



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 8TTK / pdb_00008ttk
Title : Tryptophan-6-halogenase BorH apo structure
Authors : Lingkon, K.; Bellizzi, J.J.
Deposited on : 2023-08-14
Resolution : 1.98 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

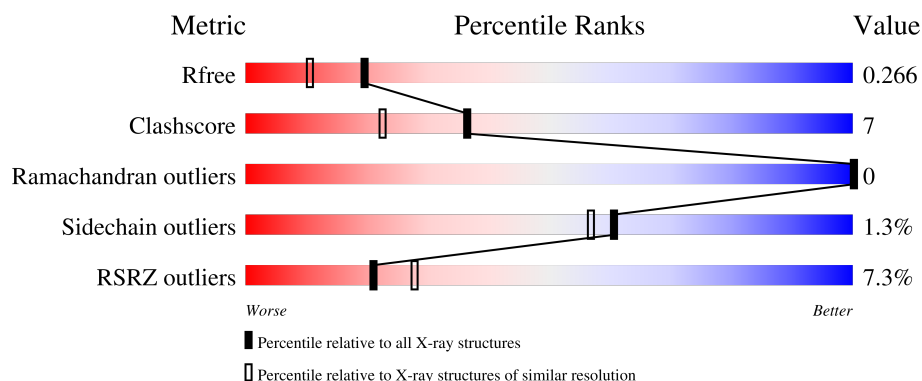
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	529	4% 87% 11% .
1	B	529	8% 81% 16% .
1	C	529	6% 82% 15% .
1	D	529	11% 81% 16% ..

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	605	-	-	X	-

2 Entry composition [i](#)

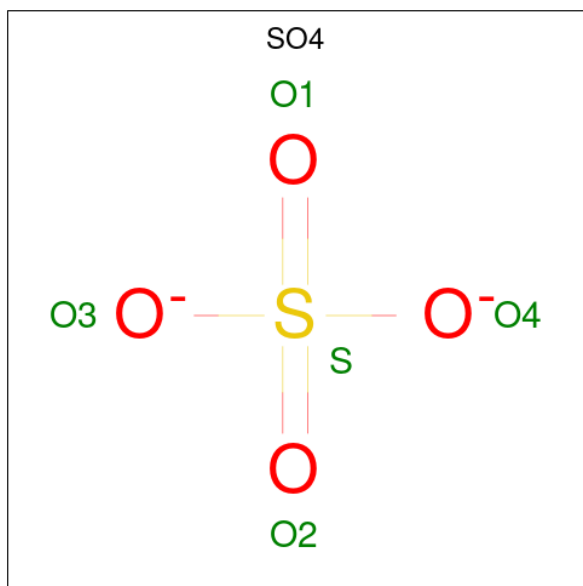
There are 3 unique types of molecules in this entry. The entry contains 17756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophan 6-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4188	2671	736	760	21			
1	B	519	Total	C	N	O	S	0	0	0
			4159	2656	728	754	21			
1	C	519	Total	C	N	O	S	0	1	0
			4156	2655	724	755	22			
1	D	517	Total	C	N	O	S	0	1	0
			4145	2648	727	748	22			

- 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	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	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		

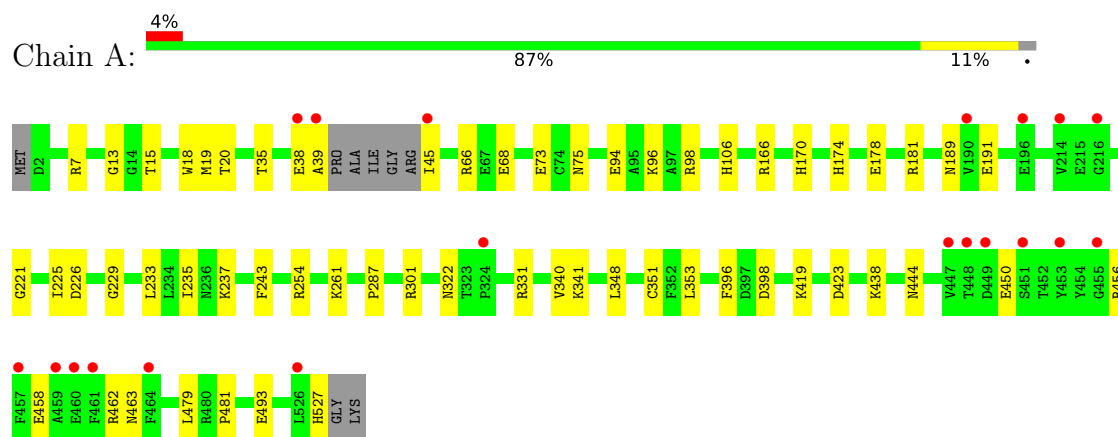
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	344	Total	O	0	0
			344	344		
3	B	306	Total	O	0	0
			306	306		
3	C	216	Total	O	0	0
			216	216		
3	D	162	Total	O	0	0
			162	162		

