326	LYS
1	C	168	LYS
1	D	328	GLY

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Mol	Chain	Res	Type
1	D	331	ASP

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	342/342 (100%)	328 (96%)	14 (4%)	41	33
1	B	342/342 (100%)	331 (97%)	11 (3%)	51	44
1	C	342/342 (100%)	333 (97%)	9 (3%)	59	54
1	D	342/342 (100%)	327 (96%)	15 (4%)	39	29
All	All	1368/1368 (100%)	1319 (96%)	49 (4%)	47	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	94	LEU
1	A	98	LEU
1	A	112	GLU
1	A	163	LEU
1	A	165	ASN
1	A	166	ARG
1	A	186	GLU
1	A	192	ARG
1	A	195	ARG
1	A	336	LEU
1	A	386	LEU
1	A	407	LEU
1	A	409	LEU
1	B	11	GLU
1	B	103	GLU
1	B	119	ARG
1	B	165	ASN
1	B	186	GLU
1	B	264	LEU
1	B	325	LEU

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Mol	Chain	Res	Type
1	B	329	LEU
1	B	398	LEU
1	B	407	LEU
1	B	409	LEU
1	C	36	LYS
1	C	155	ARG
1	C	165	ASN
1	C	186	GLU
1	C	229	GLN
1	C	244	ARG
1	C	258	LEU
1	C	336	LEU
1	C	409	LEU
1	D	95	GLU
1	D	127	LEU
1	D	134	LEU
1	D	151	GLN
1	D	155	ARG
1	D	165	ASN
1	D	186	GLU
1	D	192	ARG
1	D	195	ARG
1	D	229	GLN
1	D	244	ARG
1	D	344	GLN
1	D	386	LEU
1	D	390	LEU
1	D	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	59	HIS
1	A	165	ASN
1	A	275	HIS
1	A	344	GLN
1	B	34	GLN
1	B	41	ASN
1	B	165	ASN
1	B	238	HIS
1	C	17	HIS

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Mol	Chain	Res	Type
1	C	34	GLN
1	C	41	ASN
1	C	59	HIS
1	C	165	ASN
1	C	214	GLN
1	C	301	ASN
1	C	323	HIS
1	D	17	HIS
1	D	34	GLN
1	D	41	ASN
1	D	165	ASN
1	D	214	GLN
1	D	229	GLN
1	D	301	ASN
1	D	323	HIS
1	D	383	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 ⓘ

Of 110 ligands modelled in this entry, 8 are monoatomic - leaving 102 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	432	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	A	433	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	A	434	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	A	435	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	A	436	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	A	437	-	4,4,4	1.64	0	6,6,6	0.89	0
2	SO4	A	438	-	4,4,4	1.57	0	6,6,6	0.93	0
2	SO4	A	439	-	4,4,4	1.59	0	6,6,6	0.91	0
2	SO4	A	440	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	A	441	-	4,4,4	1.54	0	6,6,6	0.92	0
2	SO4	A	442	-	4,4,4	1.61	0	6,6,6	0.91	0
