WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 03:33 PM GMT

PDB ID   :   3RB5
Title   :   Crystal structure of calcium binding domain CBD12 of CALX1.1
Authors   :   Wu, M.; Zheng, L.
Deposited on :   2011-03-28
Resolution :   2.35 Å(reported)

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

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

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		42
Ramachandran outliers		3.8%
Sidechain outliers		14.3%
RSRZ outliers		0.6%

Worse　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
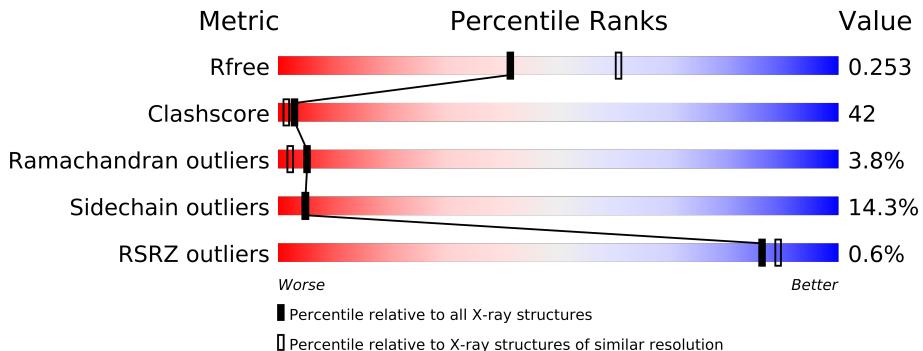
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	298	
1	B	298	
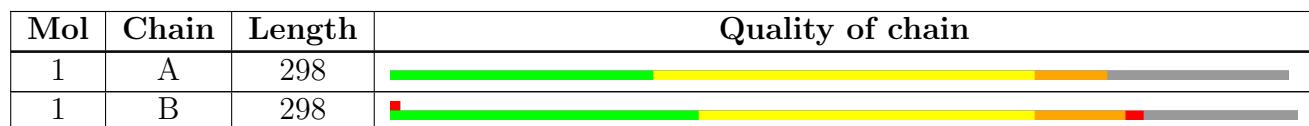
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	2	-	X
2	CA	A	3	-	X
2	CA	A	4	-	X
2	CA	B	1	-	X
2	CA	B	2	-	X
2	CA	B	4	-	X
3	MPD	A	4984	-	X

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3966 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Na/Ca exchange protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1912	1216	315	374	7			
1	B	245	Total	C	N	O	S	0	0	0
			1961	1247	319	388	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	652	GLU	GLY	SEE REMARK 999	UNP Q24413
B	652	GLU	GLY	SEE REMARK 999	UNP Q24413

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Ca	0	0
			4	4		
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
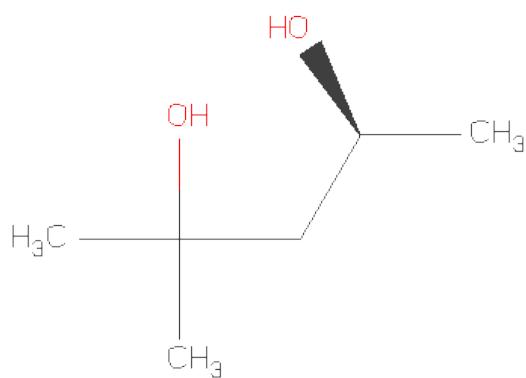
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C O			0	0
			8	6	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
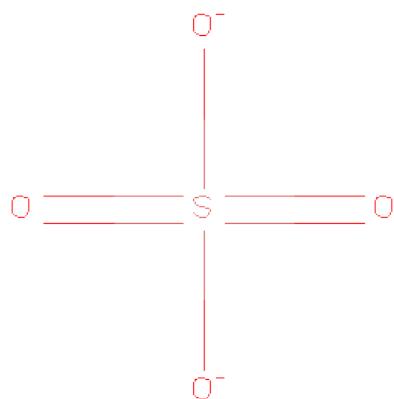
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total O S			0	0
			5	4	1		
4	A	1	Total O S			0	0
			5	4	1		
4	A	1	Total O S			0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total 21	O 21	0	0
5	B	21	Total 21	O 21	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Na/Ca exchange protein

Chain A:

- Molecule 1: Na/Ca exchange protein

Chain B:
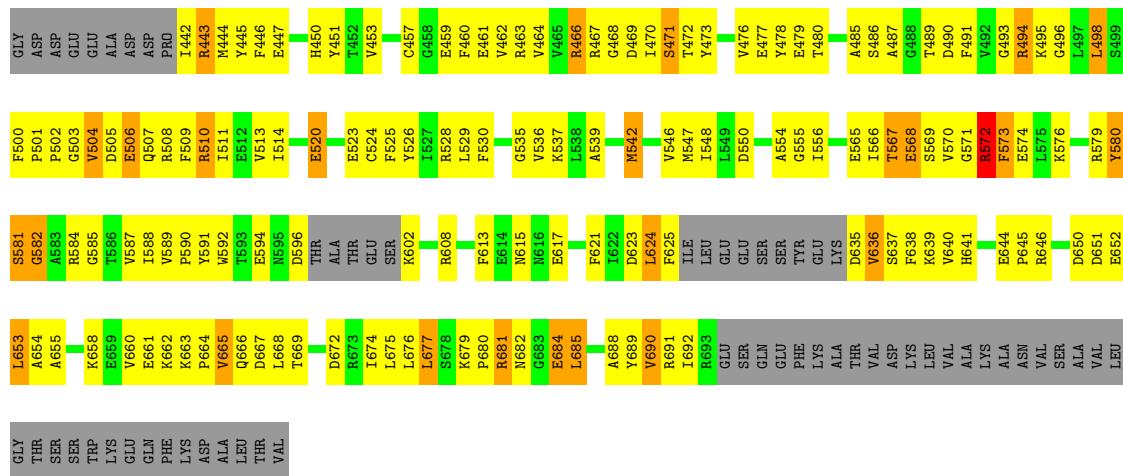
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	63.09Å 63.09Å 227.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.46 – 2.35 38.45 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.46-2.35) 98.9 (38.45-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.258 0.223 , 0.253	Depositor DCC
R_{free} test set	1819 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 29.9	EDS