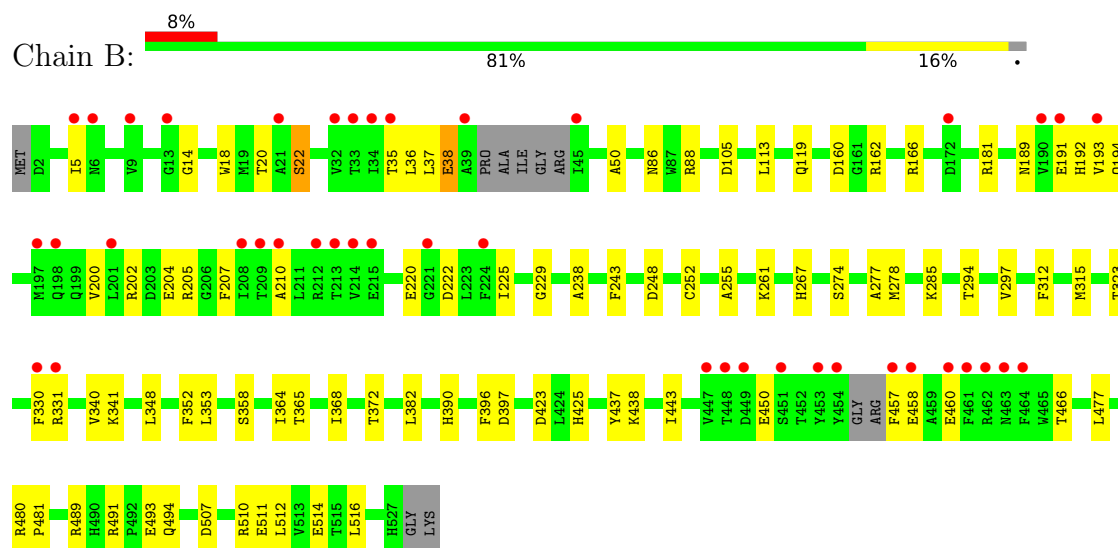
3 Residue-property plots

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.

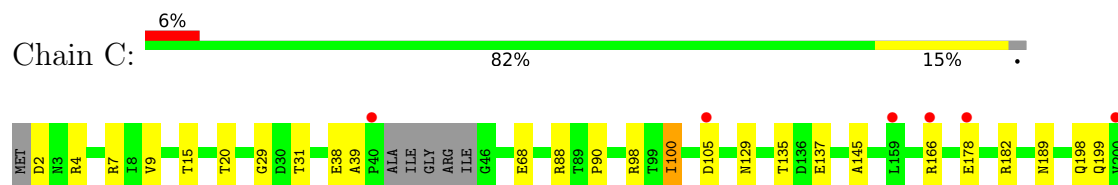
• Molecule 1: Tryptophan 6-halogenase

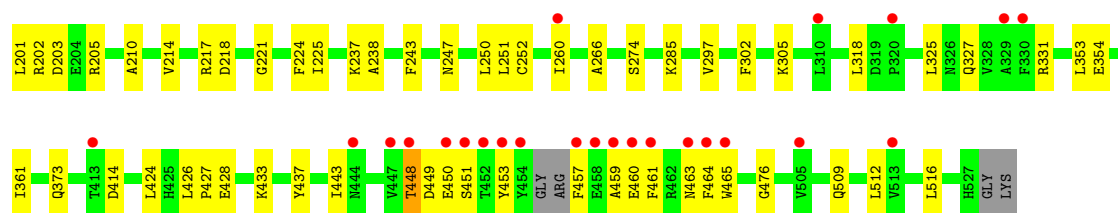


• Molecule 1: Tryptophan 6-halogenase

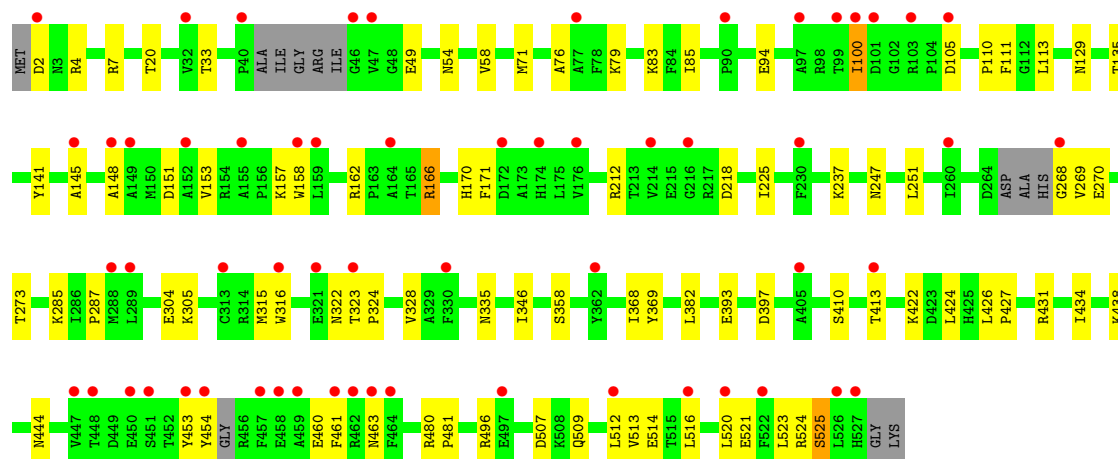
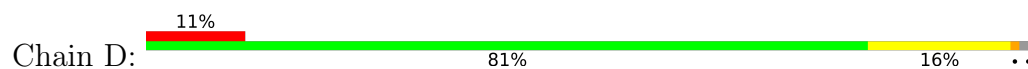


