



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 3DOR / pdb_00003dor
Title : Crystal Structure of mature CPAF
Authors : Chai, J.; Huang, Z.
Deposited on : 2008-07-06
Resolution : 2.20 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

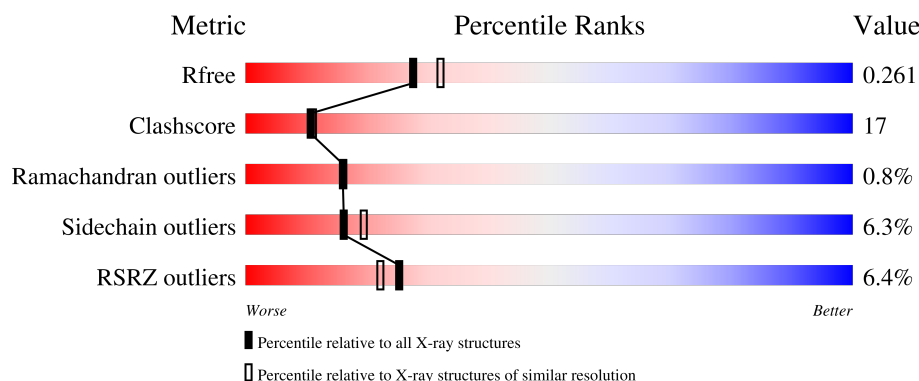
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	583	
1	B	583	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8746 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 Protein CT_858.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4105	2627	688	777	13			
1	B	527	Total	C	N	O	S	0	0	0
			4141	2652	693	783	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	HIS	-	expression tag	UNP O84866
A	611	HIS	-	expression tag	UNP O84866
A	612	HIS	-	expression tag	UNP O84866
A	613	HIS	-	expression tag	UNP O84866
A	614	HIS	-	expression tag	UNP O84866
A	615	HIS	-	expression tag	UNP O84866
B	610	HIS	-	expression tag	UNP O84866
B	611	HIS	-	expression tag	UNP O84866
B	612	HIS	-	expression tag	UNP O84866
B	613	HIS	-	expression tag	UNP O84866
B	614	HIS	-	expression tag	UNP O84866
B	615	HIS	-	expression tag	UNP O84866

- 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		
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		

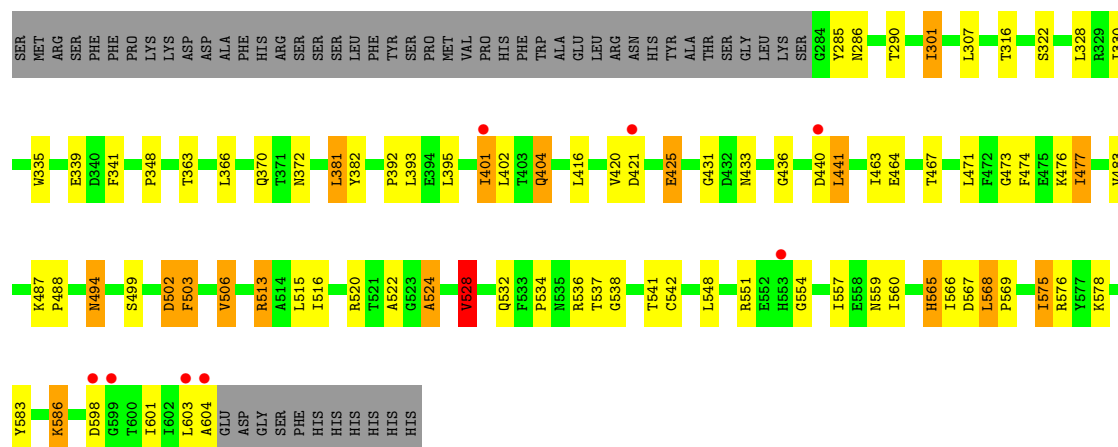
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	285	Total	O	0	0
			285	285		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 152.37Å 162.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.20 39.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.27-2.20) 99.4 (39.27-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.262 0.226 , 0.261	Depositor DCC
R_{free} test set	3937 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8746	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 3.42% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/4203 (0.0%)	0.94	16/5713 (0.3%)
1	B	0.45	0/4239	0.96	20/5763 (0.3%)
All	All	0.43	1/8442 (0.0%)	0.95	36/11476 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ALA	CA-CB	-7.46	1.42	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ILE	N-CA-C	9.52	119.48	110.53
1	B	441	LEU	N-CA-C	-8.53	101.92	111.82
1	A	192	LYS	N-CA-C	-7.63	97.62	109.76
1	B	330	ILE	N-CA-C	-7.61	100.01	107.55
1	A	452	ARG	N-CA-C	-7.57	103.03	111.28
1	B	141	GLU	N-CA-C	7.54	120.16	111.11
1	A	285	TYR	N-CA-C	-7.52	104.99	112.97
1	B	192	LYS	N-CA-C	-7.00	98.62	109.76
1	B	502	ASP	N-CA-C	-6.87	102.15	112.04
1	A	330	ILE	CA-C-N	6.80	126.40	119.19
1	A	330	ILE	C-N-CA	6.80	126.40	119.19
1	B	207	GLY	N-CA-C	6.80	121.75	113.79