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Outliers	0 of 36396 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CA, 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	0.43	0/1949	0.64	0/2631
1	B	0.48	0/1999	0.64	0/2702
All	All	0.46	0/3948	0.64	0/5333

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	ARG	Peptide
1	A	580	TYR	Peptide
1	A	581	SER	Peptide
1	A	582	GLY	Peptide
1	B	569	SER	Peptide

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1912	0	1853	158	0
1	B	1961	0	1901	182	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	8	0	14	3	0
4	A	15	0	0	1	0
4	B	20	0	0	3	0
5	A	21	0	0	1	0
5	B	21	0	0	1	0
All	All	3966	0	3768	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:602:LYS:O	1:B:603:ASP:HB2	1.44	1.07
1:B:450:HIS:HB2	5:B:35:HOH:O	1.57	1.04
1:B:569:SER:HA	1:B:626:ILE:CD1	1.88	1.03
1:A:664:PRO:HA	1:B:664:PRO:HA	1.38	1.02
1:B:585:GLY:H	1:B:615:ASN:HD22	1.14	0.96
1:B:579:ARG:HB3	1:B:618:SER:HA	1.48	0.94
1:B:600:GLU:O	1:B:601:SER:HB2	1.69	0.90
1:A:624:LEU:HA	1:A:625:PHE:HB2	1.53	0.90
1:B:569:SER:HA	1:B:626:ILE:CG1	2.02	0.89
1:A:453:VAL:HG11	1:A:513:VAL:HG21	1.53	0.88
1:B:605:GLU:CG	1:B:627:LEU:HD13	2.06	0.85
1:B:569:SER:HA	1:B:626:ILE:HD11	1.56	0.85
1:B:576:LYS:HD3	1:B:578:MET:HE2	1.59	0.84
1:B:626:ILE:O	1:B:626:ILE:HG13	1.77	0.83
1:B:569:SER:HA	1:B:626:ILE:HG13	1.58	0.83
1:B:492:VAL:CG1	1:B:512:GLU:HB2	2.11	0.81
1:B:648:ALA:HB3	1:B:651:ASP:OD2	1.81	0.81
1:A:589:VAL:HG22	1:A:645:PRO:HA	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:VAL:N	1:B:571:GLY:HA2	1.94	0.81
1:B:636:VAL:N	1:B:692:ILE:HD12	1.96	0.81
1:B:653:LEU:HD11	1:B:675:LEU:HD11	1.64	0.80
1:A:478:TYR:HE1	1:A:498:LEU:HD13	1.47	0.79
1:B:487:ALA:HA	1:B:491:PHE:O	1.81	0.79
1:B:605:GLU:HG2	1:B:627:LEU:HD13	1.64	0.79
1:A:486:SER:HB2	1:A:489:THR:OG1	1.83	0.78
1:A:494:ARG:HH22	1:A:510:ARG:HH21	1.32	0.77
1:B:600:GLU:O	1:B:601:SER:CB	2.33	0.76
1:B:576:LYS:HD3	1:B:578:MET:CE	2.15	0.76
1:B:569:SER:CA	1:B:626:ILE:HD11	2.15	0.76
1:B:620:LYS:HE3	4:B:5:SO4:O4	1.85	0.76
1:A:666:GLN:NE2	1:B:662:LYS:HA	2.01	0.75
1:B:585:GLY:H	1:B:615:ASN:ND2	1.85	0.73
1:A:476:VAL:HG23	1:A:530:PHE:O	1.88	0.73
1:A:666:GLN:HE22	1:B:662:LYS:HD2	1.52	0.72
1:A:445:TYR:HB3	1:A:539:ALA:HB3	1.69	0.72
1:A:635:ASP:HA	1:A:692:ILE:O	1.90	0.72
1:B:597:THR:HB	1:B:637:SER:H	1.54	0.71
1:B:653:LEU:O	1:B:657:ILE:HG13	1.91	0.71
