



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:42 PM UTC

PDB ID : 3IEK / pdb_00003iek
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

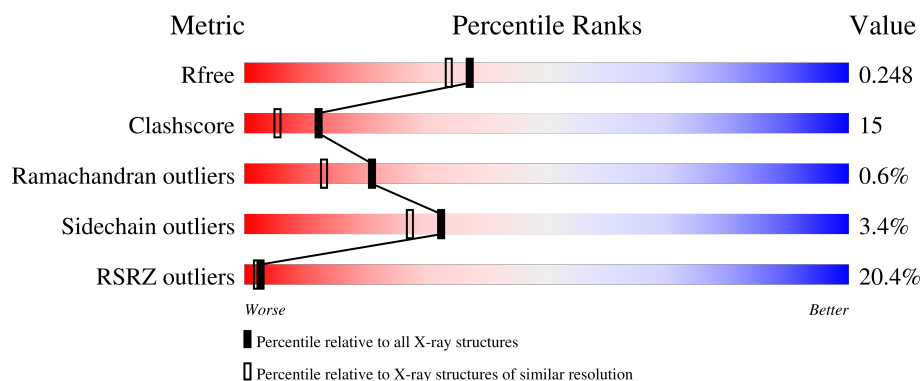
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	431	3% 81% 17% .
1	B	431	4% 74% 25% .
1	C	431	34% 64% 34% .
1	D	431	40% 58% 38% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	450	-	-	X	-
2	SO4	A	451	-	-	X	-
2	SO4	B	453	-	-	X	-
2	SO4	C	454	-	-	X	-
3	FLC	A	460	-	-	X	-
3	FLC	B	463	-	-	X	-

2 Entry composition [i](#)

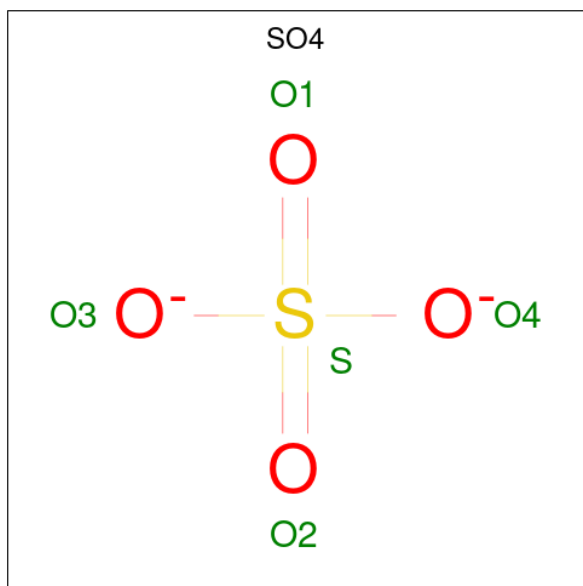
There are 5 unique types of molecules in this entry. The entry contains 14435 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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 (CCD ID: 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		

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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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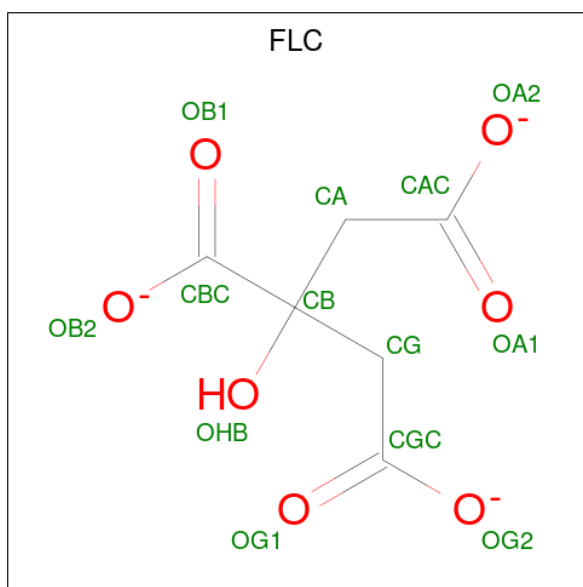
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	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 (CCD ID: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7$).



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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	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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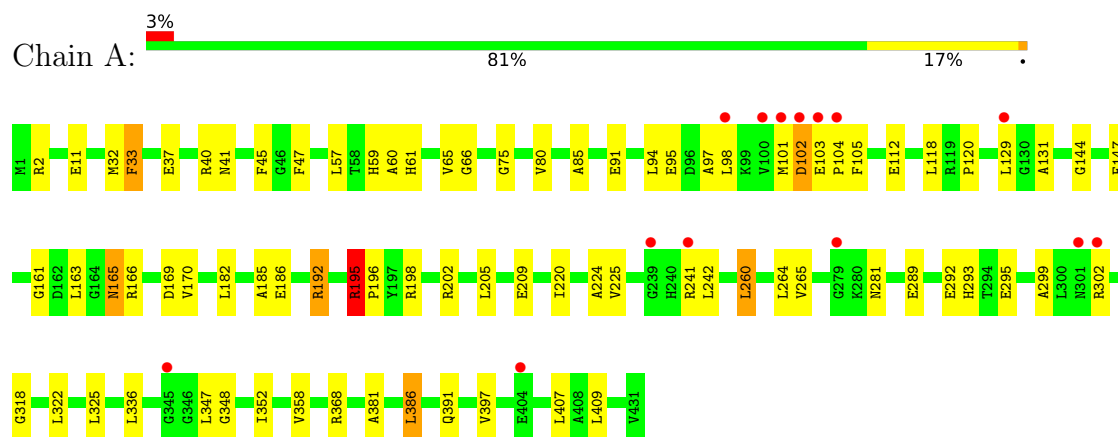
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	79	Total	O	0	0
			79	79		