2	SO4	A	443	-	4,4,4	1.54	0	6,6,6	0.89	0
2	SO4	A	444	-	4,4,4	1.63	0	6,6,6	0.87	0
2	SO4	A	445	-	4,4,4	1.57	0	6,6,6	0.91	0
2	SO4	A	446	-	4,4,4	1.57	0	6,6,6	0.89	0
2	SO4	A	447	-	4,4,4	1.58	0	6,6,6	0.91	0
2	SO4	A	448	-	4,4,4	1.59	0	6,6,6	0.88	0
2	SO4	A	449	-	4,4,4	1.43	0	6,6,6	0.81	0
2	SO4	A	450	-	4,4,4	1.60	0	6,6,6	0.88	0
2	SO4	A	451	-	4,4,4	1.59	0	6,6,6	0.86	0
2	SO4	A	452	-	4,4,4	1.58	0	6,6,6	0.93	0
2	SO4	A	453	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	A	454	-	4,4,4	1.56	0	6,6,6	0.90	0
2	SO4	A	455	-	4,4,4	1.58	0	6,6,6	0.93	0
2	SO4	A	456	-	4,4,4	1.61	0	6,6,6	0.89	0
2	SO4	A	457	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	A	458	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	A	459	-	4,4,4	1.60	0	6,6,6	0.91	0
3	FLC	A	460	-	5,12,12	4.49	2 (40%)	7,17,17	0.56	0
2	SO4	B	432	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	B	433	-	4,4,4	1.60	0	6,6,6	0.89	0
2	SO4	B	434	-	4,4,4	1.55	0	6,6,6	0.92	0
2	SO4	B	435	-	4,4,4	1.62	0	6,6,6	0.91	0
2	SO4	B	436	-	4,4,4	1.62	0	6,6,6	0.91	0
2	SO4	B	437	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	B	438	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	B	439	-	4,4,4	1.57	0	6,6,6	0.91	0
2	SO4	B	440	-	4,4,4	1.62	0	6,6,6	0.89	0
2	SO4	B	441	-	4,4,4	1.58	0	6,6,6	0.91	0
2	SO4	B	442	-	4,4,4	1.57	0	6,6,6	0.90	0
2	SO4	B	443	-	4,4,4	1.58	0	6,6,6	0.93	0
2	SO4	B	444	-	4,4,4	1.58	0	6,6,6	0.91	0
2	SO4	B	445	-	4,4,4	1.62	0	6,6,6	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	446	-	4,4,4	1.52	0	6,6,6	0.85	0
2	SO4	B	447	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	B	448	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	B	449	-	4,4,4	1.59	0	6,6,6	0.91	0
2	SO4	B	450	-	4,4,4	1.59	0	6,6,6	0.91	0
2	SO4	B	451	-	4,4,4	1.56	0	6,6,6	0.92	0
2	SO4	B	452	-	4,4,4	1.58	0	6,6,6	0.92	0
2	SO4	B	453	-	4,4,4	1.58	0	6,6,6	0.88	0
2	SO4	B	454	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	B	455	-	4,4,4	1.57	0	6,6,6	0.92	0
2	SO4	B	456	-	4,4,4	1.50	0	6,6,6	0.87	0
2	SO4	B	457	-	4,4,4	1.59	0	6,6,6	0.92	0
2	SO4	B	458	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	B	459	-	4,4,4	1.55	0	6,6,6	0.90	0
2	SO4	B	460	-	4,4,4	1.55	0	6,6,6	0.92	0
2	SO4	B	461	-	4,4,4	1.59	0	6,6,6	0.91	0
2	SO4	B	462	-	4,4,4	1.57	0	6,6,6	0.92	0