1:A:572:ARG:HA	1:A:573:PHE:HB3	1.72	0.71
1:A:490:ASP:HB3	1:A:548:ILE:HD12	1.72	0.70
1:A:460:PHE:CZ	1:A:546:VAL:HG11	2.26	0.70
1:B:598:ALA:HB2	1:B:636:VAL:N	2.07	0.70
1:B:584:ARG:HH11	1:B:615:ASN:HD21	1.38	0.70
1:A:684:GLU:HG2	1:A:685:LEU:H	1.55	0.70
1:A:596:ASP:HB3	1:A:637:SER:O	1.93	0.68
1:B:595:ASN:OD1	1:B:600:GLU:HB2	1.94	0.68
1:A:442:ILE:HD12	1:A:535:GLY:O	1.92	0.68
1:B:452:THR:HG23	1:B:547:MET:HG2	1.76	0.68
1:B:602:LYS:O	1:B:603:ASP:CB	2.32	0.68
1:B:615:ASN:O	1:B:616:ASN:HB2	1.93	0.68
1:B:564:PHE:CE2	1:B:575:LEU:HD11	2.29	0.67
1:B:570:VAL:HG23	1:B:570:VAL:O	1.95	0.67
1:B:648:ALA:CB	1:B:651:ASP:OD2	2.42	0.66
1:B:652:GLU:O	1:B:653:LEU:C	2.32	0.66
1:B:605:GLU:HG3	1:B:627:LEU:HD13	1.78	0.66
1:A:556:ILE:HD11	1:A:681:ARG:NH2	2.10	0.66
1:B:653:LEU:HG	1:B:657:ILE:HD11	1.77	0.66
1:A:446:PHE:CD2	1:A:464:VAL:HG22	2.30	0.66
1:B:569:SER:OG	1:B:628:GLU:HA	1.95	0.66
1:A:664:PRO:HA	1:B:664:PRO:CA	2.20	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:596:ASP:HB3	1:B:637:SER:O	1.96	0.65
1:A:585:GLY:H	1:A:615:ASN:ND2	1.95	0.65
1:B:475:SER:HA	1:B:498:LEU:O	1.97	0.65
1:B:570:VAL:HG12	1:B:626:ILE:HD11	1.79	0.65
1:A:478:TYR:CE1	1:A:498:LEU:HD13	2.32	0.64
1:A:585:GLY:N	1:A:615:ASN:ND2	2.45	0.64
1:A:443:ARG:HG2	1:A:467:ARG:HB2	1.78	0.64
1:A:442:ILE:CD1	1:A:469:ASP:HB3	2.28	0.64
1:B:570:VAL:CG2	1:B:570:VAL:O	2.44	0.64
1:B:568:GLU:O	1:B:626:ILE:HD12	1.98	0.64
1:B:558:ALA:HB3	1:B:580:TYR:HE2	1.63	0.64
1:B:603:ASP:O	1:B:626:ILE:HB	1.98	0.64
1:A:444:MET:CE	1:A:466:ARG:HG3	2.28	0.64
1:A:466:ARG:HH21	1:A:500:PHE:HB3	1.63	0.64
1:A:466:ARG:HB2	1:A:500:PHE:CE2	2.33	0.63
1:B:568:GLU:HG2	1:B:570:VAL:HB	1.80	0.63
1:A:464:VAL:O	1:A:506:GLU:HA	1.99	0.62
1:B:492:VAL:HG13	1:B:512:GLU:HB2	1.79	0.62
1:B:653:LEU:HG	1:B:657:ILE:CD1	2.30	0.62
1:B:652:GLU:O	1:B:655:ALA:N	2.33	0.62
1:A:668:LEU:HD11	1:B:665:VAL:CG2	2.30	0.62
1:B:568:GLU:O	1:B:626:ILE:CD1	2.48	0.62
1:A:666:GLN:HE21	1:B:662:LYS:HA	1.65	0.62
1:A:565:GLU:HG3	1:A:691:ARG:HE	1.63	0.62
1:A:569:SER:HB2	5:A:10:HOH:O	1.99	0.62
1:A:589:VAL:HG22	1:A:645:PRO:CA	2.29	0.61
1:A:613:PHE:HD1	1:A:617:GLU:O	1.84	0.61
3:A:4984:MPD:H13	1:B:481:GLN:OE1	2.01	0.61
1:B:542:MET:SD	1:B:543:ILE:HG13	2.40	0.60
1:A:442:ILE:HD13	1:A:469:ASP:HB3	1.82	0.60
1:B:475:SER:OG	1:B:497:LEU:HD11	2.01	0.60
1:A:470:ILE:O	1:A:472:THR:N	2.34	0.60
1:B:470:ILE:HG22	1:B:503:GLY:H	1.66	0.60