1	B	565	HIS	N-CA-C	-6.69	104.07	111.36
1	A	193	VAL	N-CA-C	6.61	115.17	107.77
1	A	441	LEU	N-CA-C	-6.43	104.32	111.71
1	B	431	GLY	N-CA-C	-6.25	105.67	112.04
1	B	522	ALA	N-CA-C	6.24	117.74	111.07
1	B	65	GLY	N-CA-C	-6.22	105.32	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	6.20	122.06	114.69
1	A	335	TRP	N-CA-C	5.94	118.52	111.33
1	B	503	PHE	N-CA-C	5.89	117.71	111.28
1	B	575	ILE	N-CA-C	5.79	117.32	111.00
1	B	554	GLY	N-CA-C	5.72	121.50	114.69
1	A	450	PHE	N-CA-C	-5.71	100.68	109.76
1	B	467	THR	N-CA-C	-5.69	101.93	109.84
1	B	528	VAL	CB-CA-C	-5.63	103.71	111.49
1	A	528	VAL	CB-CA-C	-5.55	103.82	111.49
1	A	402	LEU	N-CA-C	5.52	118.69	110.14
1	B	463	ILE	N-CA-C	5.47	119.39	113.43
1	A	403	THR	N-CA-C	-5.40	101.09	109.14
1	B	193	VAL	N-CA-C	5.38	113.79	107.77
1	A	502	ASP	N-CA-C	-5.33	104.37	112.04
1	B	402	LEU	N-CA-C	5.24	117.94	109.40
1	B	524	ALA	N-CA-C	-5.10	99.01	108.24
1	B	217	ARG	N-CA-C	-5.08	100.23	108.41
1	A	522	ALA	N-CA-C	5.07	116.49	111.07

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	4105	0	4043	162	0
1	B	4141	0	4088	130	0
2	A	45	0	0	1	0
2	B	30	0	0	1	0
3	A	140	0	0	2	0
3	B	285	0	0	4	0
All	All	8746	0	8131	274	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 17.

All (274) 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:B:586:LYS:HE2	1:B:603:LEU:HD23	1.40	0.99
1:B:59:TRP:HE1	1:B:559:ASN:HD22	1.07	0.98
1:A:59:TRP:HE1	1:A:559:ASN:HD22	1.10	0.95
1:A:494:ASN:HD22	1:A:496:GLN:H	0.92	0.91
1:A:494:ASN:HD22	1:A:496:GLN:N	1.65	0.91
1:B:516:ILE:H	1:B:565:HIS:HD2	1.17	0.91
1:B:586:LYS:CE	1:B:603:LEU:HD23	2.03	0.88
1:A:516:ILE:H	1:A:565:HIS:HD2	1.21	0.87
1:A:297:ILE:HB	1:A:588:LYS:HD3	1.57	0.85
1:A:432:ASP:HA	1:A:439:VAL:HB	1.57	0.84
1:A:335:TRP:HB2	1:A:348:PRO:HG3	1.60	0.84
1:B:54:TYR:CZ	1:B:56:PRO:HG2	2.14	0.82
1:A:570:PHE:HB3	1:A:575:ILE:HD11	1.61	0.81
1:A:534:PRO:HG2	1:B:49:LEU:HD22	1.62	0.80
1:A:570:PHE:HB3	1:A:575:ILE:CD1	2.12	0.79
1:B:586:LYS:CE	1:B:604:ALA:H	1.96	0.77
1:A:33:SER:O	1:A:37:LYS:HG3	1.85	0.76
1:A:427:ARG:HB3	1:A:432:ASP:HB3	1.68	0.74
1:A:133:VAL:O	1:A:578:LYS:HD3	1.88	0.73
1:A:516:ILE:H	1:A:565:HIS:CD2	2.05	0.73
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.23	0.73
1:A:57:LYS:O	1:A:61:GLU:HG3	1.89	0.72
1:A:538:GLY:HA2	1:B:404:GLN:CG	2.20	0.72
1:A:186:MET:H	1:A:191:HIS:HD2	1.39	0.70
1:A:494:ASN:ND2	1:A:496:GLN:H	1.77	0.69
1:A:404:GLN:CG	1:B:538:GLY:HA2	2.22	0.69
1:A:49:LEU:HD22	1:B:534:PRO:HG2	1.74	0.68
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.74	0.68
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.59	0.68