• Molecule 1: Tryptophan 6-halogenase





● Molecule 1: Tryptophan 6-halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.74Å 157.58Å 112.97Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	37.92 – 1.98 37.92 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.0 (37.92-1.98) 95.0 (37.92-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.221 , 0.249 (Not available) , 0.266	Depositor DCC
R_{free} test set	2000 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17756	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 19.48% 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

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	0.16	0/4305	0.36	0/5844
1	B	0.16	0/4275	0.35	0/5805
1	C	0.15	0/4276	0.34	0/5808
1	D	0.14	0/4263	0.33	0/5787
All	All	0.15	0/17119	0.35	0/23244

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4188	0	4029	42	0
1	B	4159	0	3993	61	0
1	C	4156	0	3983	67	0
1	D	4145	0	3986	64	0
2	A	30	0	0	3	0
2	B	25	0	0	2	0
2	C	10	0	0	1	0
2	D	15	0	0	0	0
3	A	344	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	306	0	0	22	0
3	C	216	0	0	36	0
3	D	162	0	0	21	1
All	All	17756	0	15991	237	1

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 7.

All (237) 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:D:4:ARG:NH1	3:D:702:HOH:O	2.05	0.90
2:C:601:SO4:O2	3:C:701:HOH:O	1.89	0.89
1:D:315:MET:O	3:D:701:HOH:O	1.89	0.89
1:C:2:ASP:N	3:C:711:HOH:O	2.07	0.85
1:C:218:ASP:O	3:C:702:HOH:O	1.94	0.85
1:D:480:ARG:NH2	3:D:706:HOH:O	2.09	0.84
1:C:354:GLU:OE2	3:C:705:HOH:O	1.97	0.82
1:C:305:LYS:NZ	3:C:713:HOH:O	2.11	0.82
1:C:199:GLN:OE1	3:C:704:HOH:O	1.96	0.81
1:B:372:THR:O	3:B:701:HOH:O	1.99	0.80
1:B:466:THR:OG1	3:B:702:HOH:O	2.00	0.79
1:C:203:ASP:OD2	1:C:205:ARG:NH1	2.16	0.79
1:B:323:THR:O	3:B:703:HOH:O	2.00	0.78
1:C:460:GLU:O	3:C:706:HOH:O	2.00	0.78
1:B:119:GLN:NE2	3:B:705:HOH:O	2.08	0.78
1:C:453:TYR:OH	3:C:703:HOH:O	1.96	0.75
1:C:459:ALA:O	3:C:708:HOH:O	2.04	0.75
1:C:464:PHE:O	3:C:707:HOH:O	2.02	0.75
1:C:238:ALA:O	3:C:709:HOH:O	2.05	0.75
2:B:602:SO4:O1	3:B:704:HOH:O	2.04	0.75
1:C:217:ARG:NH1	3:C:702:HOH:O	2.20	0.74
1:D:304:GLU:OE1	3:D:703:HOH:O	2.05	0.74
2:A:604:SO4:O1	3:A:701:HOH:O	2.05	0.73
1:C:463:ASN:O	3:C:703:HOH:O	2.05	0.73
1:C:68:GLU:OE2	3:C:710:HOH:O	2.05	0.73
1:A:73:GLU:OE1	3:A:704:HOH:O	2.07	0.73
1:B:491:ARG:NH1	3:B:706:HOH:O	2.10	0.73
1:A:398:ASP:OD1	3:A:702:HOH:O	2.05	0.73
1:A:94:GLU:OE1	3:A:703:HOH:O	2.06	0.73
1:D:393:GLU:OE1	3:D:704:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:ND2	3:A:707:HOH:O	2.25	0.70
1:C:448:THR:O	3:C:712:HOH:O	2.10	0.70
1:D:480:ARG:NH2	3:D:714:HOH:O	2.24	0.69
1:D:397:ASP:OD2	3:D:705:HOH:O	2.09	0.68
1:B:397:ASP:OD2	3:B:707:HOH:O	2.11	0.68
1:C:437:TYR:HB2	1:C:443:ILE:HD11	1.76	0.67
1:D:2:ASP:N	3:D:715:HOH:O	2.26	0.67
1:B:480:ARG:NH2	3:B:713:HOH:O	2.28	0.67
1:A:398:ASP:OD1	3:A:705:HOH:O	2.13	0.67
1:D:71:MET:SD	3:D:752:HOH:O	2.52	0.66
1:B:248:ASP:OD2	3:B:708:HOH:O	2.14	0.65
1:C:461:PHE:O	3:C:715:HOH:O	2.13	0.65
1:B:181:ARG:NH2	3:B:717:HOH:O	2.30	0.65