3	FLC	B	463	-	5,12,12	4.26	2 (40%)	7,17,17	0.33	0
2	SO4	C	432	-	4,4,4	1.61	0	6,6,6	0.89	0
2	SO4	C	433	-	4,4,4	1.58	0	6,6,6	0.89	0
2	SO4	C	434	-	4,4,4	1.61	0	6,6,6	0.86	0
2	SO4	C	435	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	C	436	-	4,4,4	1.61	0	6,6,6	0.89	0
2	SO4	C	437	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	C	438	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	C	439	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	C	440	-	4,4,4	1.59	0	6,6,6	0.92	0
2	SO4	C	441	-	4,4,4	1.57	0	6,6,6	0.90	0
2	SO4	C	442	-	4,4,4	1.61	0	6,6,6	0.90	0
2	SO4	C	443	-	4,4,4	1.61	0	6,6,6	0.89	0
2	SO4	C	444	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	C	445	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	C	446	-	4,4,4	1.61	0	6,6,6	0.90	0
2	SO4	C	447	-	4,4,4	1.60	0	6,6,6	0.89	0
2	SO4	C	448	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	C	449	-	4,4,4	1.57	0	6,6,6	0.88	0
2	SO4	C	450	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	C	451	-	4,4,4	1.58	0	6,6,6	0.91	0
2	SO4	C	452	-	4,4,4	1.61	0	6,6,6	0.90	0
2	SO4	C	453	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	C	454	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	D	432	-	4,4,4	1.59	0	6,6,6	0.96	0
2	SO4	D	433	-	4,4,4	1.60	0	6,6,6	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	434	-	4,4,4	1.57	0	6,6,6	0.91	0
2	SO4	D	435	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	D	436	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	D	437	-	4,4,4	1.55	0	6,6,6	0.94	0
2	SO4	D	438	-	4,4,4	1.58	0	6,6,6	0.92	0
2	SO4	D	439	-	4,4,4	1.56	0	6,6,6	0.91	0
2	SO4	D	440	-	4,4,4	1.60	0	6,6,6	0.91	0
2	SO4	D	441	-	4,4,4	1.60	0	6,6,6	0.90	0
2	SO4	D	442	-	4,4,4	1.59	0	6,6,6	0.90	0
2	SO4	D	443	-	4,4,4	1.51	0	6,6,6	0.89	0
2	SO4	D	444	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	D	445	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	D	446	-	4,4,4	1.61	0	6,6,6	0.86	0
2	SO4	D	447	-	4,4,4	1.59	0	6,6,6	0.89	0
2	SO4	D	448	-	4,4,4	1.56	0	6,6,6	0.91	0
2	SO4	D	449	-	4,4,4	1.61	0	6,6,6	0.89	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	432	-	-	0/0/0/0	0/0/0/0
2	SO4	A	433	-	-	0/0/0/0	0/0/0/0
2	SO4	A	434	-	-	0/0/0/0	0/0/0/0
2	SO4	A	435	-	-	0/0/0/0	0/0/0/0
2	SO4	A	436	-	-	0/0/0/0	0/0/0/0
2	SO4	A	437	-	-	0/0/0/0	0/0/0/0