1:A:54:TYR:CZ	1:A:56:PRO:HG2	2.29	0.67
1:A:105:HIS:CE1	1:A:528:VAL:HG22	2.30	0.66
1:B:105:HIS:CG	1:B:528:VAL:HG13	2.31	0.66
1:A:121:THR:HB	1:A:134:ASP:HB3	1.78	0.66
1:A:59:TRP:NE1	1:A:559:ASN:HD22	1.90	0.65
1:B:316:THR:HG22	1:B:322:SER:OG	1.96	0.65
1:B:123:GLN:HE21	1:B:133:VAL:HG11	1.62	0.64
1:B:516:ILE:H	1:B:565:HIS:CD2	2.07	0.64
1:B:395:LEU:HD21	1:B:477:ILE:HD12	1.79	0.64
1:B:586:LYS:NZ	1:B:603:LEU:HD23	2.13	0.63
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.79	0.63
1:A:186:MET:H	1:A:191:HIS:CD2	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:VAL:HA	1:A:427:ARG:NH1	2.12	0.63
1:A:538:GLY:HA2	1:B:404:GLN:HG3	1.81	0.63
1:A:404:GLN:NE2	1:A:404:GLN:H	1.97	0.62
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.35	0.62
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.33	0.62
1:A:315:VAL:HG12	1:A:323:HIS:HB2	1.81	0.62
1:A:404:GLN:HG3	1:B:538:GLY:HA2	1.80	0.62
1:A:353:ALA:HB1	1:A:483:VAL:HG11	1.82	0.62
1:A:424:VAL:O	1:A:428:LEU:HD13	2.00	0.61
1:B:87:THR:O	1:B:91:GLN:HG3	2.01	0.61
1:B:186:MET:H	1:B:191:HIS:CD2	2.19	0.60
1:B:404:GLN:H	1:B:404:GLN:NE2	1.99	0.60
1:B:64:LEU:HD23	1:B:169:LYS:HD2	1.84	0.60
1:B:59:TRP:HE1	1:B:559:ASN:ND2	1.88	0.59
1:A:63:TYR:CD2	1:A:64:LEU:HG	2.37	0.59
1:B:81:THR:HG22	1:B:81:THR:O	2.02	0.59
1:A:51:GLN:HG3	1:A:68:LEU:CD2	2.33	0.59
1:A:440:ASP:H	1:A:443:VAL:CG2	2.16	0.59
1:A:506:VAL:HG23	1:A:562:VAL:CG2	2.33	0.59
1:A:394:GLU:OE2	1:A:476:LYS:HE2	2.03	0.58
1:B:395:LEU:HD21	1:B:477:ILE:CD1	2.33	0.58
1:A:336:GLN:H	1:A:336:GLN:CD	2.10	0.58
1:B:290:THR:OG1	1:B:339:GLU:HB2	2.03	0.58
1:B:416:LEU:HD23	1:B:416:LEU:O	2.04	0.58
1:B:149:LEU:O	1:B:156:VAL:HG23	2.03	0.58
1:B:151:VAL:HB	1:B:159:VAL:HG21	1.85	0.57
1:B:328:LEU:C	1:B:328:LEU:HD13	2.29	0.57
1:B:586:LYS:HE3	3:B:860:HOH:O	2.04	0.57
1:A:538:GLY:CA	1:B:404:GLN:HG3	2.34	0.57
1:A:63:TYR:HD2	1:A:64:LEU:HG	1.67	0.57
1:A:432:ASP:CA	1:A:439:VAL:HB	2.32	0.57
1:B:33:SER:N	1:B:37:LYS:NZ	2.52	0.56
1:A:584:LEU:O	1:A:588:LYS:HG3	2.05	0.56
1:A:411:LEU:O	1:A:415:THR:HG23	2.05	0.56
1:A:554:GLY:O	1:A:555:ALA:HB3	2.06	0.56
1:B:201:LYS:HE3	1:B:209:THR:HG21	1.87	0.56
1:A:290:THR:OG1	1:A:339:GLU:HB2	2.05	0.56
1:B:401:ILE:HG12	1:B:464:GLU:O	2.05	0.56
1:A:310:ALA:HB2	1:A:328:LEU:HD23	1.88	0.55
1:A:397:LYS:HB2	1:A:468:PRO:HB2	1.88	0.55
1:A:431:GLY:C	1:A:433:ASN:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ASN:H	1:B:494:ASN:HD21	1.54	0.55
1:A:456:ASN:OD1	1:A:460:LYS:HE3	2.07	0.55
1:A:506:VAL:HG23	1:A:562:VAL:HG21	1.89	0.55
1:A:404:GLN:HG3	1:B:538:GLY:CA	2.37	0.55
1:A:538:GLY:HA2	1:B:404:GLN:HG2	1.89	0.54