1:A:189:ASN:ND2	3:A:709:HOH:O	2.30	0.65
1:B:50:ALA:O	3:B:709:HOH:O	2.14	0.65
1:C:145:ALA:HA	1:C:509:GLN:HG3	1.79	0.65
1:D:444:ASN:ND2	1:D:463:ASN:OD1	2.30	0.65
1:C:137:GLU:OE1	3:C:716:HOH:O	2.15	0.64
1:D:100:ILE:HD11	1:D:105:ASP:HA	1.78	0.64
1:C:373:GLN:NE2	3:C:724:HOH:O	2.27	0.64
1:C:39:ALA:O	3:C:717:HOH:O	2.15	0.64
1:B:341:LYS:NZ	3:B:719:HOH:O	2.32	0.63
1:C:426:LEU:HD12	1:C:427:PRO:HD2	1.81	0.62
1:B:494:GLN:HG3	3:B:715:HOH:O	1.99	0.62
1:A:166:ARG:HH21	1:A:450:GLU:HG2	1.64	0.61
1:C:68:GLU:H	1:C:68:GLU:CD	2.08	0.61
1:D:71:MET:HG2	1:D:76:ALA:HB3	1.83	0.60
1:A:254:ARG:NH2	3:A:711:HOH:O	2.31	0.60
1:C:189:ASN:ND2	3:C:725:HOH:O	2.29	0.60
1:B:20:THR:HG21	1:B:225:ILE:HG21	1.83	0.59
1:D:166:ARG:HD3	1:D:454:TYR:CE2	2.37	0.59
1:C:457:PHE:N	3:C:730:HOH:O	2.35	0.58
1:B:460:GLU:OE2	3:B:710:HOH:O	2.17	0.58
1:C:7:ARG:HB2	1:C:221:GLY:HA2	1.86	0.57
1:D:461:PHE:O	3:D:709:HOH:O	2.17	0.57
1:B:297:VAL:HG13	1:B:330:PHE:HE2	1.68	0.57
1:B:189:ASN:ND2	3:B:712:HOH:O	2.27	0.57
1:D:507:ASP:OD1	3:D:708:HOH:O	2.17	0.56
1:A:181:ARG:NH2	3:A:715:HOH:O	2.34	0.56
1:C:464:PHE:HB2	3:C:706:HOH:O	2.05	0.55
1:B:438:LYS:NZ	3:B:714:HOH:O	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:PHE:N	3:C:706:HOH:O	2.30	0.55
1:C:305:LYS:HD3	1:C:327:GLN:HG2	1.89	0.55
1:D:496:ARG:NH2	3:D:720:HOH:O	2.40	0.54
1:A:39:ALA:HB3	3:A:969:HOH:O	2.08	0.54
1:A:166:ARG:NH2	1:A:450:GLU:HG2	2.23	0.53
1:B:210:ALA:HB2	1:B:220:GLU:HG2	1.91	0.53
1:B:160:ASP:OD1	1:B:162:ARG:HG3	2.09	0.53
1:B:489:ARG:NE	3:B:723:HOH:O	2.39	0.53
1:D:166:ARG:HD3	1:D:454:TYR:CD2	2.44	0.53
1:B:113:LEU:HG	1:B:450:GLU:HG3	1.91	0.53
1:A:20:THR:HG21	1:A:225:ILE:HG21	1.91	0.52
1:A:340:VAL:HG12	1:A:341:LYS:HG3	1.90	0.52
1:D:212:ARG:NH1	1:D:218:ASP:OD1	2.42	0.52
1:A:66:ARG:NE	2:A:605:SO4:O4	2.42	0.52
1:B:507:ASP:O	1:B:511:GLU:HG3	2.09	0.52
1:C:251:LEU:HD13	1:C:302:PHE:HE2	1.74	0.52
1:D:145:ALA:HA	1:D:509:GLN:HG3	1.92	0.52
1:A:7:ARG:HB2	1:A:221:GLY:HA2	1.91	0.52
1:A:229:GLY:HA2	1:A:348:LEU:HB2	1.91	0.52
1:D:20:THR:HG21	1:D:225:ILE:HG21	1.91	0.52
1:D:157:LYS:NZ	3:D:717:HOH:O	2.32	0.52
1:D:346:ILE:HD13	1:D:368:ILE:HG13	1.93	0.51
1:B:243:PHE:CZ	1:B:331:ARG:HG2	2.45	0.51
1:B:255:ALA:HB2	1:B:330:PHE:CZ	2.46	0.51
1:C:4:ARG:NE	3:C:719:HOH:O	2.41	0.51
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.92	0.51
1:C:198:GLN:HG2	1:C:199:GLN:HG3	1.92	0.51
1:C:433:LYS:NZ	3:C:740:HOH:O	2.44	0.51
1:D:513:VAL:HG13	1:D:514:GLU:HG3	1.93	0.51
1:B:425:HIS:ND1	2:B:605:SO4:O1	2.44	0.50
1:B:423:ASP:HB2	3:B:751:HOH:O	2.12	0.50
1:C:428:GLU:OE1	3:C:718:HOH:O	2.19	0.50
1:D:54:ASN:O	1:D:58:VAL:HG12	2.10	0.50
1:D:148:ALA:HB2	1:D:509:GLN:HG2	1.94	0.50
1:C:202:ARG:NH2	3:C:741:HOH:O	2.44	0.49
1:A:301:ARG:NH2	3:A:726:HOH:O	2.41	0.49
1:C:237:LYS:HE2	1:C:237:LYS:HA	1.93	0.49
1:D:158:TRP:HE3	1:D:162:ARG:HB3	1.77	0.49
1:A:174:HIS:O	1:A:178:GLU:HG2	2.13	0.49
1:B:5:ILE:HG23	1:B:222:ASP:HB2	1.94	0.49
1:B:18:TRP:CZ2	1:B:181:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:THR:O	3:C:719:HOH:O	2.20	0.49
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.95	0.49