1:B:601:SER:O	1:B:627:LEU:CB	2.50	0.60
1:A:453:VAL:HG13	1:A:457:CYS:SG	2.42	0.59
1:B:510:ARG:NE	1:B:510:ARG:H	1.99	0.59
1:A:661:GLU:O	1:B:666:GLN:HB2	2.02	0.59
1:B:615:ASN:O	1:B:615:ASN:CG	2.40	0.59
1:B:572:ARG:HA	1:B:625:PHE:HA	1.85	0.59
1:A:663:LYS:HZ1	1:A:669:THR:HG23	1.67	0.59
1:A:478:TYR:HA	1:A:528:ARG:O	2.02	0.59
1:A:471:SER:O	1:A:502:PRO:HB3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:487:ALA:HB2	1:A:491:PHE:CZ	2.37	0.59
1:A:453:VAL:CG1	1:A:513:VAL:HG21	2.28	0.58
1:B:601:SER:O	1:B:627:LEU:HB3	2.03	0.58
1:A:539:ALA:O	1:A:542:MET:HG3	2.03	0.58
1:A:674:ILE:HA	1:A:677:LEU:CD2	2.34	0.58
1:A:460:PHE:HZ	1:A:546:VAL:HG21	1.69	0.58
1:B:611:LEU:HD13	1:B:620:LYS:HB2	1.86	0.58
1:B:576:LYS:HB2	1:B:621:PHE:CE1	2.39	0.58
1:A:660:VAL:CG1	1:A:672:ASP:HB3	2.33	0.58
1:B:639:LYS:CD	1:B:641:HIS:NE2	2.67	0.58
1:A:684:GLU:HG2	1:A:685:LEU:HG	1.86	0.57
1:B:614:GLU:O	1:B:616:ASN:N	2.36	0.57
1:B:585:GLY:N	1:B:615:ASN:HD22	1.95	0.57
1:B:597:THR:N	1:B:637:SER:O	2.32	0.57
1:A:668:LEU:HD11	1:B:665:VAL:HG21	1.87	0.57
1:B:557:PHE:HA	1:B:578:MET:O	2.04	0.57
1:A:660:VAL:CG1	1:A:668:LEU:HD22	2.34	0.56
1:A:525:PHE:CE2	1:A:546:VAL:HB	2.41	0.56
1:A:591:TYR:O	1:A:608:ARG:HA	2.05	0.56
1:B:579:ARG:HB3	1:B:618:SER:CA	2.27	0.56
1:A:588:ILE:C	1:A:589:VAL:HG23	2.26	0.56
1:B:470:ILE:HG22	1:B:470:ILE:O	2.06	0.56
1:A:637:SER:OG	1:A:691:ARG:HA	2.06	0.56
1:B:639:LYS:HD2	1:B:641:HIS:NE2	2.21	0.55
1:B:472:THR:OG1	1:B:473:TYR:N	2.40	0.55
1:B:568:GLU:CG	1:B:569:SER:H	2.18	0.55
1:B:585:GLY:O	1:B:615:ASN:HA	2.05	0.55
1:B:476:VAL:HG22	1:B:477:GLU:N	2.21	0.55
1:A:664:PRO:CA	1:B:664:PRO:HA	2.24	0.55
1:A:556:ILE:HD11	1:A:681:ARG:HH21	1.71	0.55
1:A:637:SER:HA	1:A:690:VAL:O	2.07	0.55
1:B:567:THR:O	1:B:692:ILE:HG23	2.06	0.54
1:B:463:ARG:HH21	1:B:506:GLU:CD	2.10	0.54
1:A:674:ILE:HA	1:A:677:LEU:HD22	1.87	0.54
1:B:579:ARG:CB	1:B:618:SER:HA	2.31	0.54
1:A:665:VAL:HG12	1:B:665:VAL:HG22	1.89	0.54
1:A:689:TYR:HE1	3:A:4984:MPD:H53	1.72	0.54
1:B:593:THR:HG21	1:B:606:GLY:HA2	1.89	0.54
1:A:584:ARG:HA	1:A:615:ASN:HD21	1.72	0.54
1:B:587:VAL:O	1:B:589:VAL:HG23	2.08	0.54
1:A:585:GLY:H	1:A:615:ASN:HD21	1.55	0.54
1:B:597:THR:HB	1:B:637:SER:N	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:ASP:OD1	1:A:523:GLU:OE1	2.26	0.54
1:A:645:PRO:HB2	1:A:680:PRO:HB2	1.90	0.54
1:B:524:CYS:HA	1:B:546:VAL:O	2.07	0.54
1:B:655:ALA:O	1:B:658:LYS:HG2	2.08	0.53