1:B:33:SER:N	1:B:37:LYS:HZ3	2.04	0.54
1:B:186:MET:H	1:B:191:HIS:HD2	1.52	0.54
1:A:404:GLN:H	1:A:404:GLN:CD	2.14	0.54
1:A:536:ARG:HA	1:B:404:GLN:HE22	1.73	0.54
1:A:589:LYS:HB2	1:A:589:LYS:NZ	2.23	0.54
1:A:399:ARG:HH21	1:A:465:LEU:HD23	1.73	0.53
1:A:494:ASN:ND2	1:A:496:GLN:N	2.46	0.53
1:B:301:ILE:O	1:B:301:ILE:HD12	2.08	0.53
1:B:55:ALA:CA	1:B:401:ILE:HG13	2.38	0.53
1:B:55:ALA:HA	1:B:401:ILE:HG13	1.89	0.53
1:B:420:VAL:HG13	1:B:425:GLU:HB3	1.89	0.53
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.39	0.53
1:A:570:PHE:CB	1:A:575:ILE:HD11	2.36	0.53
1:B:603:LEU:O	1:B:604:ALA:HB2	2.08	0.53
1:A:365:ALA:HB2	1:A:595:ILE:HD11	1.91	0.53
1:A:536:ARG:HA	1:B:404:GLN:NE2	2.24	0.53
1:B:603:LEU:O	1:B:604:ALA:CB	2.57	0.53
1:A:41:GLN:HG3	1:B:48:HIS:CD2	2.44	0.52
1:A:67:ASP:HB3	1:A:70:GLN:HB2	1.90	0.52
1:A:297:ILE:HB	1:A:588:LYS:CD	2.35	0.52
1:B:103:ASP:HB3	1:B:106:ALA:HB3	1.90	0.52
1:B:125:SER:OG	1:B:127:ASP:OD2	2.27	0.52
1:A:123:GLN:HE21	1:A:133:VAL:HG11	1.75	0.52
1:B:381:LEU:HD13	1:B:381:LEU:C	2.35	0.52
1:A:371:THR:HG22	1:A:494:ASN:HB2	1.92	0.52
1:A:499:SER:H	1:A:524:ALA:HB3	1.74	0.52
1:A:117:TYR:HD2	1:A:217:ARG:HD2	1.75	0.51
1:A:303:GLU:HA	1:A:311:TYR:HA	1.92	0.51
1:A:520:ARG:HD2	1:A:560:ILE:O	2.09	0.51
1:B:433:ASN:ND2	1:B:436:GLY:H	2.08	0.51
1:A:69:VAL:O	1:A:73:VAL:HG23	2.10	0.51
1:A:520:ARG:NH2	2:A:619:SO4:S	2.83	0.51
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.93	0.51
1:B:118:LEU:HD22	1:B:214:VAL:CG1	2.41	0.51
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.23	0.50
1:B:33:SER:HB3	1:B:36:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LYS:HZ1	1:B:603:LEU:HD23	1.76	0.50
1:A:415:THR:HA	1:A:418:GLU:HG3	1.92	0.50
1:A:105:HIS:CG	1:A:528:VAL:HG22	2.47	0.50
1:B:118:LEU:HG	1:B:216:TRP:CE3	2.47	0.50
1:B:566:ILE:HG23	1:B:603:LEU:HD12	1.94	0.50
1:B:586:LYS:HE2	1:B:604:ALA:H	1.76	0.50
1:A:307:LEU:HB2	1:A:351:GLU:OE1	2.12	0.49
1:A:350:GLU:O	1:A:354:LYS:HG2	2.12	0.49
1:A:105:HIS:ND1	1:A:528:VAL:HG22	2.27	0.49
1:B:568:LEU:HD13	1:B:583:TYR:CD1	2.47	0.49
1:B:586:LYS:HE2	1:B:603:LEU:CD2	2.28	0.49
1:A:516:ILE:N	1:A:565:HIS:HD2	2.01	0.49
1:A:43:LEU:HD13	1:A:43:LEU:C	2.38	0.49
1:A:431:GLY:O	1:A:432:ASP:CG	2.55	0.49
1:A:365:ALA:CB	1:A:595:ILE:HD11	2.43	0.49
1:B:393:LEU:HD21	1:B:513:ARG:HG3	1.94	0.49
1:A:447:LEU:O	1:A:450:PHE:O	2.30	0.49
1:A:315:VAL:HG23	1:A:588:LYS:HB3	1.95	0.49
1:A:356:ILE:HG23	1:A:485:TYR:HB2	1.94	0.49
1:B:55:ALA:HB2	1:B:401:ILE:HG13	1.95	0.49
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.43	0.48
1:B:537:THR:O	1:B:537:THR:HG22	2.13	0.48
1:B:499:SER:O	1:B:502:ASP:HB2	2.13	0.48