1:C:318:LEU:HA	3:C:738:HOH:O	2.13	0.49
1:D:110:PRO:O	3:D:711:HOH:O	2.20	0.49
1:D:512:LEU:HD22	1:D:516:LEU:HD11	1.95	0.49
1:D:323:THR:O	3:D:710:HOH:O	2.20	0.48
1:D:285:LYS:HD2	1:D:316:TRP:HH2	1.76	0.48
1:A:94:GLU:OE2	1:A:98:ARG:NH1	2.43	0.48
1:A:419:LYS:NZ	3:A:725:HOH:O	2.40	0.48
1:C:20:THR:HG21	1:C:225:ILE:HG21	1.96	0.48
1:C:449:ASP:O	1:C:453:TYR:N	2.47	0.48
1:B:200:VAL:HG12	1:B:202:ARG:HG3	1.95	0.48
1:B:204:GLU:H	1:B:204:GLU:CD	2.22	0.48
1:A:419:LYS:HE3	1:A:419:LYS:HB2	1.67	0.48
1:D:268:GLY:N	3:D:726:HOH:O	2.47	0.47
1:D:49:GLU:N	1:D:171:PHE:O	2.44	0.47
1:B:88:ARG:HD3	1:B:477:LEU:C	2.39	0.47
1:C:15:THR:HG21	1:C:361:ILE:HD11	1.96	0.47
1:B:18:TRP:O	1:B:22:SER:OG	2.25	0.47
1:C:457:PHE:HA	3:C:854:HOH:O	2.14	0.47
1:B:166:ARG:HD3	3:B:930:HOH:O	2.14	0.47
1:A:261:LYS:HB3	1:A:261:LYS:HE2	1.65	0.47
1:B:20:THR:OG1	1:B:368:ILE:HD11	2.15	0.47
1:C:98:ARG:O	1:C:105:ASP:N	2.42	0.46
1:C:38:GLU:OE1	3:C:717:HOH:O	2.20	0.46
1:D:335:ASN:HB2	3:D:758:HOH:O	2.14	0.46
1:C:247:ASN:ND2	1:C:250:LEU:O	2.45	0.46
1:D:83:LYS:HD3	1:D:85:ILE:HD11	1.97	0.46
1:C:465:TRP:HA	1:C:465:TRP:CE3	2.50	0.46
1:A:13:GLY:HA3	1:A:38:GLU:CD	2.41	0.46
1:A:15:THR:O	1:A:19:MET:HG3	2.15	0.46
1:A:106:HIS:CE1	3:A:917:HOH:O	2.69	0.46
1:C:260:ILE:HD11	1:C:318:LEU:HD11	1.97	0.46
1:A:423:ASP:CG	3:A:712:HOH:O	2.58	0.46
1:C:100:ILE:HD11	1:C:105:ASP:HA	1.98	0.46
1:A:462:ARG:HD3	1:A:462:ARG:HA	1.73	0.45
1:D:7:ARG:HG2	1:D:33:THR:OG1	2.15	0.45
1:C:325:LEU:HD23	1:C:327:GLN:HE22	1.81	0.45
1:A:243:PHE:CE2	1:A:331:ARG:HG2	2.51	0.45
1:B:510:ARG:O	1:B:514:GLU:HG2	2.16	0.45
1:C:199:GLN:NE2	3:C:704:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LEU:HD12	3:C:823:HOH:O	2.16	0.45
1:D:79:LYS:NZ	1:D:358:SER:OG	2.50	0.45
1:D:369:TYR:OH	3:D:712:HOH:O	2.20	0.45
1:D:520:LEU:O	1:D:524:ARG:HG2	2.16	0.45
1:A:456:ARG:NE	1:A:458:GLU:OE1	2.41	0.45
1:B:425:HIS:HB3	3:B:923:HOH:O	2.17	0.45
1:D:129:ASN:HB3	1:D:135:THR:HG22	1.99	0.44
1:C:457:PHE:HE1	1:C:461:PHE:CD1	2.36	0.44
1:C:166:ARG:NH2	1:C:450:GLU:HG2	2.32	0.44
1:B:438:LYS:HA	1:B:481:PRO:HA	1.98	0.44
1:B:457:PHE:CD2	1:B:458:GLU:N	2.86	0.44
1:A:35:THR:HG23	1:A:191:GLU:HG2	1.99	0.44
1:B:340:VAL:HG12	1:B:341:LYS:HG2	2.00	0.44
1:B:200:VAL:HG21	1:B:238:ALA:HB2	1.98	0.44
1:C:512:LEU:HD22	1:C:516:LEU:HD11	2.00	0.44
1:D:453:TYR:CE1	1:D:460:GLU:HA	2.52	0.44
1:B:35:THR:HG22	1:B:191:GLU:HB3	1.98	0.43
1:D:170:HIS:NE2	1:D:273:THR:OG1	2.44	0.43
1:B:512:LEU:HD22	1:B:516:LEU:HD11	2.00	0.43
1:B:38:GLU:HG3	1:B:192:HIS:CE1	2.52	0.43
1:B:229:GLY:HA2	1:B:348:LEU:HB2	2.01	0.43
1:D:251:LEU:HD21	1:D:424:LEU:HD21	2.01	0.43
1:A:170:HIS:CE1	1:A:287:PRO:HD2	2.54	0.43
1:B:14:GLY:N	3:B:729:HOH:O	2.43	0.43
1:C:90:PRO:HB3	1:C:414:ASP:HB3	1.99	0.43
1:C:252:CYS:HB3	1:C:297:VAL:HG12	2.01	0.43
1:C:129:ASN:HB3	1:C:135:THR:HG22	2.01	0.43
1:D:438:LYS:HA	1:D:481:PRO:HA	2.01	0.43
1:B:86:ASN:HA	1:B:105:ASP:OD2	2.19	0.43
1:D:153:VAL:HG12	1:D:270:GLU:HA	2.01	0.43
1:D:431:ARG:NH1	3:D:721:HOH:O	2.40	0.43
1:C:274:SER:HB2	1:C:285:LYS:HB3	2.01	0.43
1:D:521:GLU:O	1:D:525:SER:OG	2.36	0.43
1:B:493:GLU:OE1	1:B:493:GLU:N	2.47	0.43