1:A:588:ILE:O	1:A:589:VAL:CG2	2.55	0.53
1:A:485:ALA:N	1:A:524:CYS:O	2.39	0.53
1:A:594:GLU:O	1:A:638:PHE:HB2	2.09	0.53
1:A:588:ILE:O	1:A:589:VAL:HG23	2.09	0.53
1:A:461:GLU:CD	1:A:508:ARG:HD3	2.28	0.53
1:A:498:LEU:HD21	1:A:509:PHE:CD1	2.43	0.53
1:B:573:PHE:CD2	1:B:574:GLU:N	2.77	0.53
1:B:569:SER:CA	1:B:626:ILE:CD1	2.73	0.53
1:B:557:PHE:HB2	1:B:682:ASN:HD22	1.74	0.53
1:B:536:VAL:HG22	1:B:537:LYS:O	2.09	0.52
1:A:660:VAL:HG21	1:A:675:LEU:HD23	1.91	0.52
1:A:660:VAL:HG13	1:A:672:ASP:HB3	1.91	0.52
1:B:572:ARG:HA	1:B:625:PHE:HB3	1.91	0.52
1:A:470:ILE:HD12	1:A:470:ILE:H	1.75	0.52
1:B:564:PHE:HE2	1:B:688:ALA:HB1	1.74	0.52
1:A:520:GLU:OE2	1:A:523:GLU:OE1	2.28	0.52
1:B:564:PHE:CZ	1:B:575:LEU:HD11	2.44	0.52
1:B:656:LYS:O	1:B:660:VAL:HG12	2.10	0.52
1:A:660:VAL:HG12	1:A:668:LEU:HD22	1.91	0.52
1:B:576:LYS:CD	1:B:578:MET:HE2	2.36	0.51
1:A:444:MET:HE3	1:A:466:ARG:HG3	1.92	0.51
1:A:573:PHE:CD1	1:A:573:PHE:O	2.64	0.51
1:A:501:PRO:O	1:A:504:VAL:HG13	2.11	0.51
1:B:589:VAL:HG21	1:B:613:PHE:CD2	2.46	0.51
1:B:676:LEU:O	1:B:679:LYS:HE3	2.11	0.51
1:B:568:GLU:CG	1:B:569:SER:N	2.75	0.50
1:A:478:TYR:CZ	1:A:496:GLY:HA3	2.47	0.50
1:A:478:TYR:CD1	1:A:498:LEU:HD22	2.47	0.50
1:B:475:SER:CB	1:B:497:LEU:HD11	2.42	0.50
1:A:466:ARG:HB2	1:A:500:PHE:CD2	2.46	0.50
1:A:592:TRP:CE2	1:A:641:HIS:HB2	2.47	0.50
1:A:666:GLN:NE2	1:B:662:LYS:HD2	2.23	0.50
1:B:469:ASP:C	1:B:471:SER:H	2.14	0.50
1:B:584:ARG:HH11	1:B:584:ARG:HA	1.76	0.50
1:B:444:MET:O	1:B:539:ALA:N	2.44	0.50
1:B:593:THR:HB	1:B:607:ALA:O	2.11	0.49
1:B:515:ASP:OD2	1:B:516:ASP:N	2.45	0.49
1:B:584:ARG:NH1	1:B:615:ASN:HD21	2.08	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:652:GLU:O	1:B:654:ALA:N	2.45	0.49
1:A:468:GLY:O	1:A:470:ILE:HD12	2.12	0.49
1:B:525:PHE:CE2	1:B:546:VAL:HG11	2.47	0.49
1:A:638:PHE:CE1	1:A:690:VAL:HB	2.47	0.49
1:A:663:LYS:O	1:A:664:PRO:C	2.49	0.49
1:B:651:ASP:O	1:B:652:GLU:C	2.51	0.49
1:B:583:ALA:HB3	1:B:616:ASN:HD22	1.76	0.49
1:A:568:GLU:HG2	1:A:569:SER:H	1.77	0.49
1:A:470:ILE:HG22	1:A:503:GLY:H	1.78	0.49
1:B:651:ASP:O	1:B:654:ALA:N	2.46	0.49
1:A:473:TYR:C	1:A:473:TYR:CD2	2.85	0.49
1:A:667:ASP:O	1:A:668:LEU:C	2.51	0.49
1:A:636:VAL:HG23	1:A:692:ILE:HB	1.94	0.49
1:A:684:GLU:HG2	1:A:685:LEU:N	2.24	0.48
1:A:450:HIS:HB3	4:A:732:SO4:O4	2.13	0.48
1:B:585:GLY:N	1:B:615:ASN:ND2	2.58	0.48
1:B:615:ASN:O	1:B:616:ASN:CB	2.57	0.48