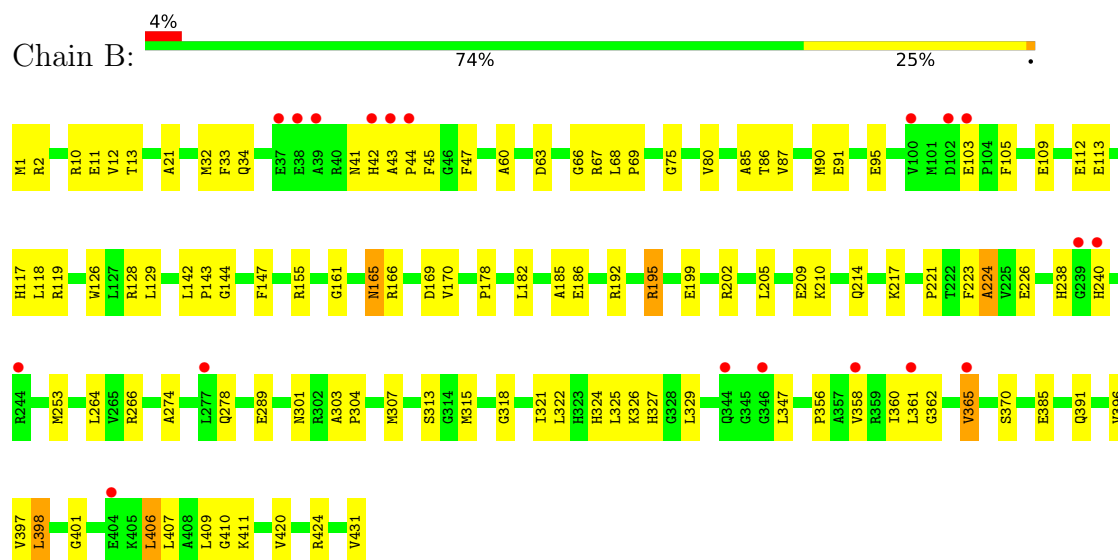
3 Residue-property plots

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

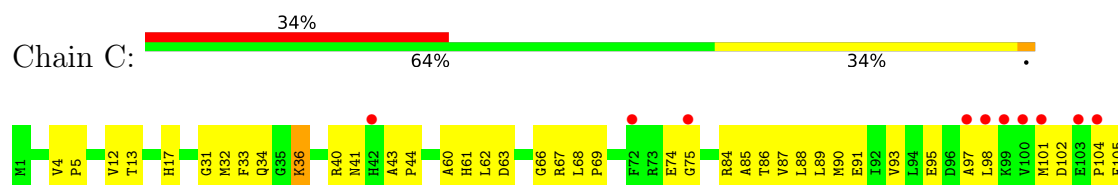
• Molecule 1: Ribonuclease TTHA0252

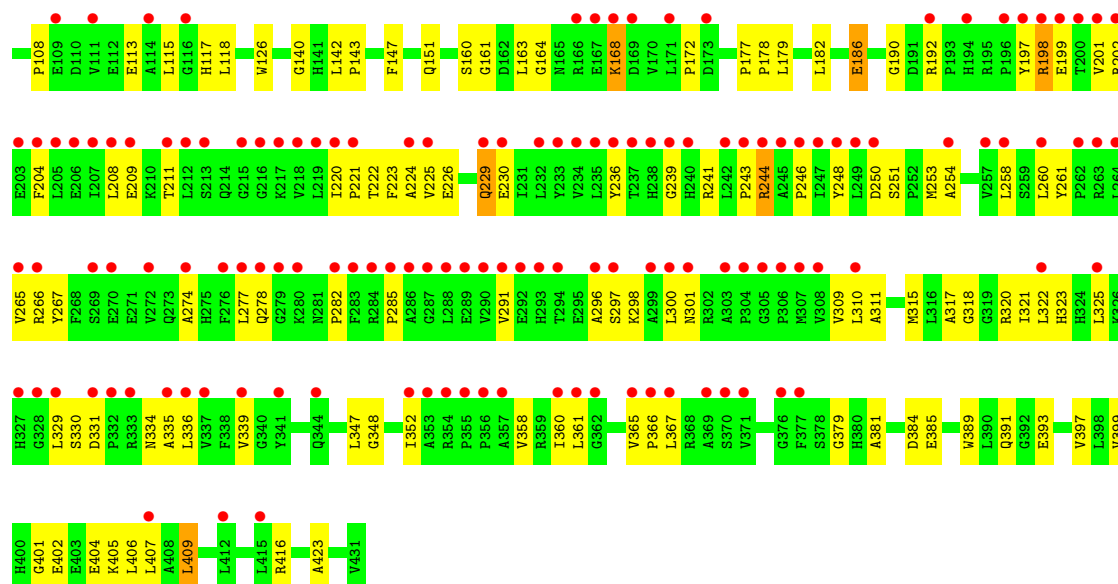


• Molecule 1: Ribonuclease TTHA0252

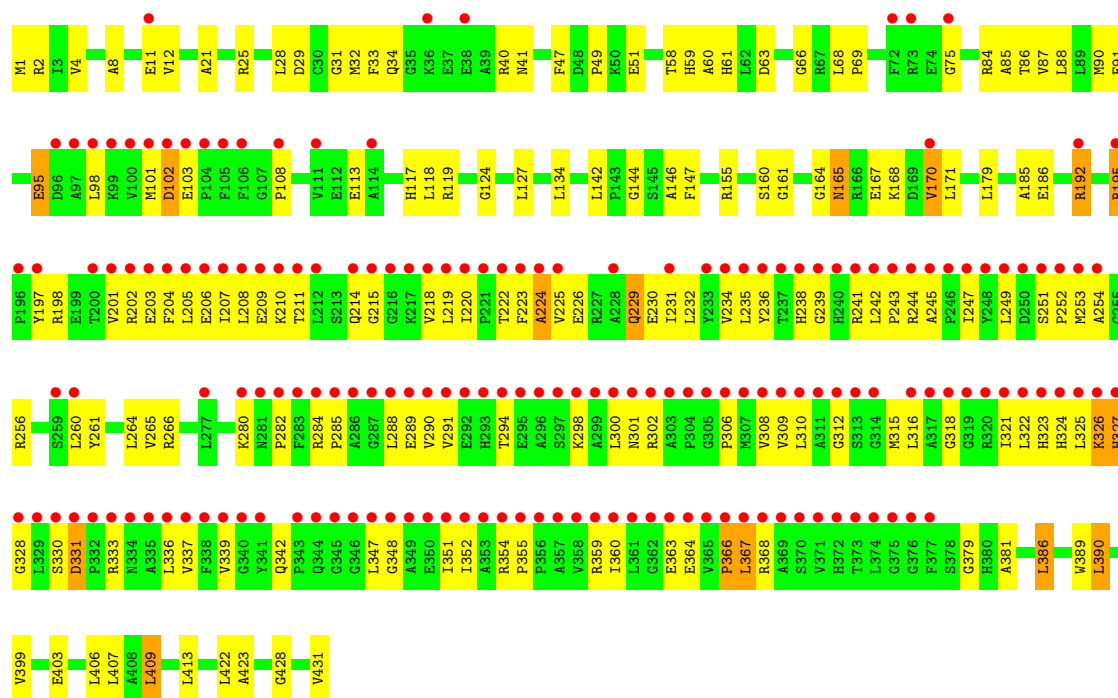
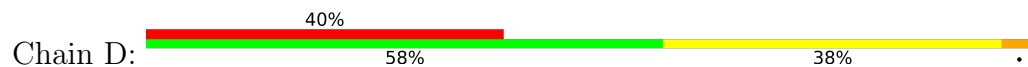