2	SO4	A	438	-	-	0/0/0/0	0/0/0/0
2	SO4	A	439	-	-	0/0/0/0	0/0/0/0
2	SO4	A	440	-	-	0/0/0/0	0/0/0/0
2	SO4	A	441	-	-	0/0/0/0	0/0/0/0
2	SO4	A	442	-	-	0/0/0/0	0/0/0/0
2	SO4	A	443	-	-	0/0/0/0	0/0/0/0
2	SO4	A	444	-	-	0/0/0/0	0/0/0/0
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	A	446	-	-	0/0/0/0	0/0/0/0
2	SO4	A	447	-	-	0/0/0/0	0/0/0/0
2	SO4	A	448	-	-	0/0/0/0	0/0/0/0
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0
2	SO4	A	450	-	-	0/0/0/0	0/0/0/0
2	SO4	A	451	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	452	-	-	0/0/0/0	0/0/0/0
2	SO4	A	453	-	-	0/0/0/0	0/0/0/0
2	SO4	A	454	-	-	0/0/0/0	0/0/0/0
2	SO4	A	455	-	-	0/0/0/0	0/0/0/0
2	SO4	A	456	-	-	0/0/0/0	0/0/0/0
2	SO4	A	457	-	-	0/0/0/0	0/0/0/0
2	SO4	A	458	-	-	0/0/0/0	0/0/0/0
2	SO4	A	459	-	-	0/0/0/0	0/0/0/0
3	FLC	A	460	-	-	0/6/16/16	0/0/0/0
2	SO4	B	432	-	-	0/0/0/0	0/0/0/0
2	SO4	B	433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	434	-	-	0/0/0/0	0/0/0/0
2	SO4	B	435	-	-	0/0/0/0	0/0/0/0
2	SO4	B	436	-	-	0/0/0/0	0/0/0/0
2	SO4	B	437	-	-	0/0/0/0	0/0/0/0
2	SO4	B	438	-	-	0/0/0/0	0/0/0/0
2	SO4	B	439	-	-	0/0/0/0	0/0/0/0
2	SO4	B	440	-	-	0/0/0/0	0/0/0/0
2	SO4	B	441	-	-	0/0/0/0	0/0/0/0
2	SO4	B	442	-	-	0/0/0/0	0/0/0/0
2	SO4	B	443	-	-	0/0/0/0	0/0/0/0
2	SO4	B	444	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	446	-	-	0/0/0/0	0/0/0/0
2	SO4	B	447	-	-	0/0/0/0	0/0/0/0
2	SO4	B	448	-	-	0/0/0/0	0/0/0/0
2	SO4	B	449	-	-	0/0/0/0	0/0/0/0
2	SO4	B	450	-	-	0/0/0/0	0/0/0/0
2	SO4	B	451	-	-	0/0/0/0	0/0/0/0
2	SO4	B	452	-	-	0/0/0/0	0/0/0/0
2	SO4	B	453	-	-	0/0/0/0	0/0/0/0
2	SO4	B	454	-	-	0/0/0/0	0/0/0/0
2	SO4	B	455	-	-	0/0/0/0	0/0/0/0
2	SO4	B	456	-	-	0/0/0/0	0/0/0/0
2	SO4	B	457	-	-	0/0/0/0	0/0/0/0
2	SO4	B	458	-	-	0/0/0/0	0/0/0/0
2	SO4	B	459	-	-	0/0/0/0	0/0/0/0
2	SO4	B	460	-	-	0/0/0/0	0/0/0/0
2	SO4	B	461	-	-	0/0/0/0	0/0/0/0
2	SO4	B	462	-	-	0/0/0/0	0/0/0/0
3	FLC	B	463	-	-	0/6/16/16	0/0/0/0
2	SO4	C	432	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	433	-	-	0/0/0/0	0/0/0/0
2	SO4	C	434	-	-	0/0/0/0	0/0/0/0
2	SO4	C	435	-	-	0/0/0/0	0/0/0/0
2	SO4	C	436	-	-	0/0/0/0	0/0/0/0
2	SO4	C	437	-	-	0/0/0/0	0/0/0/0
2	SO4	C	438	-	-	0/0/0/0	0/0/0/0
2	SO4	C	439	-	-	0/0/0/0	0/0/0/0
2	SO4	C	440	-	-	0/0/0/0	0/0/0/0
2	SO4	C	441	-	-	0/0/0/0	0/0/0/0
2	SO4	C	442	-	-	0/0/0/0	0/0/0/0