1:C:29:GLY:O	3:C:722:HOH:O	2.22	0.43
1:D:285:LYS:HD2	1:D:316:TRP:CH2	2.53	0.43
1:A:444:ASN:HB3	1:A:463:ASN:OD1	2.19	0.43
1:C:9:VAL:HB	1:C:224:PHE:CD2	2.54	0.43
1:C:266:ALA:O	3:C:720:HOH:O	2.21	0.42
1:D:410:SER:O	1:D:422:LYS:NZ	2.46	0.42
1:D:141:TYR:OH	1:D:151:ASP:OD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HD2	1:B:192:HIS:CD2	2.55	0.42
1:D:237:LYS:HA	1:D:237:LYS:HD3	1.78	0.42
1:D:269:VAL:HG21	1:D:523:LEU:HD12	2.02	0.42
1:D:316:TRP:HA	3:D:701:HOH:O	2.18	0.42
1:A:226:ASP:OD2	1:A:235:ILE:HG22	2.20	0.42
1:B:205:ARG:HG3	1:B:207:PHE:CD1	2.55	0.42
1:B:353:LEU:HG	1:B:396:PHE:CE1	2.53	0.42
1:C:243:PHE:CE2	1:C:331:ARG:HG2	2.55	0.41
1:D:158:TRP:CD1	1:D:516:LEU:HD23	2.55	0.41
1:B:364:ILE:O	1:B:368:ILE:HG12	2.20	0.41
1:A:351:CYS:HB2	1:A:396:PHE:CE2	2.55	0.41
1:B:252:CYS:HB3	1:B:297:VAL:HG12	2.01	0.41
1:D:158:TRP:CE3	1:D:162:ARG:HB3	2.55	0.41
1:D:305:LYS:HB2	1:D:305:LYS:HE2	1.77	0.41
1:D:324:PRO:HA	3:D:784:HOH:O	2.20	0.41
1:B:36:LEU:HD23	1:B:37:LEU:N	2.35	0.41
1:B:277:ALA:O	1:B:278:MET:HE2	2.20	0.41
1:B:294:THR:HG23	1:B:312:PHE:HZ	1.86	0.41
1:D:434:ILE:HG22	1:D:438:LYS:HE3	2.01	0.41
1:A:233:LEU:O	1:A:237:LYS:HB2	2.20	0.41
1:A:438:LYS:HE2	1:A:479:LEU:HD11	2.01	0.41
1:B:331:ARG:O	1:B:352:PHE:HB3	2.21	0.41
1:D:426:LEU:HD12	1:D:427:PRO:HD2	2.03	0.41
1:C:4:ARG:HD3	3:C:773:HOH:O	2.21	0.41
1:C:178:GLU:O	1:C:182:ARG:HG3	2.20	0.41
1:A:353:LEU:HG	1:A:396:PHE:CE2	2.56	0.41
1:B:191:GLU:HG2	1:B:193:VAL:HG23	2.02	0.41
1:B:261:LYS:HA	1:B:261:LYS:HD2	1.89	0.41
1:C:88:ARG:HD2	1:C:476:GLY:O	2.21	0.41
1:C:201:LEU:HD12	1:C:210:ALA:HB3	2.01	0.41
1:A:68:GLU:N	2:A:605:SO4:O1	2.52	0.41
1:B:390:HIS:CD2	3:B:734:HOH:O	2.73	0.41
1:D:94:GLU:HA	1:D:315:MET:HG3	2.03	0.41
1:A:438:LYS:HA	1:A:481:PRO:HA	2.02	0.40
1:C:250:LEU:HD23	1:C:250:LEU:HA	1.91	0.40
1:D:148:ALA:CB	1:D:509:GLN:HG2	2.51	0.40
1:D:270:GLU:O	1:D:287:PRO:HG2	2.21	0.40
1:A:75:ASN:HA	1:A:527:HIS:CE1	2.56	0.40
1:A:493:GLU:OE1	1:A:493:GLU:N	2.47	0.40
1:D:413:THR:O	1:D:413:THR:OG1	2.35	0.40
1:A:18:TRP:CZ2	1:A:181:ARG:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:PHE:HB3	1:D:166:ARG:HG2	2.02	0.40
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:782:HOH:O	3:D:834:HOH:O[1_655]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/529 (98%)	504 (98%)	13 (2%)	0	100	100
1	B	513/529 (97%)	496 (97%)	17 (3%)	0	100	100
1	C	514/529 (97%)	499 (97%)	15 (3%)	0	100	100
1	D	510/529 (96%)	492 (96%)	18 (4%)	0	100	100
All	All	2054/2116 (97%)	1991 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/436 (99%)	429 (100%)	2 (0%)	81	79
1	B	427/436 (98%)	419 (98%)	8 (2%)	50	44
1	C	427/436 (98%)	422 (99%)	5 (1%)	63	58
1	D	426/436 (98%)	419 (98%)	7 (2%)	55	50
All	All	1711/1744 (98%)	1689 (99%)	22 (1%)	61	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	96	LYS
1	B	22	SER
1	B	38	GLU
1	B	194	GLN
1	B	267	HIS
1	B	315	MET
1	B	358	SER
1	B	365	THR
1	B	382	LEU
1	C	100	ILE
1	C	214	VAL
1	C	353	LEU
1	C	448	THR
1	C	451	SER
1	D	100	ILE
1	D	113	LEU
1	D	166	ARG
1	D	247	ASN
1	D	322	ASN
1	D	328	VAL
1	D	525	SER