• Molecule 1: Ribonuclease TTHA0252





• Molecule 1: Ribonuclease TTHA0252



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 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.05) 94.4 (50.00-2.05)	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	14389 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/3407	0.96	17/4621 (0.4%)
1	B	0.40	0/3407	0.94	12/4621 (0.3%)
1	C	0.34	0/3407	0.90	11/4621 (0.2%)
1	D	0.34	0/3407	0.89	14/4621 (0.3%)
All	All	0.37	0/13628	0.92	54/18484 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	N-CA-C	9.73	116.89	108.13
1	D	192	ARG	N-CA-C	8.47	115.75	108.13
1	D	225	VAL	N-CA-C	7.77	117.88	110.42
1	A	224	ALA	N-CA-C	7.54	122.48	113.28
1	A	161	GLY	N-CA-C	-7.42	98.30	111.80
1	B	224	ALA	N-CA-C	7.41	122.32	113.28
1	B	192	ARG	N-CA-C	7.38	114.86	108.22
1	A	220	ILE	N-CA-C	7.28	115.36	108.15
1	A	170	VAL	N-CA-C	7.22	118.01	110.72
1	A	60	ALA	N-CA-C	7.10	121.80	113.20
1	B	195	ARG	N-CA-C	-7.00	100.94	109.83
1	B	161	GLY	N-CA-C	-6.95	99.41	111.50
1	B	60	ALA	N-CA-C	6.90	121.53	113.18
1	D	12	VAL	N-CA-C	6.80	117.42	110.82
1	D	161	GLY	N-CA-C	-6.74	99.54	111.80
1	B	170	VAL	N-CA-C	6.68	117.47	110.72
1	A	169	ASP	N-CA-C	6.67	121.70	113.50
1	C	75	GLY	N-CA-C	6.67	120.71	113.58
1	C	60	ALA	N-CA-C	6.53	121.08	113.18
1	A	225	VAL	N-CA-C	6.47	118.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GLY	N-CA-C	6.45	120.70	112.83
1	D	60	ALA	N-CA-C	6.28	120.66	113.19
1	C	161	GLY	N-CA-C	-6.27	100.60	111.50
1	A	147	PHE	N-CA-C	-6.24	100.48	110.14
1	C	225	VAL	N-CA-C	6.18	116.34	110.53
1	D	147	PHE	N-CA-C	-6.09	100.70	110.14
1	B	185	ALA	N-CA-C	5.98	119.28	109.72
1	D	224	ALA	N-CA-C	5.95	120.27	112.89
1	A	265	VAL	N-CA-C	5.89	117.33	110.62
1	A	293	HIS	N-CA-C	5.83	119.06	109.85
1	C	192	ARG	N-CA-C	5.82	115.00	108.25
1	C	160	SER	N-CA-C	5.79	118.54	111.82
1	C	147	PHE	N-CA-C	-5.70	101.76	110.14
1	A	75	GLY	N-CA-C	5.70	121.55	114.37
1	B	169	ASP	N-CA-C	5.69	121.25	113.97
1	D	170	VAL	N-CA-C	5.69	117.20	111.00
1	C	4	VAL	N-CA-C	5.67	113.66	107.60
1	A	33	PHE	N-CA-C	-5.62	101.38	110.32
1	C	393	GLU	CA-C-N	5.57	124.76	118.97
1	C	393	GLU	C-N-CA	5.57	124.76	118.97
1	A	185	ALA	N-CA-C	5.48	118.15	109.50
1	C	66	GLY	N-CA-C	5.44	120.51	113.27
1	D	160	SER	N-CA-C	5.39	118.07	111.82
1	D	66	GLY	N-CA-C	5.27	119.26	112.83
1	A	292	GLU	N-CA-C	5.24	118.14	111.69
1	A	66	GLY	N-CA-C	5.23	120.69	113.99
1	D	4	VAL	N-CA-C	5.21	113.67	107.73
1	B	365	VAL	N-CA-C	5.20	113.16	107.60
1	A	195	ARG	N-CA-C	-5.15	102.98	110.08
1	D	265	VAL	N-CA-C	5.10	116.43	110.62
1	D	185	ALA	N-CA-C	5.09	117.87	109.72
1	B	75	GLY	N-CA-C	5.07	120.75	114.37
1	D	75	GLY	N-CA-C	5.03	121.68	114.64
1	B	147	PHE	N-CA-C	-5.02	101.92	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3351	58	0
1	B	3326	0	3351	87	0
1	C	3326	0	3351	133	0
1	D	3326	0	3351	151	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	6	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	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:H	1:C:244:ARG:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:H	1:A:41:ASN:HD21	1.12	0.90
1:B:87:VAL:HA	1:B:90:MET:HE3	1.53	0.90
1:B:33:PHE:H	1:B:41:ASN:HD21	0.89	0.88
1:A:101:MET:HE3	1:A:104:PRO:HA	1.53	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
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:C:101:MET:HE3	1:C:104:PRO:HA	1.60	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:C:229:GLN:CD	1:C:229:GLN:H	1.90	0.77
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:C:198:ARG:HE	1:C:198:ARG:HA	1.53	0.74
1:D:331:ASP:N	1:D:368:ARG:HB2	2.03	0.74
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.70	0.74
1:D:86:THR:HG22	1:D:90:MET:HE2	1.69	0.73
1:A:120:PRO:CB	2:A:451:SO4:O3	2.35	0.73
1:D:87:VAL:HA	1:D:90:MET:HE3	1.69	0.73
1:C:209:GLU:HG2	1:C:243:PRO:HD3	1.69	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:HA	1:C:198:ARG:NE	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:C:32:MET:HE2	1:C:105:PHE:HZ	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:VAL:HG11	1:D:324:HIS:NE2	2.07	0.69
1:A:131:ALA:HB1	2:A:450:SO4:O1	1.93	0.69
1:C:244:ARG:H	1:C:244:ARG:CD	2.05	0.69
1:D:207:ILE:O	1:D:211:THR:HG22	1.91	0.69
1:D:229:GLN:H	1:D:229:GLN:CD	1.99	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: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:32:MET:HE1	1:D:101:MET:HE1	1.76	0.67
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:B:289:GLU:HG3	5:B:527:HOH:O	1.93	0.67
1:C:168:LYS:HE3	1:C:230:GLU:OE1	1.94	0.67
1:B:87:VAL:HA	1:B:90:MET:CE	2.24	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:A:102:ASP:CG	1:A:103:GLU:H	2.03	0.66
1:D:34:GLN:NE2	1:D:63:ASP:HB3	2.11	0.65
1:C:329:LEU:HD23	1:C:367:LEU:HD13	1.77	0.64
1:D:205:LEU:HD13	1:D:241:ARG:HD2	1.77	0.64
1:D:33:PHE:N	1:D:41:ASN:HD21	1.87	0.64
1:D:195:ARG:H	1:D:195:ARG:HD2	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:B:32:MET:HE2	1:B:105:PHE:HZ	1.64	0.63
1:D:294:THR:HG22	1:D:298:LYS:NZ	2.14	0.63
1:D:309:VAL:C	1:D:310:LEU:HD12	2.24	0.63
1:D:61:HIS:CE1	1:D:142:LEU:HD11	2.34	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:C:86:THR:HG22	1:C:90:MET:CE	2.29	0.61
1:C:404:GLU:CD	1:C:404:GLU:H	2.08	0.61
1:D:34:GLN:HE21	1:D:63:ASP:HB3	1.65	0.61
1:C:33:PHE:H	1:C:41:ASN:ND2	1.93	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:318:GLY:HA2	1:A:322:LEU:HD11	1.83	0.61
1:C:250:ASP:HA	1:C:291:VAL:HB	1.83	0.61
1:D:348:GLY:O	1:D:352:ILE:HG13	2.00	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:90:MET:HE1	1:D:118:LEU:HD22	1.83	0.60
1:B:34:GLN:HE21	1:B:63:ASP:HB3	1.67	0.59
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:D:229:GLN:H	1:D:229:GLN:NE2	1.99	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:101:MET:HE3	1:C:104:PRO:CA	2.31	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:B:385:GLU:CD	5:B:551:HOH:O	2.47	0.58
1:B:326:LYS:HD2	1:B:361:LEU:HB2	1.86	0.57
1:D:155:ARG:NH2	2:D:449:SO4:O1	2.33	0.57
1:D:325:LEU:C	1:D:327:HIS:H	2.11	0.57
1:B:90:MET:HE1	1:B:118:LEU:HD22	1.86	0.57
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.87	0.57
1:D:239:GLY:HA2	1:D:242:LEU:CG	2.34	0.57
1:D:309:VAL:HG11	1:D:324:HIS:CD2	2.39	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:260:LEU:HD22	1:A:264:LEU:HD11	1.85	0.56
1:A:281:ASN:HB2	3:A:460:FLC:OB2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:O	1:D:206:GLU:HG3	2.05	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:B:266:ARG:HG2	5:B:573:HOH:O	2.06	0.55
1:D:223:PHE:CZ	1:D:315:MET:HG3	2.41	0.55
1:B:396:VAL:HG12	1:B:398:LEU:HD13	1.88	0.55
1:D:236:TYR:OH	1:D:280:LYS:HD3	2.05	0.55
1:B:91:GLU:O	1:B:95:GLU:HG2	2.07	0.55
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.88	0.55
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.88	0.55
1:C:322:LEU:HB3	1:C:361:LEU:HD11	1.87	0.55
1:A:289:GLU:HG3	5:A:603:HOH:O	2.07	0.55
1:C:211:THR:HG21	1:C:335:ALA:HB2	1.87	0.55
1:B:223:PHE:HZ	1:B:315:MET:HE2	1.70	0.55
1:B:205:LEU:O	1:B:209:GLU:HG3	2.07	0.55
1:B:401:GLY:HA3	1:B:406:LEU:HD13	1.88	0.55
1:B:202:ARG:NE	2:B:458:SO4:O3	2.35	0.54
1:D:302:ARG:HG2	1:D:302:ARG:HH21	1.70	0.54
1:D:102:ASP:CG	1:D:103:GLU:H	2.14	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:C:236:TYR:HD1	1:C:285:PRO:HA	1.73	0.54
1:D:224:ALA:HB3	1:D:253:MET:CE	2.38	0.54
1:B:362:GLY:N	2:B:451:SO4:O1	2.41	0.54
1:D:84:ARG:HD2	1:D:266:ARG:HH12	1.73	0.53
1:D:244:ARG:HD2	1:D:244:ARG:N	2.24	0.53
1:B:128:ARG:O	1:B:129:LEU:HD23	2.07	0.53
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.90	0.53
1:C:321:ILE:O	1:C:325:LEU:HD13	2.09	0.53
1:D:381:ALA:HB3	1:D:386:LEU:HD13	1.91	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:A:11:GLU:CD	1:A:40:ARG:HH12	2.17	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:B:155:ARG:HD2	1:B:431:VAL:O	2.09	0.52
1:C:86:THR:O	1:C:90:MET:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:THR:HG21	1:C:335:ALA:CB	2.39	0.52
1:C:229:GLN:CD	1:C:229:GLN:N	2.66	0.52
2:A:450:SO4:O2	1:D:179:LEU:HD21	2.09	0.52
1:C:358:VAL:O	1:C:365:VAL:HG22	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:B:165:ASN:HD22	1:B:165:ASN:C	2.16	0.52
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.90	0.52
1:D:165:ASN:C	1:D:165:ASN:HD22	2.18	0.52