2	SO4	C	443	-	-	0/0/0/0	0/0/0/0
2	SO4	C	444	-	-	0/0/0/0	0/0/0/0
2	SO4	C	445	-	-	0/0/0/0	0/0/0/0
2	SO4	C	446	-	-	0/0/0/0	0/0/0/0
2	SO4	C	447	-	-	0/0/0/0	0/0/0/0
2	SO4	C	448	-	-	0/0/0/0	0/0/0/0
2	SO4	C	449	-	-	0/0/0/0	0/0/0/0
2	SO4	C	450	-	-	0/0/0/0	0/0/0/0
2	SO4	C	451	-	-	0/0/0/0	0/0/0/0
2	SO4	C	452	-	-	0/0/0/0	0/0/0/0
2	SO4	C	453	-	-	0/0/0/0	0/0/0/0
2	SO4	C	454	-	-	0/0/0/0	0/0/0/0
2	SO4	D	432	-	-	0/0/0/0	0/0/0/0
2	SO4	D	433	-	-	0/0/0/0	0/0/0/0
2	SO4	D	434	-	-	0/0/0/0	0/0/0/0
2	SO4	D	435	-	-	0/0/0/0	0/0/0/0
2	SO4	D	436	-	-	0/0/0/0	0/0/0/0
2	SO4	D	437	-	-	0/0/0/0	0/0/0/0
2	SO4	D	438	-	-	0/0/0/0	0/0/0/0
2	SO4	D	439	-	-	0/0/0/0	0/0/0/0
2	SO4	D	440	-	-	0/0/0/0	0/0/0/0
2	SO4	D	441	-	-	0/0/0/0	0/0/0/0
2	SO4	D	442	-	-	0/0/0/0	0/0/0/0
2	SO4	D	443	-	-	0/0/0/0	0/0/0/0
2	SO4	D	444	-	-	0/0/0/0	0/0/0/0
2	SO4	D	445	-	-	0/0/0/0	0/0/0/0
2	SO4	D	446	-	-	0/0/0/0	0/0/0/0
2	SO4	D	447	-	-	0/0/0/0	0/0/0/0
2	SO4	D	448	-	-	0/0/0/0	0/0/0/0
2	SO4	D	449	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	460	FLC	CG-CGC	7.21	1.54	1.49
3	B	463	FLC	CA-CAC	6.80	1.53	1.49
3	A	460	FLC	CA-CAC	6.78	1.53	1.49
3	B	463	FLC	CG-CGC	6.59	1.53	1.49

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	431/431 (100%)	-0.15	1 (0%) 93 95	13, 22, 39, 65	0
1	B	431/431 (100%)	-0.09	3 (0%) 84 87	14, 26, 44, 62	0
1	C	431/431 (100%)	0.61	49 (11%) 6 5	17, 45, 75, 91	0
1	D	431/431 (100%)	0.98	95 (22%) 1 1	16, 42, 92, 103	0
All	All	1724/1724 (100%)	0.34	148 (8%) 11 10	13, 31, 78, 103	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	8.4
1	C	242	LEU	7.3
1	D	242	LEU	7.1
1	D	300	LEU	7.0
1	D	306	PRO	6.7
1	C	277	LEU	6.6
1	D	212	LEU	5.8
1	D	332	PRO	5.6
1	D	325	LEU	5.5
1	D	304	PRO	5.2
1	C	415	LEU	5.0
1	D	335	ALA	5.0
1	D	208	LEU	4.9
1	C	335	ALA	4.9
1	D	239	GLY	4.8
1	D	104	PRO	4.8
1	D	324	HIS	4.8
1	D	368	ARG	4.7
1	D	241	ARG	4.7
1	D	286	ALA	4.6
1	D	362	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	306	PRO	4.5
1	D	210	LYS	4.5
1	D	317	ALA	4.4
1	D	333	ARG	4.4
1	C	216	GLY	4.4
1	D	334	ASN	4.3
1	D	240	HIS	4.3
1	D	297	SER	4.3
1	C	212	LEU	4.2
1	D	98	LEU	4.1
1	D	299	ALA	4.1
1	C	213	SER	4.1
1	D	327	HIS	4.1
1	D	244	ARG	4.0
1	D	367	LEU	4.0
1	C	333	ARG	4.0
1	D	249	LEU	3.9
1	D	213	SER	3.9
1	C	354	ARG	3.8
1	D	296	ALA	3.8
1	D	310	LEU	3.7
1	D	248	TYR	3.7