1:A:87:THR:O	1:A:91:GLN:HG3	2.13	0.48
1:B:117:TYR:O	1:B:217:ARG:HB2	2.13	0.48
1:B:60:LYS:NZ	1:B:559:ASN:HD21	2.12	0.48
1:B:286:ASN:HB2	3:B:673:HOH:O	2.13	0.48
1:A:328:LEU:HD13	1:A:328:LEU:C	2.38	0.47
1:B:55:ALA:HA	1:B:401:ILE:CG1	2.44	0.47
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.96	0.47
1:B:601:ILE:HD12	1:B:601:ILE:N	2.29	0.47
1:A:495:GLU:CD	1:A:495:GLU:H	2.21	0.47
1:A:82:GLN:HG3	1:A:89:PHE:CE2	2.49	0.47
1:A:591:VAL:O	1:A:595:ILE:HD12	2.14	0.47
1:A:117:TYR:OH	1:A:136:MET:HE2	2.14	0.47
1:A:301:ILE:HD12	1:A:301:ILE:C	2.38	0.47
1:B:499:SER:H	1:B:524:ALA:HB3	1.79	0.47
1:A:371:THR:CG2	1:A:494:ASN:HB2	2.45	0.47
1:B:155:PRO:HG2	1:B:158:ASP:OD2	2.14	0.47
1:B:341:PHE:CE1	1:B:348:PRO:HD3	2.50	0.47
1:A:134:ASP:OD2	1:A:136:MET:SD	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:N	1:A:231:PRO:HD2	2.30	0.47
1:A:134:ASP:C	1:A:135:ILE:HD12	2.39	0.47
1:A:423:ASN:O	1:A:427:ARG:HG3	2.15	0.47
1:A:536:ARG:HG3	1:B:52:VAL:HG13	1.96	0.46
1:B:180:ARG:NE	2:B:617:SO4:O4	2.48	0.46
1:B:433:ASN:HD22	1:B:436:GLY:H	1.64	0.46
1:B:586:LYS:NZ	1:B:604:ALA:H	2.13	0.46
1:B:118:LEU:HD22	1:B:214:VAL:HG11	1.97	0.46
1:A:105:HIS:CE1	1:A:526:GLY:O	2.69	0.46
1:B:516:ILE:HD12	1:B:516:ILE:N	2.31	0.46
1:A:54:TYR:CE2	1:A:56:PRO:HG2	2.50	0.46
1:A:575:ILE:HD12	1:A:575:ILE:N	2.29	0.46
1:A:319:ASP:OD2	1:A:319:ASP:N	2.49	0.46
1:A:470:PRO:HB2	1:A:474:PHE:O	2.16	0.46
1:B:129:ARG:CZ	1:B:131:TYR:OH	2.64	0.46
1:B:392:PRO:HB2	1:B:476:LYS:HD3	1.97	0.46
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.98	0.46
1:A:53:LYS:HG3	1:B:534:PRO:CB	2.46	0.45
1:A:130:PHE:HE2	1:A:179:LEU:HD21	1.81	0.45
1:A:404:GLN:HE22	1:B:536:ARG:HA	1.82	0.45
1:A:558:GLU:O	1:A:559:ASN:HB2	2.15	0.45
3:A:739:HOH:O	1:B:404:GLN:HG2	2.16	0.45
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.51	0.45
1:A:371:THR:HB	1:A:494:ASN:HB2	1.99	0.45
1:A:335:TRP:NE1	1:A:336:GLN:HE21	2.15	0.45
1:A:404:GLN:HG2	1:B:538:GLY:HA2	1.96	0.45
1:A:53:LYS:HG3	1:B:534:PRO:HB2	1.99	0.45
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.52	0.45
1:A:591:VAL:O	1:A:595:ILE:CD1	2.66	0.45
1:B:57:LYS:O	1:B:61:GLU:HG3	2.18	0.44
1:B:103:ASP:OD1	1:B:105:HIS:HB2	2.17	0.44
1:A:149:LEU:O	1:A:156:VAL:HG23	2.16	0.44
1:A:494:ASN:ND2	1:A:495:GLU:N	2.65	0.44
1:A:440:ASP:H	1:A:443:VAL:HG23	1.82	0.44
1:B:59:TRP:NE1	1:B:559:ASN:HD22	1.91	0.44
1:A:285:TYR:CE1	1:A:578:LYS:HD2	2.53	0.44
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.53	0.44
1:B:381:LEU:HD12	1:B:382:TYR:CD1	2.53	0.44
1:B:404:GLN:H	1:B:404:GLN:CD	2.25	0.44
1:B:575:ILE:O	1:B:576:ARG:C	2.60	0.44