1:D:219:LEU:HD12	1:D:219:LEU:N	2.24	0.52
1:B:327:HIS:O	2:B:438:SO4:O4	2.28	0.52
1:C:402:GLU:HB2	1:C:405:LYS:HG2	1.92	0.52
1:D:218:VAL:HB	1:D:308:VAL:HG22	1.92	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:A:166:ARG:NH2	1:A:166:ARG:HB2	2.25	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:D:119:ARG:HD2	5:D:585:HOH:O	2.11	0.51
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.46	0.51
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:B:223:PHE:CZ	1:B:315:MET:HE2	2.46	0.50
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:B:68:LEU:HB3	1:B:69:PRO:HD3	1.93	0.50
1:D:85:ALA:HB3	1:D:144:GLY:HA3	1.94	0.50
1:D:321:ILE:C	1:D:323:HIS:H	2.19	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:C:391:GLN:HA	1:C:416:ARG:NH2	2.26	0.50
1:D:326:LYS:HB2	1:D:360:ILE:HG21	1.93	0.50
1:B:410:GLY:C	3:B:463:FLC:HG2	2.36	0.50
1:D:171:LEU:HD11	1:D:226:GLU:OE1	2.11	0.50
1:D:325:LEU:N	1:D:325:LEU:HD12	2.26	0.50
1:D:336:LEU:HD23	1:D:336:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:HE21	1:C:63:ASP:HB3	1.78	0.49
1:A:102:ASP:CG	1:A:103:GLU:N	2.70	0.49
1:B:210:LYS:O	1:B:214:GLN:HG2	2.13	0.49
1:D:234:VAL:O	1:D:238:HIS:HB2	2.12	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:D:87:VAL:HA	1:D:90:MET:CE	2.40	0.48
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.48	0.48
1:C:98:LEU:C	1:C:98:LEU:HD23	2.37	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:C:86:THR:HG22	1:C:90:MET:HE3	1.94	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:B:113:GLU:OE2	1:B:117:HIS:HE1	1.97	0.48
1:B:318:GLY:HA2	1:B:322:LEU:CD1	2.43	0.48
1:B:398:LEU:HB3	1:B:406:LEU:HG	1.95	0.48
1:C:68:LEU:HB3	1:C:69:PRO:HD3	1.96	0.48
1:D:171:LEU:HD12	1:D:171:LEU:N	2.28	0.48
1:C:190:GLY:HA3	1:C:409:LEU:HB2	1.96	0.48
1:A:33:PHE:N	1:A:41:ASN:HD21	1.94	0.48
1:B:360:ILE:HD12	1:B:365:VAL:HG11	1.96	0.47
1:C:298:LYS:HA	1:C:301:ASN:ND2	2.29	0.47
1:D:203:GLU:O	1:D:207:ILE:HG13	2.13	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:C:36:LYS:HB2	1:C:36:LYS:NZ	2.29	0.47
1:C:246:PRO:HG2	1:C:248:TYR:HE1	1.80	0.47
1:D:253:MET:HA	1:D:256:ARG:NH1	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:A:209:GLU:HG2	1:A:242:LEU:HD23	1.96	0.47
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.15	0.47
1:D:224:ALA:HB3	1:D:253:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:GLY:C	5:D:526:HOH:O	2.57	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:C:88:LEU:HD13	1:C:260:LEU:HD11	1.96	0.46
1:C:163:LEU:HD11	1:C:389:TRP:CE3	2.51	0.46
1:D:1:MET:HB3	1:D:431:VAL:HB	1.97	0.46
1:D:252:PRO:HD2	5:D:495:HOH:O	2.16	0.46
1:D:315:MET:HA	1:D:342:GLN:HE22	1.80	0.46
1:C:221:PRO:HA	1:C:311:ALA:O	2.15	0.46
1:C:32:MET:HE2	1:C:105:PHE:CZ	2.43	0.46
1:A:198:ARG:HH21	1:A:198:ARG:HG3	1.80	0.46
1:B:85:ALA:HB3	1:B:144:GLY:HA3	1.98	0.46
1:D:403:GLU:O	1:D:407:LEU:HD23	2.15	0.46
1:C:265:VAL:HG23	1:C:266:ARG:N	2.31	0.46
1:A:198:ARG:HG3	1:A:198:ARG:NH2	2.31	0.46
1:A:209:GLU:OE2	1:A:241:ARG:NH2	2.48	0.46
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:B:12:VAL:HG23	1:B:13:THR:HG23	1.98	0.45
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	0.45
1:C:89:LEU:O	1:C:93:VAL:HG23	2.16	0.45
1:C:222:THR:HG22	1:C:339:VAL:CG2	2.46	0.45
1:D:363:GLU:CG	1:D:364:GLU:H	2.09	0.45
1:B:396:VAL:O	1:B:420:VAL:HA	2.17	0.45
1:C:239:GLY:C	1:C:241:ARG:H	2.23	0.45
1:C:320:ARG:HA	1:C:323:HIS:HD2	1.81	0.45
1:C:325:LEU:O	1:C:329:LEU:HD13	2.16	0.45
1:D:58:THR:HB	1:D:146:ALA:O	2.17	0.45
1:A:165:ASN:C	1:A:165:ASN:HD22	2.24	0.45
1:B:109:GLU:O	1:B:112:GLU:HG2	2.17	0.45
1:C:204:PHE:CE1	1:C:208:LEU:HD11	2.51	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:B:224:ALA:HB3	1:B:253:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:LEU:HD12	1:D:310:LEU:N	2.32	0.45
1:A:59:HIS:CD2	1:A:61:HIS:H	2.30	0.45
1:A:281:ASN:HB3	3:A:460:FLC:HG2	1.99	0.45
1:D:61:HIS:NE2	1:D:142:LEU:HD11	2.31	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:B:109:GLU:HA	1:B:112:GLU:HG2	1.99	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:D:197:TYR:O	1:D:201:VAL:HG23	2.17	0.45
1:D:209:GLU:C	1:D:211:THR:H	2.25	0.45
1:A:32:MET:HE2	1:A:105:PHE:HZ	1.81	0.44
1:A:59:HIS:HE2	1:A:61:HIS:HB2	1.82	0.44
1:B:34:GLN:NE2	1:B:63:ASP:HB3	2.30	0.44
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.98	0.44
1:C:32:MET:HA	1:C:67:ARG:HG3	1.98	0.44
1:C:98:LEU:HD23	1:C:98:LEU:O	2.16	0.44
1:C:172:PRO:HA	2:C:442:SO4:O3	2.17	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:C:209:GLU:HG2	1:C:243:PRO:CD	2.42	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:A:85:ALA:HB3	1:A:144:GLY:HA3	1.99	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:C:88:LEU:O	1:C:91:GLU:HB3	2.18	0.44
1:D:28:LEU:O	1:D:29:ASP:HB2	2.17	0.44
1:D:86:THR:O	1:D:90:MET:HG3	2.18	0.44
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: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:312:GLY:O	1:D:321:ILE:HB	2.18	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:88:LEU:HD12	1:D:264:LEU:HD21	2.01	0.43
1:D:220:ILE:HG23	1:D:339:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:GLY:HA2	1:D:322:LEU:CD1	2.46	0.43
1:A:281:ASN:CB	3:A:460:FLC:HG2	2.48	0.43
1:D:325:LEU:C	1:D:327:HIS:N	2.76	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: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: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:B:86:THR:HG22	1:B:90:MET:HE2	2.00	0.43
1:C:5:PRO:HA	1:C:17:HIS:HD2	1.83	0.43
1:C:365:VAL:HG23	1:C:365:VAL:O	2.18	0.43
1:D:210:LYS:HG3	1:D:210:LYS:O	2.19	0.43
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.53	0.43
1:C:309:VAL:C	1:C:310:LEU:HD12	2.44	0.43
1:D:90:MET:O	1:D:91:GLU:C	2.62	0.42
1:D:239:GLY:HA2	1:D:242:LEU:CD1	2.49	0.42
1:D:31:GLY:HA3	1:D:63:ASP:C	2.44	0.42
1:C:224:ALA:HB1	1:C:254:ALA:HA	2.02	0.42
1:C:310:LEU:HD12	1:C:310:LEU:N	2.33	0.42
1:B:1:MET:N	2:B:453:SO4:O3	2.43	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:214:GLN:NE2	1:D:333:ARG:HA	2.34	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
1:C:113:GLU:OE2	1:C:117:HIS:HE1	2.03	0.42
1:C:186:GLU:HA	1:C:399:VAL:O	2.19	0.42
1:D:165:ASN:C	1:D:165:ASN:ND2	2.76	0.42
1:D:326:LYS:HD2	1:D:360:ILE:HG22	2.01	0.42
1:B:109:GLU:HA	1:B:112:GLU:OE2	2.20	0.42
1:B:365:VAL:HG13	1:B:365:VAL:O	2.19	0.42
1:D:244:ARG:N	1:D:244:ARG:CD	2.83	0.42
1:A:166:ARG:CB	1:A:166:ARG:HH21	2.33	0.42
1:B:10:ARG:NH1	1:B:424:ARG:HA	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NH2	5:A:479:HOH:O	2.53	0.41
1:C:384:ASP:OD2	1:C:384:ASP:N	2.53	0.41
1:D:102:ASP:CG	1:D:103:GLU:N	2.78	0.41
1:D:224:ALA:HB3	1:D:253:MET:HE2	2.01	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:C:12:VAL:HG23	1:C:13:THR:HG23	2.01	0.41
1:D:389:TRP:CE3	1:D:390:LEU:HD13	2.52	0.41
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.50	0.41
1:C:347:LEU:HD11	1:C:358:VAL:HG11	2.03	0.41
1:C:224:ALA:HB1	1:C:254:ALA:CA	2.50	0.41
1:C:322:LEU:HB3	1:C:361:LEU:CD1	2.51	0.41
1:B:166:ARG:HG2	1:B:385:GLU:CD	2.45	0.41
1:C:151:GLN:HB2	2:C:448:SO4:O3	2.21	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:D:8:ALA:HA	1:D:11:GLU:HG3	2.03	0.41
1:D:25:ARG:NH1	1:D:51:GLU:HB3	2.36	0.41
1:D:232:LEU:HB3	1:D:285:PRO:HD3	2.03	0.41
1:D:284:ARG:HD3	1:D:288:LEU:HD23	2.03	0.41
1:D:285:PRO:HG2	1:D:288:LEU:HB2	2.03	0.41
1:D:316:LEU:CD1	1:D:347:LEU:HD12	2.49	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:D:330:SER:O	1:D:331:ASP:HB2	2.21	0.41
1:C:236:TYR:CD2	1:C:282:PRO:HA	2.56	0.40
1:B:142:LEU:O	1:B:143:PRO:C	2.64	0.40
1:C:360:ILE:HD12	1:C:365:VAL:HG21	2.03	0.40
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.55	0.40
1:D:209:GLU:HG2	1:D:243:PRO:CD	2.41	0.40
1:D:347:LEU:CD1	1:D:351:ILE:HD11	2.51	0.40
1:C:93:VAL:HA	1:C:253:MET:HE1	2.03	0.40
1:A:302:ARG:HD3	1:B:304:PRO:HD2	2.02	0.40
1:A:57:LEU:HD13	1:A:65:VAL:HG12	2.03	0.40
1:C:31:GLY:HA3	1:C:63:ASP:C	2.46	0.40
1:C:229:GLN:HG3	1:C:261:TYR:CE1	2.56	0.40
1:D:113:GLU:OE2	1:D:117:HIS:HE1	2.04	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%)	43	37
1	B	429/431 (100%)	416 (97%)	13 (3%)	0	100	100
1	C	429/431 (100%)	400 (93%)	26 (6%)	3 (1%)	18	10
1	D	429/431 (100%)	394 (92%)	28 (6%)	7 (2%)	7	2
All	All	1716/1724 (100%)	1628 (95%)	77 (4%)	11 (1%)	21	13