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

Mol	Chain	Res	Type
1	A	119	GLN
1	B	192	HIS
1	B	247	ASN
1	C	6	ASN
1	C	119	GLN

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Mol	Chain	Res	Type
1	D	117	HIS
1	D	326	ASN
1	D	373	GLN
1	D	444	ASN

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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	601	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	B	603	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	C	601	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	D	602	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	602	-	4,4,4	0.27	0	6,6,6	0.15	0
2	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	602	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	D	601	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	604	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	D	603	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	A	602	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	B	605	-	4,4,4	0.44	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	SO4	1	0
2	C	601	SO4	1	0
2	A	605	SO4	2	0
2	B	602	SO4	1	0
2	B	605	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	521/529 (98%)	0.32	20 (3%)	44 54	14, 29, 51, 64	0
1	B	519/529 (98%)	0.63	42 (8%)	18 25	16, 35, 68, 91	0
1	C	519/529 (98%)	0.74	30 (5%)	29 37	18, 40, 65, 87	1 (0%)
1	D	517/529 (97%)	0.98	59 (11%)	10 13	22, 45, 72, 93	1 (0%)
All	All	2076/2116 (98%)	0.67	151 (7%)	21 28	14, 37, 67, 93	2 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	7.3
1	D	457	PHE	7.0
1	B	39	ALA	6.9
1	C	454	TYR	6.4
1	D	454	TYR	5.9
1	C	463	ASN	5.2
1	B	457	PHE	5.0
1	C	457	PHE	4.8
1	B	214	VAL	4.8
1	C	461	PHE	4.6
1	D	464	PHE	4.5
1	C	464	PHE	4.1
1	D	459	ALA	4.0
1	C	453	TYR	4.0
1	A	457	PHE	3.9
1	D	100	ILE	3.9
1	A	45	ILE	3.8
1	C	459	ALA	3.8
1	D	461	PHE	3.8
1	A	453	TYR	3.7
1	A	448	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	450	GLU	3.6
1	D	40	PRO	3.6
1	B	453	TYR	3.5
1	D	413	THR	3.5
1	A	461	PHE	3.4
1	D	148	ALA	3.4
1	D	101	ASP	3.4
1	C	448	THR	3.4
1	B	32	VAL	3.3
1	D	316	TRP	3.3
1	B	461	PHE	3.3
1	D	159	LEU	3.2
1	D	174	HIS	3.2
1	B	447	VAL	3.2
1	D	289	LEU	3.1
1	B	460	GLU	3.1
1	B	34	ILE	3.1
1	D	453	TYR	3.1
1	B	448	THR	3.1
1	D	512	LEU	3.1
1	C	458	GLU	3.0
1	A	455	GLY	3.0
1	D	448	THR	2.9
1	B	209	THR	2.9
1	B	454	TYR	2.9
1	D	158	TRP	2.9
1	B	458	GLU	2.8
1	B	9	VAL	2.8
1	B	190	VAL	2.8
1	B	210	ALA	2.8
1	B	193	VAL	2.8
1	B	197	MET	2.8