1:B:201:LYS:CE	1:B:209:THR:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:NH2	3:A:647:HOH:O	2.48	0.44
1:A:441:LEU:HD13	1:A:441:LEU:C	2.42	0.44
1:B:536:ARG:HG3	1:B:536:ARG:HH11	1.81	0.44
1:A:168:HIS:CE1	1:A:170:GLY:HA2	2.51	0.44
1:A:450:PHE:HB2	1:A:473:GLY:CA	2.48	0.44
1:A:493:ILE:HD11	1:A:564:PRO:HB3	2.00	0.44
1:B:105:HIS:CG	1:B:528:VAL:CG1	3.01	0.44
1:B:503:PHE:O	1:B:506:VAL:HG12	2.17	0.44
1:A:506:VAL:HG23	1:A:562:VAL:HG22	1.98	0.43
1:A:432:ASP:OD1	1:A:432:ASP:C	2.60	0.43
1:B:55:ALA:CB	1:B:401:ILE:HG13	2.49	0.43
1:A:130:PHE:CE2	1:A:179:LEU:HD21	2.53	0.43
1:A:335:TRP:HB2	1:A:348:PRO:CG	2.40	0.43
1:B:566:ILE:CG2	1:B:603:LEU:HD12	2.48	0.43
1:B:168:HIS:CE1	1:B:170:GLY:HA2	2.54	0.43
1:B:520:ARG:HD3	1:B:560:ILE:O	2.19	0.43
1:A:504:PHE:HB3	1:A:505:PRO:HD3	2.00	0.43
1:A:537:THR:HG22	1:A:537:THR:O	2.18	0.43
1:B:551:ARG:HD2	1:B:557:ILE:CD1	2.49	0.43
1:A:98:ILE:HG13	1:A:108:VAL:CG2	2.49	0.42
1:A:575:ILE:CD1	1:A:575:ILE:N	2.82	0.42
1:B:114:GLU:OE2	1:B:218:TYR:OH	2.28	0.42
1:B:208:THR:HB	3:B:748:HOH:O	2.20	0.42
1:A:318:GLY:C	1:A:320:GLY:H	2.26	0.42
1:B:474:PHE:N	1:B:474:PHE:CD1	2.87	0.42
1:B:586:LYS:HA	1:B:586:LYS:HD3	1.62	0.42
1:A:132:PHE:HB3	1:A:135:ILE:HD11	2.01	0.42
1:A:304:SER:O	1:A:306:GLY:N	2.52	0.42
1:A:285:TYR:HE1	1:A:578:LYS:HD2	1.85	0.42
1:B:285:TYR:OH	1:B:578:LYS:HG2	2.20	0.42
1:A:127:ASP:OD2	1:A:127:ASP:C	2.62	0.42
1:A:424:VAL:HA	1:A:427:ARG:HH12	1.84	0.42
1:A:155:PRO:HG2	1:A:158:ASP:OD2	2.19	0.42
1:A:301:ILE:HD12	1:A:302:TRP:HB2	2.02	0.42
1:A:427:ARG:HD3	1:A:432:ASP:HB2	2.02	0.42
1:A:470:PRO:HG2	1:A:473:GLY:HA2	2.02	0.42
1:B:551:ARG:CG	1:B:557:ILE:HD11	2.50	0.42
1:A:371:THR:CB	1:A:494:ASN:HB2	2.50	0.42
1:B:56:PRO:HB3	1:B:548:LEU:HD21	2.01	0.41
1:A:148:LEU:HG	1:A:156:VAL:CG2	2.50	0.41
1:A:229:ILE:C	1:A:231:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD1	1:A:572:ALA:HB2	2.20	0.41
1:A:217:ARG:CG	1:A:217:ARG:NH1	2.84	0.41
1:B:56:PRO:O	1:B:60:LYS:HG2	2.19	0.41
1:A:398:HIS:CD2	1:A:471:LEU:HG	2.55	0.41
1:A:498:PHE:N	1:A:501:ALA:HB3	2.35	0.41
1:B:471:LEU:C	1:B:473:GLY:N	2.78	0.41
1:A:72:SER:O	1:A:76:GLN:HG3	2.21	0.41
1:A:453:GLN:HB3	1:A:469:ILE:HD12	2.03	0.41
1:A:570:PHE:HB3	1:A:575:ILE:HD13	1.95	0.41
1:B:105:HIS:ND1	1:B:528:VAL:HG13	2.35	0.41
1:B:199:THR:OG1	1:B:213:ARG:HD3	2.21	0.41
1:A:103:ASP:HB3	1:A:106:ALA:HB3	2.03	0.41
1:B:565:HIS:HE1	3:B:650:HOH:O	2.04	0.41
1:A:83:GLU:O	1:A:84:ASN:C	2.63	0.41
1:B:55:ALA:HA	1:B:401:ILE:HD11	2.02	0.41
1:A:51:GLN:HG3	1:A:68:LEU:HD21	2.02	0.41
1:B:416:LEU:HD23	1:B:416:LEU:C	2.45	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.94	0.40