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
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%)	27	21
1	B	342/342 (100%)	330 (96%)	12 (4%)	32	27
1	C	342/342 (100%)	333 (97%)	9 (3%)	40	37
1	D	342/342 (100%)	330 (96%)	12 (4%)	32	27
All	All	1368/1368 (100%)	1321 (97%)	47 (3%)	32	27

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	98	LEU
1	A	112	GLU
1	A	163	LEU
1	A	165	ASN
1	A	186	GLU
1	A	192	ARG
1	A	195	ARG
1	A	260	LEU
1	A	325	LEU
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
1	B	329	LEU
1	B	398	LEU
1	B	406	LEU
1	B	407	LEU
1	B	409	LEU
1	C	36	LYS
1	C	40	ARG
1	C	186	GLU
1	C	229	GLN
1	C	244	ARG
1	C	258	LEU
1	C	336	LEU

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Mol	Chain	Res	Type
1	C	407	LEU
1	C	409	LEU
1	D	95	GLU
1	D	127	LEU
1	D	134	LEU
1	D	165	ASN
1	D	186	GLU
1	D	192	ARG
1	D	195	ARG
1	D	229	GLN
1	D	386	LEU
1	D	390	LEU
1	D	406	LEU
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	301	ASN
1	A	344	GLN
1	B	34	GLN
1	B	41	ASN
1	B	165	ASN
1	B	238	HIS
1	B	293	HIS
1	B	391	GLN
1	C	17	HIS
1	C	34	GLN
1	C	41	ASN
1	C	165	ASN
1	C	214	GLN
1	C	278	GLN
1	C	301	ASN
1	C	323	HIS
1	C	372	HIS
1	D	17	HIS
1	D	34	GLN
1	D	41	ASN