1:A:485:ALA:HB2	1:A:523:GLU:HB3	1.96	0.48
1:A:466:ARG:HB3	1:A:505:ASP:HA	1.95	0.48
1:B:501:PRO:O	1:B:504:VAL:HG13	2.14	0.48
1:B:531:ASN:N	1:B:532:PRO:CD	2.76	0.48
1:B:651:ASP:O	1:B:654:ALA:HB3	2.13	0.48
1:A:587:VAL:HG12	1:A:589:VAL:HG23	1.96	0.48
1:B:579:ARG:HD3	1:B:617:GLU:O	2.14	0.48
1:B:519:PHE:CD1	1:B:678:SER:HB3	2.49	0.48
1:B:603:ASP:O	1:B:627:LEU:O	2.32	0.47
1:B:554:ALA:HB3	1:B:555:GLY:HA2	1.96	0.47
1:A:469:ASP:C	1:A:469:ASP:OD1	2.52	0.47
1:A:651:ASP:O	1:A:653:LEU:N	2.48	0.47
1:A:676:LEU:HD21	1:B:665:VAL:HG11	1.96	0.47
1:A:555:GLY:O	1:A:680:PRO:HA	2.15	0.47
1:A:523:GLU:O	1:A:547:MET:HG3	2.15	0.47
1:A:624:LEU:N	1:A:624:LEU:HD12	2.29	0.47
1:B:519:PHE:HD1	1:B:678:SER:HB3	1.80	0.47
1:A:485:ALA:HB3	1:A:524:CYS:O	2.15	0.46
1:A:507:GLN:HA	1:A:507:GLN:OE1	2.15	0.46
1:A:460:PHE:CZ	1:A:546:VAL:HG21	2.49	0.46
1:A:444:MET:HE2	1:A:466:ARG:HG3	1.98	0.46
1:A:660:VAL:HG11	1:A:672:ASP:HB3	1.96	0.46
1:B:672:ASP:O	1:B:673:ARG:C	2.53	0.46
1:A:677:LEU:HD22	1:A:677:LEU:H	1.80	0.46
1:A:480:THR:OG1	1:A:493:GLY:HA2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:494:ARG:HH12	1:B:510:ARG:CZ	2.29	0.46
1:A:446:PHE:CE2	1:A:464:VAL:HG22	2.51	0.46
1:A:508:ARG:O	1:A:509:PHE:HB3	2.15	0.46
1:B:568:GLU:C	1:B:626:ILE:HD11	2.36	0.46
1:B:605:GLU:HB2	1:B:625:PHE:O	2.16	0.46
1:B:454:MET:CE	1:B:551:ASP:HB3	2.46	0.46
1:B:534:GLU:HG2	1:B:534:GLU:H	1.56	0.46
1:B:617:GLU:HG3	1:B:619:GLU:H	1.80	0.45
1:A:579:ARG:NH2	1:A:584:ARG:O	2.49	0.45
1:A:500:PHE:HD2	1:A:504:VAL:O	1.99	0.45
1:A:651:ASP:O	1:A:654:ALA:N	2.49	0.45
1:A:663:LYS:NZ	1:A:669:THR:HG23	2.32	0.45
1:B:485:ALA:HB1	1:B:490:ASP:HB3	1.98	0.45
1:A:554:ALA:N	1:A:555:GLY:HA2	2.32	0.45
1:A:479:GLU:CB	1:A:495:LYS:HD3	2.47	0.45
1:B:481:GLN:NE2	1:B:528:ARG:HD3	2.31	0.45
1:A:662:LYS:O	1:B:664:PRO:HB3	2.17	0.45
1:B:557:PHE:HB2	1:B:682:ASN:ND2	2.31	0.45
1:A:567:THR:O	1:A:568:GLU:C	2.55	0.45
1:B:455:GLU:O	1:B:455:GLU:HG2	2.16	0.45
1:B:485:ALA:HB1	1:B:490:ASP:CB	2.46	0.45
1:A:459:GLU:HB2	1:A:511:ILE:O	2.18	0.44
1:B:564:PHE:CE2	1:B:688:ALA:HB1	2.53	0.44
1:A:676:LEU:CD2	1:B:665:VAL:HG11	2.47	0.44
1:B:623:ASP:OD2	1:B:623:ASP:N	2.50	0.44
1:B:599:THR:O	1:B:601:SER:N	2.50	0.44
1:B:510:ARG:H	1:B:510:ARG:HE	1.62	0.44
1:B:664:PRO:HG2	1:B:667:ASP:OD2	2.18	0.43
1:A:689:TYR:OH	3:A:4984:MPD:H31	2.17	0.43
1:B:454:MET:HE3	1:B:551:ASP:HB3	2.00	0.43
1:B:569:SER:CA	1:B:626:ILE:HG13	2.39	0.43