1:B:433:ASN:ND2	1:B:433:ASN:C	2.79	0.40
1:B:541:THR:HG22	1:B:542:CYS:N	2.36	0.40
1:A:483:VAL:O	1:A:483:VAL:CG2	2.68	0.40
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.61	0.40
1:A:399:ARG:NH2	1:B:237:GLN:O	2.54	0.40
1:B:567:ASP:OD1	1:B:569:PRO:HD3	2.22	0.40
1:B:230:ALA:N	1:B:231:PRO:HD2	2.36	0.40
1:B:471:LEU:C	1:B:473:GLY:H	2.28	0.40
1:B:551:ARG:HD2	1:B:557:ILE:HD11	2.04	0.40
1:B:586:LYS:NZ	1:B:604:ALA:O	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/583 (89%)	487 (94%)	25 (5%)	6 (1%)	10	8
1	B	523/583 (90%)	504 (96%)	17 (3%)	2 (0%)	30	34
All	All	1041/1166 (89%)	991 (95%)	42 (4%)	8 (1%)	16	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	B	83	GLU
1	A	598	ASP
1	B	139	SER
1	A	317	ASP
1	A	306	GLY
1	A	555	ALA
1	A	432	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	451/506 (89%)	424 (94%)	27 (6%)	17	21
1	B	455/506 (90%)	425 (93%)	30 (7%)	15	18
All	All	906/1012 (90%)	849 (94%)	57 (6%)	16	19

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	175	GLU
1	A	179	LEU
1	A	182	LEU
1	A	192	LYS
1	A	209	THR
1	A	213	ARG
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	307	LEU
1	A	319	ASP
1	A	363	THR
1	A	364	GLU
1	A	366	LEU
1	A	370	GLN
1	A	381	LEU
1	A	404	GLN
1	A	445	GLU
1	A	477	ILE
1	A	483	VAL
1	A	495	GLU
1	A	513	ARG
1	A	515	LEU
1	A	528	VAL
1	A	532	GLN
1	A	562	VAL
1	A	568	LEU
1	A	589	LYS
1	B	43	LEU
1	B	140	SER
1	B	179	LEU
1	B	182	LEU
1	B	208	THR
1	B	214	VAL
1	B	217	ARG
1	B	301	ILE
1	B	307	LEU
1	B	363	THR
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	401	ILE
1	B	404	GLN
1	B	421	ASP
1	B	425	GLU
1	B	440	ASP
1	B	441	LEU
1	B	477	ILE
1	B	483	VAL
1	B	494	ASN
1	B	506	VAL

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Mol	Chain	Res	Type
1	B	513	ARG
1	B	515	LEU
1	B	528	VAL
1	B	532	GLN
1	B	568	LEU
1	B	586	LYS
1	B	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	70	GLN
1	A	84	ASN
1	A	123	GLN
1	A	168	HIS
1	A	191	HIS
1	A	286	ASN
1	A	404	GLN
1	A	494	ASN
1	A	559	ASN
1	A	565	HIS
1	A	593	GLN
1	A	596	ASN
1	B	41	GLN
1	B	48	HIS
1	B	76	GLN
1	B	84	ASN
1	B	102	ASN
1	B	123	GLN
1	B	168	HIS
1	B	191	HIS
1	B	357	GLN
1	B	404	GLN
1	B	433	ASN
1	B	453	GLN
1	B	456	ASN
1	B	494	ASN
1	B	559	ASN
1	B	565	HIS
1	B	596	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](#)

15 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	620	-	4,4,4	0.91	0	6,6,6	0.35	0
2	SO4	A	619	-	4,4,4	0.92	0	6,6,6	0.37	0
2	SO4	A	624	-	4,4,4	0.68	0	6,6,6	0.37	0
2	SO4	A	623	-	4,4,4	0.61	0	6,6,6	0.24	0
2	SO4	B	621	-	4,4,4	0.90	0	6,6,6	0.39	0
2	SO4	B	620	-	4,4,4	0.74	0	6,6,6	0.38	0