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Mol	Chain	Res	Type
1	D	165	ASN
1	D	214	GLN
1	D	229	GLN
1	D	238	HIS
1	D	301	ASN
1	D	323	HIS
1	D	342	GLN
1	D	372	HIS
1	D	383	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	440	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	B	436	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	433	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	444	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	440	-	4,4,4	1.08	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	461	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	C	437	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	442	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	B	456	-	4,4,4	0.99	0	6,6,6	0.55	0
2	SO4	A	447	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	B	447	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	458	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	439	-	4,4,4	1.04	0	6,6,6	0.57	0
2	SO4	A	435	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	459	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	A	444	-	4,4,4	1.09	0	6,6,6	0.55	0
2	SO4	D	435	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	438	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	454	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	453	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	449	-	4,4,4	0.96	0	6,6,6	0.56	0
2	SO4	D	443	-	4,4,4	1.03	0	6,6,6	0.55	0
2	SO4	B	457	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	B	452	-	4,4,4	1.05	0	6,6,6	0.56	0
2	SO4	C	448	-	4,4,4	1.06	0	6,6,6	0.57	0
3	FLC	B	463	-	12,12,12	1.43	2 (16%)	17,17,17	1.36	1 (5%)
2	SO4	C	433	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	442	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	D	434	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	D	441	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	448	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	B	441	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	450	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	440	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	453	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	445	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	D	449	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	451	-	4,4,4	1.04	0	6,6,6	0.58	0
2	SO4	D	446	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	D	442	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	C	442	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	A	452	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	B	435	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	A	440	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	444	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	455	-	4,4,4	1.05	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	448	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	D	438	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	432	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	453	-	4,4,4	1.06	0	6,6,6	0.56	0
2	SO4	C	445	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	458	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	443	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	434	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	446	-	4,4,4	1.04	0	6,6,6	0.55	0
2	SO4	D	445	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	450	-	4,4,4	1.06	0	6,6,6	0.56	0
3	FLC	A	460	-	12,12,12	1.59	5 (41%)	17,17,17	1.35	1 (5%)
2	SO4	A	443	-	4,4,4	1.04	0	6,6,6	0.58	0
2	SO4	A	459	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	433	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	B	460	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	449	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	451	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	450	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	A	457	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	B	438	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	433	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	434	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	437	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	439	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	439	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	435	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	B	432	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	D	444	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	462	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	447	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	B	454	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	446	-	4,4,4	1.05	0	6,6,6	0.57	0
2	SO4	B	439	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	449	-	4,4,4	1.05	0	6,6,6	0.57	0
2	SO4	C	434	-	4,4,4	1.07	0	6,6,6	0.55	0
2	SO4	C	438	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	455	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	441	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	A	432	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	452	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	456	-	4,4,4	1.07	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	448	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	447	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	D	437	-	4,4,4	1.04	0	6,6,6	0.58	0
2	SO4	C	446	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	451	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	441	-	4,4,4	1.04	0	6,6,6	0.58	0
2	SO4	A	437	-	4,4,4	1.10	0	6,6,6	0.57	0
2	SO4	A	454	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	443	-	4,4,4	1.04	0	6,6,6	0.59	0
2	SO4	D	432	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	A	445	-	4,4,4	1.06	0	6,6,6	0.58	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
3	FLC	B	463	-	-	0/16/16/16	-
3	FLC	A	460	-	-	0/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	463	FLC	OG2-CGC	-2.64	1.22	1.30
3	B	463	FLC	OA2-CAC	-2.61	1.22	1.30
3	A	460	FLC	OG2-CGC	-2.49	1.22	1.30
3	A	460	FLC	OA2-CAC	-2.47	1.22	1.30
3	A	460	FLC	CA-CB	2.20	1.56	1.54
3	A	460	FLC	CG-CB	2.15	1.56	1.54
3	A	460	FLC	OB1-CBC	2.00	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	FLC	OB2-CBC-CB	3.92	120.67	113.14
3	B	463	FLC	OB2-CBC-CB	3.89	120.60	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	458	SO4	1	0
2	A	435	SO4	1	0
2	D	435	SO4	1	0
2	C	454	SO4	4	0
2	B	457	SO4	1	0
2	C	448	SO4	1	0
3	B	463	FLC	5	0
2	D	449	SO4	1	0
2	B	451	SO4	1	0
2	D	446	SO4	1	0
2	C	442	SO4	1	0
2	B	455	SO4	1	0
2	B	453	SO4	3	0
3	A	460	FLC	4	0
2	A	451	SO4	2	0
2	A	450	SO4	2	0
2	B	438	SO4	1	0
2	B	454	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.02	14 (3%)	50	50	13, 22, 39, 65	0
1	B	431/431 (100%)	0.23	19 (4%)	39	39	14, 26, 44, 62	0
1	C	431/431 (100%)	1.45	145 (33%)	1	0	17, 45, 75, 91	0
1	D	431/431 (100%)	1.81	173 (40%)	0	0	16, 42, 92, 103	0
All	All	1724/1724 (100%)	0.87	351 (20%)	3	2	13, 31, 78, 103	0