1:B:466:ARG:NH2	1:B:500:PHE:HB3	2.33	0.43
1:B:532:PRO:O	1:B:533:SER:C	2.56	0.43
1:B:492:VAL:HG11	1:B:512:GLU:HB2	1.97	0.43
1:B:593:THR:HB	1:B:607:ALA:H	1.83	0.43
1:A:576:LYS:HG3	1:A:621:PHE:CE1	2.54	0.43
1:A:478:TYR:O	1:A:495:LYS:HA	2.18	0.43
1:A:466:ARG:NH2	1:A:500:PHE:O	2.51	0.43
1:A:477:GLU:O	1:A:529:LEU:HA	2.18	0.43
1:B:596:ASP:CB	1:B:637:SER:O	2.66	0.43
1:A:447:GLU:O	1:A:463:ARG:HB3	2.19	0.43
1:A:635:ASP:CA	1:A:692:ILE:O	2.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:481:GLN:NE2	1:B:528:ARG:CD	2.82	0.43
1:B:481:GLN:HE22	1:B:528:ARG:HD2	1.84	0.43
1:B:466:ARG:HH21	1:B:500:PHE:HB3	1.84	0.42
1:A:574:GLU:OE1	1:A:623:ASP:OD2	2.37	0.42
1:A:596:ASP:HB2	1:A:638:PHE:HA	2.01	0.42
1:B:519:PHE:HA	1:B:550:ASP:OD2	2.19	0.42
1:A:501:PRO:HD2	1:A:504:VAL:HG11	2.01	0.42
1:B:536:VAL:HG22	1:B:537:LYS:N	2.34	0.42
1:B:604:TYR:CD1	1:B:638:PHE:HB3	2.53	0.42
1:B:568:GLU:HG2	1:B:570:VAL:CB	2.48	0.42
1:B:475:SER:HB2	1:B:497:LEU:HD11	2.02	0.42
1:A:580:TYR:O	1:A:582:GLY:N	2.52	0.42
1:A:466:ARG:O	1:A:505:ASP:HB2	2.19	0.42
1:B:562:SER:HB3	1:B:685:LEU:HD21	2.01	0.42
1:A:665:VAL:HA	1:A:668:LEU:HG	2.02	0.42
1:A:451:TYR:CE2	1:A:462:VAL:HG13	2.55	0.42
1:A:491:PHE:HA	1:A:514:ILE:HG13	2.02	0.42
1:B:609:GLY:O	1:B:610:GLU:HG3	2.18	0.42
1:A:684:GLU:CD	1:A:684:GLU:H	2.23	0.42
1:A:466:ARG:NH2	1:A:500:PHE:HB3	2.31	0.42
1:A:567:THR:OG1	1:A:570:VAL:HG23	2.20	0.42
1:A:639:LYS:HA	1:A:688:ALA:O	2.20	0.42
1:B:616:ASN:HD22	1:B:616:ASN:HA	1.54	0.42
1:B:470:ILE:HG22	1:B:503:GLY:N	2.33	0.42
1:B:476:VAL:CG2	1:B:477:GLU:N	2.82	0.42
1:B:579:ARG:NH1	1:B:613:PHE:HB3	2.35	0.41
1:A:485:ALA:HA	1:A:490:ASP:OD1	2.19	0.41
1:A:494:ARG:HH12	1:A:510:ARG:HE	1.69	0.41
1:A:473:TYR:HA	1:A:500:PHE:O	2.20	0.41
1:B:518:VAL:HG12	1:B:518:VAL:O	2.19	0.41
1:B:601:SER:O	1:B:627:LEU:HB2	2.19	0.41
1:A:572:ARG:CA	1:A:573:PHE:HB3	2.42	0.41
1:B:584:ARG:HA	1:B:615:ASN:ND2	2.36	0.41
1:B:652:GLU:HG2	1:B:652:GLU:H	1.44	0.41
1:B:636:VAL:HA	1:B:637:SER:HA	1.72	0.41
1:A:498:LEU:HA	1:A:498:LEU:HD12	1.77	0.41
1:B:653:LEU:CD1	1:B:675:LEU:HD11	2.42	0.41
1:A:536:VAL:CG2	1:A:537:LYS:N	2.83	0.41
1:A:536:VAL:HG22	1:A:537:LYS:N	2.36	0.41
1:B:451:TYR:O	1:B:547:MET:N	2.36	0.41
1:B:451:TYR:CZ	1:B:462:VAL:HG13	2.56	0.41
1:A:674:ILE:HA	1:A:677:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:565:GLU:HA	1:B:691:ARG:HB3	2.03	0.41
1:B:467:ARG:HB3	4:B:6:SO4:O2	2.21	0.41