1	B	451	SER	2.8
1	B	21	ALA	2.8
1	B	224	PHE	2.7
1	C	451	SER	2.7
1	A	214	VAL	2.7
1	D	47	VAL	2.7
1	A	459	ALA	2.7
1	D	97	ALA	2.7
1	B	330	PHE	2.7
1	B	201	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	2.7
1	C	460	GLU	2.7
1	A	449	ASP	2.6
1	C	452	THR	2.6
1	B	45	ILE	2.6
1	B	33	THR	2.6
1	C	40	PRO	2.6
1	A	464	PHE	2.6
1	D	516	LEU	2.6
1	D	313	CYS	2.5
1	D	330	PHE	2.5
1	D	447	VAL	2.5
1	D	164	ALA	2.5
1	C	413	THR	2.5
1	C	513	VAL	2.5
1	D	214	VAL	2.5
1	D	149	ALA	2.4
1	B	462	ARG	2.4
1	D	103	ARG	2.4
1	B	215	GLU	2.4
1	C	450	GLU	2.4
1	D	176	VAL	2.4
1	B	464	PHE	2.4
1	C	330	PHE	2.4
1	D	260	ILE	2.4
1	A	38	GLU	2.4
1	D	463	ASN	2.4
1	D	451	SER	2.4
1	B	449	ASP	2.3
1	D	362	TYR	2.3
1	D	230	PHE	2.3
1	D	321	GLU	2.3
1	C	465	TRP	2.3
1	C	178	GLU	2.3
1	D	497	GLU	2.3
1	D	526	LEU	2.3
1	D	99	THR	2.3
1	D	46	GLY	2.3
1	B	213	THR	2.3
1	D	527	HIS	2.3
1	D	77	ALA	2.3
1	A	451	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	196	GLU	2.2
1	D	90	PRO	2.2
1	D	522	PHE	2.2
1	B	35	THR	2.2
1	C	159	LEU	2.2
1	D	520	LEU	2.2
1	D	2	ASP	2.2
1	C	444	ASN	2.2
1	D	288	MET	2.2
1	B	198	GLN	2.2
1	D	268	GLY	2.2
1	C	329	ALA	2.2
1	D	155	ALA	2.2
1	C	260	ILE	2.2
1	B	6	ASN	2.2
1	B	212	ARG	2.2
1	A	190	VAL	2.2
1	C	310	LEU	2.2
1	D	172	ASP	2.1
1	A	447	VAL	2.1
1	A	324	PRO	2.1
1	C	320	PRO	2.1
1	B	191	GLU	2.1
1	D	458	GLU	2.1
1	D	145	ALA	2.1
1	D	152	ALA	2.1
1	B	208	ILE	2.1
1	D	216	GLY	2.1
1	D	462	ARG	2.1
1	A	526	LEU	2.1
1	D	105	ASP	2.1
1	C	166	ARG	2.1
1	A	460	GLU	2.1
1	D	323	THR	2.1
1	C	447	VAL	2.1
1	D	405	ALA	2.1
1	C	105	ASP	2.1
1	A	216	GLY	2.0
1	B	13	GLY	2.0
1	B	221	GLY	2.0
1	B	172	ASP	2.0
1	B	331	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	463	ASN	2.0
1	C	200	VAL	2.0
1	C	505	VAL	2.0
1	D	32	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	606	5/5	0.63	0.15	41,53,60,81	0
2	SO4	B	602	5/5	0.73	0.13	43,48,57,62	0
2	SO4	D	603	5/5	0.74	0.14	47,48,59,69	0
2	SO4	C	602	5/5	0.80	0.12	42,43,60,66	0
2	SO4	B	605	5/5	0.81	0.13	67,75,79,82	0
2	SO4	B	603	5/5	0.84	0.09	57,58,71,73	0
2	SO4	B	604	5/5	0.85	0.09	54,55,63,70	0
2	SO4	A	605	5/5	0.86	0.30	41,41,58,58	0
2	SO4	D	602	5/5	0.87	0.10	43,47,49,54	5
2	SO4	B	601	5/5	0.89	0.20	46,49,55,61	0
2	SO4	A	603	5/5	0.90	0.08	50,52,56,60	0
2	SO4	A	604	5/5	0.93	0.17	32,40,54,55	0
2	SO4	C	601	5/5	0.94	0.12	39,46,52,57	0
2	SO4	A	602	5/5	0.95	0.15	40,45,50,52	0
2	SO4	D	601	5/5	0.95	0.08	39,47,51,51	0
2	SO4	A	601	5/5	0.98	0.06	22,23,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.