All (351) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	9.1
1	D	325	LEU	8.2
1	D	361	LEU	7.8
1	D	362	GLY	7.5
1	D	328	GLY	7.4
1	D	299	ALA	7.3
1	D	219	LEU	7.1
1	D	296	ALA	7.0
1	C	277	LEU	6.9
1	D	300	LEU	6.9
1	D	366	PRO	6.8
1	D	365	VAL	6.6
1	D	360	ILE	6.3
1	C	335	ALA	6.3
1	D	242	LEU	6.1
1	D	327	HIS	6.1
1	D	208	LEU	6.0
1	D	334	ASN	6.0
1	D	339	VAL	5.9
1	D	367	LEU	5.9
1	D	250	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	42	HIS	5.8
1	D	297	SER	5.7
1	D	330	SER	5.6
1	D	294	THR	5.5
1	D	312	GLY	5.3
1	D	207	ILE	5.3
1	D	338	PHE	5.3
1	D	306	PRO	5.3
1	C	216	GLY	5.2
1	D	358	VAL	5.2
1	D	336	LEU	5.2
1	D	322	LEU	5.1
1	D	249	LEU	5.1
1	D	335	ALA	5.1
1	D	332	PRO	5.0
1	D	248	TYR	5.0
1	C	242	LEU	4.9
1	D	309	VAL	4.9
1	D	220	ILE	4.9
1	D	247	ILE	4.9
1	D	324	HIS	4.9
1	D	321	ILE	4.9
1	C	100	VAL	4.8
1	D	357	ALA	4.8
1	C	205	LEU	4.8
1	D	210	LYS	4.7
1	C	204	PHE	4.7
1	D	369	ALA	4.7
1	D	323	HIS	4.6
1	D	326	LYS	4.6
1	D	347	LEU	4.6
1	D	351	ILE	4.6
1	C	308	VAL	4.6
1	D	239	GLY	4.5
1	D	331	ASP	4.5
1	D	337	VAL	4.5
1	C	245	ALA	4.4
1	C	208	LEU	4.4
1	C	207	ILE	4.4
1	D	240	HIS	4.3
1	D	311	ALA	4.3
1	D	310	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	205	LEU	4.3
1	C	306	PRO	4.3
1	D	246	PRO	4.3
1	D	341	TYR	4.3
1	D	217	LYS	4.2
1	C	291	VAL	4.2
1	D	218	VAL	4.2
1	B	39	ALA	4.2
1	D	286	ALA	4.1
1	C	232	LEU	4.1
1	D	98	LEU	4.1
1	D	302	ARG	4.1
1	C	246	PRO	4.0
1	D	243	PRO	4.0
1	D	356	PRO	4.0
1	C	247	ILE	4.0
1	D	363	GLU	4.0
1	C	101	MET	4.0
1	D	244	ARG	4.0
1	D	236	TYR	3.9
1	D	293	HIS	3.9
1	C	243	PRO	3.9
1	D	307	MET	3.9
1	C	301	ASN	3.9
1	D	290	VAL	3.9
1	C	283	PHE	3.9
1	D	304	PRO	3.9
1	D	204	PHE	3.8
1	C	212	LEU	3.8
1	C	310	LEU	3.8
1	C	415	LEU	3.8
1	C	288	LEU	3.8
1	D	371	VAL	3.8
1	D	223	PHE	3.8
1	C	274	ALA	3.7
1	D	211	THR	3.7
1	D	298	LYS	3.7
1	C	365	VAL	3.7
1	C	367	LEU	3.7
1	C	233	TYR	3.7
1	D	368	ARG	3.7
1	C	236	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	212	LEU	3.6
1	D	104	PRO	3.6
1	D	252	PRO	3.6
1	D	333	ARG	3.6
1	D	100	VAL	3.6
1	D	349	ALA	3.6
1	D	221	PRO	3.6
1	A	302	ARG	3.6
1	D	253	MET	3.5
1	C	198	ARG	3.5
1	D	301	ASN	3.5
1	D	352	ILE	3.5
1	C	239	GLY	3.5
1	D	288	LEU	3.4
1	D	320	ARG	3.4
1	C	211	THR	3.4
1	D	346	GLY	3.4
1	C	280	LYS	3.4
1	C	197	TYR	3.4
1	C	265	VAL	3.4
1	B	43	ALA	3.4
1	C	98	LEU	3.4
1	C	200	THR	3.4
1	D	222	THR	3.4
1	C	215	GLY	3.4
1	D	237	THR	3.3
1	D	291	VAL	3.3
1	D	377	PHE	3.3
1	D	285	PRO	3.3
1	D	305	GLY	3.3
1	D	303	ALA	3.3
1	C	307	MET	3.3
1	A	102	ASP	3.3
1	D	343	PRO	3.3
1	C	234	VAL	3.3
1	D	292	GLU	3.3
1	D	105	PHE	3.3
1	C	370	SER	3.2
1	D	355	PRO	3.2
1	C	371	VAL	3.2
1	D	374	LEU	3.2
1	C	202	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	237	THR	3.2
1	C	240	HIS	3.2
1	C	282	PRO	3.2
1	C	201	VAL	3.2
1	C	218	VAL	3.2
1	D	317	ALA	3.2
1	C	333	ARG	3.2
1	D	364	GLU	3.2
1	D	225	VAL	3.1
1	D	197	TYR	3.1
1	D	214	GLN	3.1
1	C	353	ALA	3.1
1	D	224	ALA	3.1
1	C	305	GLY	3.1
1	D	313	SER	3.1
1	B	277	LEU	3.0
1	C	337	VAL	3.0
1	D	234	VAL	3.0
1	D	215	GLY	3.0
1	D	287	GLY	3.0
1	B	37	GLU	3.0
1	C	99	LYS	3.0
1	C	290	VAL	3.0
1	C	328	GLY	3.0
1	D	295	GLU	3.0
1	C	276	PHE	3.0
1	C	377	PHE	3.0
1	C	357	ALA	3.0
1	D	354	ARG	3.0
1	C	248	TYR	3.0
1	C	369	ALA	2.9
1	C	235	LEU	2.9
1	D	348	GLY	2.9
1	D	200	THR	2.9
1	C	304	PRO	2.9
1	C	103	GLU	2.9
1	C	336	LEU	2.9
1	C	361	LEU	2.9
1	D	319	GLY	2.9
1	D	308	VAL	2.9
1	C	224	ALA	2.9
1	C	219	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	278	GLN	2.9
1	D	359	ARG	2.9
1	D	282	PRO	2.9
1	C	299	ALA	2.9
1	C	303	ALA	2.9
1	C	238	HIS	2.9
1	C	166	ARG	2.8
1	D	201	VAL	2.8
1	C	269	SER	2.8
1	D	233	TYR	2.8
1	A	101	MET	2.8
1	C	171	LEU	2.8
1	D	206	GLU	2.8
1	A	104	PRO	2.8
1	B	244	ARG	2.8
1	D	344	GLN	2.8
1	C	329	LEU	2.8
1	C	262	PRO	2.8
1	B	240	HIS	2.7
1	C	325	LEU	2.7
1	C	257	VAL	2.7
1	D	238	HIS	2.7
1	D	251	SER	2.7
1	C	279	GLY	2.7
1	C	362	GLY	2.7
1	D	284	ARG	2.7
1	D	283	PHE	2.7
1	D	316	LEU	2.7
1	D	373	THR	2.7
1	C	206	GLU	2.7
1	C	293	HIS	2.7
1	C	354	ARG	2.7
1	C	376	GLY	2.7
1	D	314	GLY	2.7
1	C	167	GLU	2.6
1	C	322	LEU	2.6
1	D	101	MET	2.6
1	C	221	PRO	2.6
1	B	365	VAL	2.6
1	C	111	VAL	2.6
1	A	239	GLY	2.6
1	D	228	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	245	ALA	2.6
1	C	300	LEU	2.6
1	D	36	LYS	2.6
1	B	344	GLN	2.6
1	C	72	PHE	2.6
1	A	404	GLU	2.6
1	D	203	GLU	2.6
1	D	209	GLU	2.6
1	C	104	PRO	2.6
1	C	194	HIS	2.5
1	C	294	THR	2.5
1	C	296	ALA	2.5
1	D	75	GLY	2.5
1	D	350	GLU	2.5
1	A	241	ARG	2.5
1	D	241	ARG	2.5
1	C	341	TYR	2.5
1	C	332	PRO	2.5
1	D	353	ALA	2.5
1	B	239	GLY	2.5
1	C	225	VAL	2.4
1	C	407	LEU	2.4
1	D	99	LYS	2.4
1	C	42	HIS	2.4
1	B	100	VAL	2.4
1	D	192	ARG	2.4
1	D	195	ARG	2.4
1	A	98	LEU	2.4
1	D	375	GLY	2.4
1	B	103	GLU	2.4
1	C	272	VAL	2.4
1	D	114	ALA	2.4
1	A	129	LEU	2.4
1	C	264	LEU	2.4
1	A	103	GLU	2.4
1	C	109	GLU	2.4
1	A	100	VAL	2.4
1	D	111	VAL	2.4
1	D	370	SER	2.4
1	C	199	GLU	2.3
1	D	97	ALA	2.3
1	B	361	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	344	GLN	2.3
1	D	340	GLY	2.3
1	D	102	ASP	2.3
1	D	106	PHE	2.3
1	D	289	GLU	2.3
1	A	279	GLY	2.3
1	C	352	ILE	2.3
1	D	231	ILE	2.3
1	D	72	PHE	2.3
1	B	44	PRO	2.3
1	C	355	PRO	2.3
1	C	97	ALA	2.3
1	C	114	ALA	2.3
1	D	254	ALA	2.3
1	D	318	GLY	2.3
1	D	345	GLY	2.3
1	C	203	GLU	2.2
1	C	297	SER	2.2
1	C	356	PRO	2.2
1	D	170	VAL	2.2
1	C	192	ARG	2.2
1	D	281	ASN	2.2
1	C	75	GLY	2.2
1	C	286	ALA	2.2
1	C	287	GLY	2.2
1	C	289	GLU	2.2
1	A	301	ASN	2.2
1	D	280	LYS	2.2
1	D	96	ASP	2.2
1	C	209	GLU	2.2
1	D	38	GLU	2.2
1	C	339	VAL	2.2
1	D	11	GLU	2.2
1	D	372	HIS	2.2
1	C	260	LEU	2.2
1	D	235	LEU	2.2
1	B	102	ASP	2.2
1	C	250	ASP	2.2
1	C	366	PRO	2.1
1	D	196	PRO	2.1
1	B	38	GLU	2.1