2	SO4	B	619	-	4,4,4	0.83	0	6,6,6	0.34	0
2	SO4	A	618	-	4,4,4	0.86	0	6,6,6	0.39	0
2	SO4	B	616	-	4,4,4	0.95	0	6,6,6	0.37	0
2	SO4	B	617	-	4,4,4	0.69	0	6,6,6	0.32	0
2	SO4	B	618	-	4,4,4	0.65	0	6,6,6	0.32	0
2	SO4	A	622	-	4,4,4	0.65	0	6,6,6	0.30	0
2	SO4	A	616	-	4,4,4	0.89	0	6,6,6	0.35	0
2	SO4	A	621	-	4,4,4	0.92	0	6,6,6	0.37	0
2	SO4	A	617	-	4,4,4	0.87	0	6,6,6	0.48	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	619	SO4	1	0
2	B	617	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	522/583 (89%)	0.67	45 (8%) 16 14	27, 43, 66, 87	0
1	B	527/583 (90%)	0.09	22 (4%) 40 37	20, 32, 52, 71	0
All	All	1049/1166 (89%)	0.38	67 (6%) 25 22	20, 38, 62, 87	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	599	GLY	5.6
1	B	598	ASP	4.6
1	A	428	LEU	4.4
1	B	238	LEU	4.3
1	B	604	ALA	4.2
1	A	432	ASP	4.2
1	B	401	ILE	4.0
1	A	318	GLY	3.8
1	B	138	PHE	3.8
1	A	494	ASN	3.6
1	A	440	ASP	3.6
1	A	553	HIS	3.6
1	A	598	ASP	3.5
1	A	420	VAL	3.5
1	A	451	GLY	3.4
1	A	306	GLY	3.4
1	A	286	ASN	3.4
1	B	603	LEU	3.3
1	A	314	SER	3.2
1	B	231	PRO	3.1
1	B	599	GLY	3.1
1	A	424	VAL	3.0
1	A	63	TYR	3.0
1	B	140	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	81	THR	2.9
1	B	440	ASP	2.8
1	A	285	TYR	2.8
1	B	77	GLN	2.8
1	B	139	SER	2.7
1	A	479	PRO	2.7
1	B	234	ARG	2.7
1	A	482	ARG	2.6
1	A	322	SER	2.6
1	A	442	GLN	2.6
1	A	363	THR	2.6
1	A	305	GLU	2.5
1	A	430	LEU	2.5
1	A	359	PHE	2.5
1	A	304	SER	2.5
1	A	321	LYS	2.5
1	A	284	GLY	2.5
1	A	554	GLY	2.5
1	A	319	ASP	2.4
1	A	595	ILE	2.4
1	A	237	GLN	2.4
1	A	477	ILE	2.3
1	A	478	HIS	2.3
1	B	553	HIS	2.3
1	A	64	LEU	2.2
1	B	236	PRO	2.2
1	A	320	GLY	2.2
1	A	315	VAL	2.2
1	A	234	ARG	2.2
1	A	62	GLN	2.2
1	B	421	ASP	2.2
1	B	237	GLN	2.2
1	A	597	ASN	2.2
1	A	592	CYS	2.2
1	A	419	ASN	2.1
1	B	83	GLU	2.1
1	A	180	ARG	2.1
1	B	213	ARG	2.1
1	A	555	ALA	2.1
1	A	357	GLN	2.1
1	A	427	ARG	2.1
1	B	37	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLN	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	623	5/5	0.50	0.17	77,77,77,79	0
2	SO4	A	624	5/5	0.56	0.17	70,71,71,72	0
2	SO4	A	620	5/5	0.64	0.15	76,76,77,78	0
2	SO4	B	618	5/5	0.66	0.14	72,72,73,75	0
2	SO4	A	621	5/5	0.78	0.12	75,75,75,76	0
2	SO4	A	622	5/5	0.79	0.13	69,70,70,70	0
2	SO4	A	619	5/5	0.85	0.13	71,71,71,71	0
2	SO4	B	616	5/5	0.88	0.15	61,61,62,63	0
2	SO4	A	618	5/5	0.88	0.13	56,57,58,59	0
2	SO4	B	621	5/5	0.91	0.18	62,63,64,64	0
2	SO4	B	620	5/5	0.93	0.12	60,61,62,63	0
2	SO4	A	617	5/5	0.96	0.09	34,36,37,39	0
2	SO4	B	619	5/5	0.97	0.08	37,40,41,42	0
2	SO4	A	616	5/5	0.98	0.07	35,35,37,38	0
2	SO4	B	617	5/5	0.98	0.10	46,49,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.