1	C	205	LEU	3.7
1	D	209	GLU	3.6
1	D	374	LEU	3.5
1	B	42	HIS	3.5
1	D	354	ARG	3.5
1	D	100	VAL	3.5
1	D	366	PRO	3.5
1	D	247	ILE	3.4
1	D	365	VAL	3.4
1	D	36	LYS	3.4
1	D	357	ALA	3.4
1	D	101	MET	3.3
1	C	198	ARG	3.3
1	C	295	GLU	3.3
1	D	336	LEU	3.2
1	D	373	THR	3.2
1	C	209	GLU	3.2
1	D	198	ARG	3.2
1	D	309	VAL	3.2
1	D	211	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	241	ARG	3.1
1	D	369	ALA	3.1
1	D	243	PRO	3.1
1	C	288	LEU	3.1
1	C	308	VAL	3.1
1	D	330	SER	3.1
1	C	204	PHE	3.0
1	C	208	LEU	3.0
1	D	245	ALA	3.0
1	C	207	ILE	3.0
1	D	102	ASP	3.0
1	D	359	ARG	3.0
1	D	358	VAL	3.0
1	C	239	GLY	3.0
1	C	240	HIS	2.9
1	D	219	LEU	2.9
1	D	108	PRO	2.9
1	D	207	ILE	2.8
1	C	210	LYS	2.8
1	C	344	GLN	2.8
1	D	214	GLN	2.8
1	D	218	VAL	2.8
1	D	318	GLY	2.8
1	C	99	LYS	2.8
1	C	202	ARG	2.7
1	D	302	ARG	2.7
1	D	250	ASP	2.7
1	D	322	LEU	2.7
1	D	361	LEU	2.7
1	D	293	HIS	2.7
1	D	206	GLU	2.6
1	D	352	ILE	2.6
1	D	285	PRO	2.6
1	D	307	MET	2.6
1	D	220	ILE	2.5
1	C	238	HIS	2.5
1	C	214	GLN	2.5
1	A	302	ARG	2.5
1	C	244	ARG	2.5
1	B	244	ARG	2.5
1	C	206	GLU	2.5
1	D	238	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	293	HIS	2.4
1	D	109	GLU	2.4
1	C	280	LYS	2.4
1	D	234	VAL	2.4
1	B	39	ALA	2.4
1	D	202	ARG	2.4
1	C	305	GLY	2.4
1	C	236	TYR	2.3
1	D	301	ASN	2.3
1	D	308	VAL	2.3
1	D	295	GLU	2.3
1	D	205	LEU	2.3
1	D	339	VAL	2.3
1	C	248	TYR	2.3
1	D	294	THR	2.3
1	D	291	VAL	2.3
1	C	109	GLU	2.3
1	D	237	THR	2.3
1	C	370	SER	2.2
1	C	215	GLY	2.2
1	C	377	PHE	2.2
1	D	344	GLN	2.2
1	D	360	ILE	2.2
1	D	337	VAL	2.2
1	C	325	LEU	2.2
1	C	369	ALA	2.2
1	C	246	PRO	2.2
1	D	338	PHE	2.2
1	C	367	LEU	2.2
1	D	99	LYS	2.2
1	D	280	LYS	2.1
1	C	304	PRO	2.1
1	D	203	GLU	2.1
1	C	365	VAL	2.1
1	D	288	LEU	2.1
1	D	303	ALA	2.1
1	C	211	THR	2.1
1	D	312	GLY	2.1
1	C	411	LYS	2.1
1	C	100	VAL	2.1
1	C	301	ASN	2.1
1	D	347	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	353	ALA	2.1

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	B	449	5/5	0.31	38.09	84,86,86,86	0
2	SO4	D	434	5/5	0.46	33.25	103,103,103,103	0
2	SO4	C	448	5/5	0.56	29.05	122,122,123,123	0
3	FLC	B	463	13/13	0.53	23.59	96,97,98,99	0
2	SO4	A	432	5/5	0.26	19.15	118,118,118,118	0
2	SO4	B	458	5/5	0.31	18.98	102,102,102,102	0
2	SO4	C	450	5/5	0.51	16.87	120,120,120,121	0
2	SO4	C	436	5/5	0.28	15.87	108,108,108,108	0