1	C	270	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	358	VAL	2.1
1	C	229	GLN	2.1
1	C	327	HIS	2.1
1	C	258	LEU	2.1
1	C	266	ARG	2.1
1	C	412	LEU	2.1
1	D	277	LEU	2.1
1	C	213	SER	2.1
1	C	292	GLU	2.1
1	C	220	ILE	2.1
1	B	346	GLY	2.1
1	D	260	LEU	2.1
1	D	103	GLU	2.1
1	C	169	ASP	2.1
1	C	173	ASP	2.1
1	C	331	ASP	2.1
1	C	263	ARG	2.1
1	C	230	GLU	2.1
1	C	196	PRO	2.1
1	C	285	PRO	2.1
1	D	108	PRO	2.1
1	C	116	GLY	2.1
1	C	217	LYS	2.1
1	C	360	ILE	2.1
1	C	244	ARG	2.0
1	C	284	ARG	2.0
1	D	73	ARG	2.0
1	A	345	GLY	2.0
1	D	216	GLY	2.0
1	D	376	GLY	2.0
1	B	404	GLU	2.0
1	D	259	SER	2.0
1	C	254	ALA	2.0
1	C	249	LEU	2.0
1	D	202	ARG	2.0
1	C	168	LYS	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	440	5/5	0.42	0.16	118,118,118,118	0
2	SO4	D	434	5/5	0.51	0.15	103,103,103,103	0
2	SO4	D	449	5/5	0.52	0.17	125,125,125,125	0
2	SO4	C	440	5/5	0.55	0.18	123,124,124,124	0
2	SO4	D	444	5/5	0.55	0.23	137,137,138,138	0
2	SO4	B	439	5/5	0.55	0.16	105,105,106,106	0
2	SO4	C	446	5/5	0.56	0.15	136,136,137,137	0
2	SO4	B	453	5/5	0.58	0.28	129,129,129,130	0
2	SO4	D	433	5/5	0.58	0.16	107,107,108,108	0
2	SO4	A	434	5/5	0.58	0.16	118,118,118,118	0
2	SO4	B	457	5/5	0.59	0.32	128,128,128,128	0
2	SO4	D	445	5/5	0.59	0.16	124,124,124,124	0
2	SO4	B	450	5/5	0.59	0.20	121,121,121,121	0
2	SO4	B	447	5/5	0.61	0.19	126,126,126,126	0
2	SO4	A	433	5/5	0.61	0.17	116,116,117,117	0
2	SO4	C	444	5/5	0.62	0.14	114,114,114,114	0
3	FLC	A	460	13/13	0.62	0.27	69,73,75,75	0
2	SO4	A	450	5/5	0.63	0.19	131,131,131,131	0
2	SO4	C	451	5/5	0.63	0.16	121,121,121,121	0
2	SO4	C	432	5/5	0.63	0.24	140,140,141,141	0
2	SO4	A	432	5/5	0.65	0.17	118,118,118,118	0
2	SO4	A	454	5/5	0.66	0.20	77,78,78,79	0
2	SO4	B	445	5/5	0.66	0.17	99,100,100,100	0
2	SO4	C	437	5/5	0.67	0.16	115,115,115,115	0
2	SO4	C	436	5/5	0.67	0.15	108,108,108,108	0
2	SO4	A	445	5/5	0.69	0.20	90,91,91,92	0
2	SO4	B	436	5/5	0.69	0.20	124,124,124,124	0
2	SO4	A	446	5/5	0.70	0.19	95,95,96,96	0
2	SO4	A	453	5/5	0.70	0.17	125,125,125,125	0
2	SO4	B	433	5/5	0.71	0.21	128,128,128,129	0
2	SO4	A	442	5/5	0.71	0.19	87,88,88,88	0
2	SO4	C	453	5/5	0.71	0.12	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	435	5/5	0.71	0.11	105,105,105,105	0
2	SO4	C	435	5/5	0.71	0.14	92,92,92,92	0
2	SO4	B	462	5/5	0.72	0.15	93,93,93,93	0
2	SO4	A	436	5/5	0.72	0.19	94,94,95,95	0
2	SO4	A	459	5/5	0.72	0.22	114,114,114,114	0
2	SO4	B	437	5/5	0.72	0.16	113,113,114,114	0
2	SO4	D	436	5/5	0.72	0.13	89,90,90,90	0
2	SO4	C	438	5/5	0.73	0.20	128,128,128,128	0
2	SO4	A	451	5/5	0.73	0.30	118,118,118,119	0
2	SO4	D	448	5/5	0.74	0.14	85,85,86,86	0
2	SO4	D	441	5/5	0.75	0.17	101,101,101,102	0
2	SO4	B	448	5/5	0.75	0.15	99,99,99,100	0
2	SO4	D	435	5/5	0.75	0.15	99,99,100,100	0
2	SO4	B	438	5/5	0.76	0.22	113,113,113,113	0
2	SO4	B	440	5/5	0.76	0.20	108,108,108,109	0
2	SO4	C	442	5/5	0.78	0.17	84,84,84,84	0
2	SO4	A	440	5/5	0.78	0.18	107,107,107,107	0
2	SO4	A	456	5/5	0.78	0.19	104,104,104,105	0
2	SO4	C	441	5/5	0.78	0.14	78,78,79,79	0
2	SO4	C	445	5/5	0.79	0.15	97,97,97,97	0
2	SO4	B	442	5/5	0.79	0.18	110,110,110,110	0
2	SO4	C	439	5/5	0.79	0.12	91,91,91,91	0
2	SO4	C	452	5/5	0.79	0.15	91,91,91,91	0
2	SO4	C	454	5/5	0.80	0.26	90,90,90,92	0
2	SO4	A	438	5/5	0.80	0.17	101,101,101,101	0
2	SO4	B	458	5/5	0.80	0.13	102,102,102,102	0
2	SO4	B	449	5/5	0.80	0.17	84,86,86,86	0
2	SO4	B	454	5/5	0.81	0.18	90,91,91,92	0
2	SO4	B	441	5/5	0.81	0.13	79,79,79,79	0
2	SO4	A	448	5/5	0.81	0.15	101,101,101,101	0
2	SO4	B	444	5/5	0.81	0.24	69,70,71,73	0
2	SO4	C	448	5/5	0.81	0.31	122,122,123,123	0
2	SO4	D	442	5/5	0.82	0.13	89,89,89,90	0
2	SO4	B	461	5/5	0.82	0.15	76,76,76,77	0
2	SO4	D	437	5/5	0.82	0.26	102,102,103,103	0
2	SO4	B	455	5/5	0.83	0.16	79,79,80,80	0
2	SO4	A	447	5/5	0.83	0.18	95,96,96,96	0
2	SO4	A	437	5/5	0.83	0.15	68,68,69,69	0
2	SO4	D	439	5/5	0.83	0.12	98,98,98,98	0
3	FLC	B	463	13/13	0.83	0.41	96,97,98,99	0
2	SO4	B	451	5/5	0.84	0.15	68,68,68,69	0
2	SO4	C	447	5/5	0.84	0.12	72,72,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	447	5/5	0.86	0.15	66,66,67,68	0
2	SO4	C	450	5/5	0.86	0.31	120,120,120,121	0
2	SO4	B	434	5/5	0.86	0.12	56,56,57,58	0
2	SO4	A	452	5/5	0.86	0.13	65,65,66,66	0
2	SO4	A	439	5/5	0.86	0.12	100,100,101,101	0
2	SO4	B	459	5/5	0.87	0.14	64,64,66,66	0
2	SO4	A	444	5/5	0.87	0.12	56,57,57,57	0
2	SO4	D	446	5/5	0.88	0.11	73,73,74,74	0
2	SO4	C	434	5/5	0.89	0.12	65,65,66,66	0
2	SO4	A	455	5/5	0.89	0.11	69,69,70,70	0
2	SO4	B	443	5/5	0.89	0.17	53,54,55,56	0
2	SO4	B	460	5/5	0.90	0.10	70,71,72,72	0
2	SO4	C	443	5/5	0.91	0.09	64,64,65,65	0
2	SO4	D	432	5/5	0.92	0.12	51,51,52,53	0
2	SO4	B	435	5/5	0.92	0.09	67,67,68,68	0
2	SO4	C	433	5/5	0.93	0.11	50,50,51,52	0
2	SO4	B	452	5/5	0.94	0.10	48,49,50,51	0
2	SO4	B	432	5/5	0.94	0.10	48,48,49,50	0
4	ZN	C	455	1/1	0.94	0.13	65,65,65,65	0
2	SO4	A	441	5/5	0.95	0.09	53,53,54,56	0
2	SO4	D	438	5/5	0.95	0.10	50,50,51,51	0
2	SO4	D	443	5/5	0.95	0.09	42,43,45,46	0
2	SO4	A	457	5/5	0.96	0.09	48,48,49,49	0
4	ZN	A	462	1/1	0.97	0.22	50,50,50,50	0
4	ZN	B	465	1/1	0.97	0.18	53,53,53,53	0
2	SO4	C	449	5/5	0.97	0.07	42,43,44,44	0
4	ZN	C	456	1/1	0.97	0.09	61,61,61,61	0
4	ZN	D	450	1/1	0.97	0.13	63,63,63,63	0
4	ZN	B	464	1/1	0.98	0.17	46,46,46,46	0
2	SO4	B	446	5/5	0.98	0.08	31,32,33,34	0
2	SO4	A	443	5/5	0.98	0.14	32,32,35,35	0
2	SO4	A	449	5/5	0.98	0.05	18,23,25,25	0
2	SO4	A	458	5/5	0.98	0.06	35,37,39,40	0
4	ZN	D	451	1/1	0.98	0.13	54,54,54,54	0
4	ZN	A	461	1/1	0.99	0.14	47,47,47,47	0
2	SO4	B	456	5/5	0.99	0.05	20,22,23,23	0

6.5 Other polymers

There are no such residues in this entry.