2	SO4	D	437	5/5	0.31	15.80	102,102,103,103	0
2	SO4	B	437	5/5	0.31	15.68	113,113,114,114	0
2	SO4	A	450	5/5	0.67	15.11	131,131,131,131	0
2	SO4	B	444	5/5	0.34	11.10	69,70,71,73	0
2	SO4	B	457	5/5	0.38	10.65	128,128,128,128	0
2	SO4	C	454	5/5	0.27	8.68	90,90,90,92	0
2	SO4	A	451	5/5	0.30	8.47	118,118,118,119	0
3	FLC	A	460	13/13	0.35	7.64	69,73,75,75	0
2	SO4	D	436	5/5	0.17	7.45	89,90,90,90	0
2	SO4	A	435	5/5	0.17	7.38	105,105,105,105	0
2	SO4	B	443	5/5	0.18	7.23	53,54,55,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	447	5/5	0.17	6.29	95,96,96,96	0
2	SO4	D	433	5/5	0.30	6.09	107,107,108,108	0
2	SO4	A	456	5/5	0.16	6.05	104,104,104,105	0
2	SO4	A	446	5/5	0.18	5.79	95,95,96,96	0
2	SO4	B	433	5/5	0.32	5.41	128,128,128,129	0
2	SO4	A	439	5/5	0.14	4.87	100,100,101,101	0
2	SO4	B	454	5/5	0.22	4.53	90,91,91,92	0
2	SO4	C	438	5/5	0.35	4.24	128,128,128,128	0
2	SO4	A	445	5/5	0.21	4.07	90,91,91,92	0
2	SO4	B	436	5/5	0.29	3.96	124,124,124,124	0
2	SO4	C	432	5/5	0.31	3.90	140,140,141,141	0
2	SO4	B	448	5/5	0.28	3.78	99,99,99,100	0
2	SO4	B	453	5/5	0.25	3.73	129,129,129,130	0
2	SO4	A	454	5/5	0.20	3.40	77,78,78,79	0
2	SO4	B	450	5/5	0.28	3.33	121,121,121,121	0
2	SO4	B	438	5/5	0.27	3.23	113,113,113,113	0
2	SO4	B	455	5/5	0.23	3.14	79,79,80,80	0
2	SO4	B	447	5/5	0.19	2.70	126,126,126,126	0
2	SO4	A	453	5/5	0.20	2.69	125,125,125,125	0
2	SO4	A	433	5/5	0.15	2.43	116,116,117,117	0
2	SO4	A	444	5/5	0.18	2.35	56,57,57,57	0
2	SO4	D	449	5/5	0.20	2.30	125,125,125,125	0
2	SO4	B	440	5/5	0.27	2.07	108,108,108,109	0
2	SO4	A	437	5/5	0.13	1.65	68,68,69,69	0
2	SO4	C	440	5/5	0.25	1.44	123,124,124,124	0
2	SO4	B	445	5/5	0.17	1.13	99,100,100,100	0
2	SO4	B	461	5/5	0.17	1.13	76,76,76,77	0
2	SO4	B	456	5/5	0.11	1.10	20,22,23,23	0
2	SO4	C	444	5/5	0.17	1.08	114,114,114,114	0
2	SO4	C	446	5/5	0.27	1.04	136,136,137,137	0
2	SO4	D	441	5/5	0.14	0.99	101,101,101,102	0
2	SO4	A	434	5/5	0.20	0.99	118,118,118,118	0
2	SO4	A	449	5/5	0.10	0.69	18,23,25,25	0
2	SO4	A	442	5/5	0.16	0.69	87,88,88,88	0
2	SO4	C	451	5/5	0.27	0.65	121,121,121,121	0
2	SO4	C	439	5/5	0.13	0.65	91,91,91,91	0
2	SO4	A	440	5/5	0.19	0.53	107,107,107,107	0
2	SO4	A	436	5/5	0.14	0.49	94,94,95,95	0
2	SO4	A	459	5/5	0.17	0.43	114,114,114,114	0
2	SO4	A	443	5/5	0.11	0.38	32,32,35,35	0
2	SO4	D	446	5/5	0.15	0.37	73,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	462	5/5	0.14	0.31	93,93,93,93	0
2	SO4	D	435	5/5	0.15	0.28	99,99,100,100	0
2	SO4	A	458	5/5	0.12	0.05	35,37,39,40	0
2	SO4	D	448	5/5	0.17	-0.01	85,85,86,86	0
2	SO4	A	452	5/5	0.12	-0.04	65,65,66,66	0
2	SO4	B	459	5/5	0.12	-0.04	64,64,66,66	0
2	SO4	C	452	5/5	0.16	-0.05	91,91,91,91	0
2	SO4	B	435	5/5	0.11	-0.09	67,67,68,68	0
2	SO4	C	447	5/5	0.11	-0.11	72,72,73,73	0
2	SO4	C	441	5/5	0.21	-0.18	78,78,79,79	0
2	SO4	C	445	5/5	0.19	-0.20	97,97,97,97	0
2	SO4	B	442	5/5	0.14	-0.24	110,110,110,110	0
2	SO4	A	438	5/5	0.20	-0.25	101,101,101,101	0
2	SO4	D	442	5/5	0.16	-0.26	89,89,89,90	0
2	SO4	B	432	5/5	0.12	-0.31	48,48,49,50	0
2	SO4	A	448	5/5	0.15	-0.31	101,101,101,101	0
2	SO4	D	444	5/5	0.23	-0.39	137,137,138,138	0
2	SO4	C	449	5/5	0.13	-0.43	42,43,44,44	0
2	SO4	B	441	5/5	0.17	-0.44	79,79,79,79	0
2	SO4	C	434	5/5	0.14	-0.47	65,65,66,66	0
2	SO4	D	432	5/5	0.11	-0.48	51,51,52,53	0
2	SO4	D	447	5/5	0.14	-0.63	66,66,67,68	0
2	SO4	A	441	5/5	0.10	-0.67	53,53,54,56	0
2	SO4	C	453	5/5	0.15	-0.91	101,101,101,101	0
2	SO4	D	445	5/5	0.14	-0.92	124,124,124,124	0
2	SO4	C	433	5/5	0.08	-0.94	50,50,51,52	0
2	SO4	B	434	5/5	0.09	-0.96	56,56,57,58	0
2	SO4	B	451	5/5	0.12	-1.02	68,68,68,69	0
2	SO4	D	440	5/5	0.19	-1.12	118,118,118,118	0
2	SO4	D	443	5/5	0.08	-1.14	42,43,45,46	0
2	SO4	A	457	5/5	0.10	-1.14	48,48,49,49	0
2	SO4	C	437	5/5	0.12	-1.20	115,115,115,115	0
2	SO4	B	452	5/5	0.12	-1.34	48,49,50,51	0
4	ZN	B	464	1/1	0.08	-1.48	46,46,46,46	0
2	SO4	D	439	5/5	0.21	-1.59	98,98,98,98	0
4	ZN	B	465	1/1	0.08	-1.66	53,53,53,53	0
2	SO4	D	438	5/5	0.10	-1.71	50,50,51,51	0
2	SO4	A	455	5/5	0.08	-1.73	69,69,70,70	0
2	SO4	C	443	5/5	0.10	-1.87	64,64,65,65	0
4	ZN	A	462	1/1	0.09	-2.10	50,50,50,50	0
2	SO4	C	435	5/5	0.10	-2.18	92,92,92,92	0
2	SO4	B	446	5/5	0.08	-2.25	31,32,33,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	442	5/5	0.14	-2.85	84,84,84,84	0
2	SO4	B	460	5/5	0.06	-3.01	70,71,72,72	0
4	ZN	D	450	1/1	0.04	-4.21	63,63,63,63	0
4	ZN	A	461	1/1	0.06	-4.33	47,47,47,47	0
4	ZN	D	451	1/1	0.04	-4.33	54,54,54,54	0
4	ZN	C	456	1/1	0.06	-5.10	61,61,61,61	0
4	ZN	C	455	1/1	0.05	-8.55	65,65,65,65	0
2	SO4	B	439	5/5	0.20	-	105,105,106,106	0

6.5 Other polymers ⓘ

There are no such residues in this entry.