1:A:655:ALA:O	1:A:658:LYS:N	2.54	0.41
1:B:655:ALA:HA	1:B:658:LYS:HD2	2.03	0.40
1:B:597:THR:CB	1:B:637:SER:H	2.28	0.40
1:A:498:LEU:HD21	1:A:509:PHE:CE1	2.56	0.40
1:A:442:ILE:C	1:A:536:VAL:HG23	2.41	0.40
1:A:589:VAL:HA	1:A:590:PRO:HD2	1.65	0.40
1:B:654:ALA:O	1:B:658:LYS:HB3	2.21	0.40
1:B:620:LYS:HE3	4:B:5:SO4:S	2.61	0.40
1:A:571:GLY:O	1:A:572:ARG:HB3	2.21	0.40
1:A:684:GLU:CG	1:A:685:LEU:H	2.28	0.40
1:A:588:ILE:C	1:A:589:VAL:CG2	2.89	0.40
1:A:565:GLU:O	1:A:566:ILE:HG23	2.21	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	232/298 (78%)	199 (86%)	28 (12%)	5 (2%)	10	7
1	B	241/298 (81%)	207 (86%)	21 (9%)	13 (5%)	3	1
All	All	473/596 (79%)	406 (86%)	49 (10%)	18 (4%)	5	2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	SER
1	A	568	GLU
1	A	573	PHE
1	B	600	GLU
1	B	601	SER
1	B	603	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	616	ASN
1	B	649	PRO
1	B	652	GLU
1	A	652	GLU
1	B	554	ALA
1	B	567	THR
1	B	615	ASN
1	A	684	GLU
1	B	627	LEU
1	B	673	ARG
1	B	470	ILE
1	B	501	PRO

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	207/259 (80%)	178 (86%)	29 (14%)	5	5
1	B	213/259 (82%)	182 (85%)	31 (15%)	5	4
All	All	420/518 (81%)	360 (86%)	60 (14%)	5	5

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	466	ARG
1	A	494	ARG
1	A	498	LEU
1	A	504	VAL
1	A	506	GLU
1	A	510	ARG
1	A	520	GLU
1	A	526	TYR
1	A	542	MET
1	A	550	ASP
1	A	567	THR
1	A	572	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	581	SER
1	A	602	LYS
1	A	624	LEU
1	A	636	VAL
1	A	640	VAL
1	A	644	GLU
1	A	646	ARG
1	A	650	ASP
1	A	653	LEU
1	A	665	VAL
1	A	677	LEU
1	A	679	LYS
1	A	681	ARG
1	A	682	ASN
1	A	685	LEU
1	A	690	VAL
1	B	443	ARG
1	B	466	ARG
1	B	472	THR
1	B	475	SER
1	B	492	VAL
1	B	504	VAL
1	B	510	ARG
1	B	534	GLU
1	B	562	SER
1	B	567	THR
1	B	568	GLU
1	B	570	VAL
1	B	593	THR
1	B	595	ASN
1	B	599	THR
1	B	601	SER
1	B	602	LYS
1	B	603	ASP
1	B	604	TYR
1	B	605	GLU
1	B	616	ASN
1	B	623	ASP
1	B	624	LEU
1	B	625	PHE
1	B	628	GLU
1	B	639	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	640	VAL
1	B	652	GLU
1	B	660	VAL
1	B	666	GLN
1	B	679	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	ASN
1	A	615	ASN
1	A	666	GLN
1	A	682	ASN
1	B	615	ASN
1	B	616	ASN
1	B	682	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	MPD	A	4984	-	7,7,7	0.35	0	10,10,10	0.36	0
4	SO4	A	7	-	4,4,4	0.05	0	6,6,6	0.18	0
4	SO4	A	731	-	4,4,4	0.13	0	6,6,6	0.18	0
4	SO4	A	732	-	4,4,4	0.07	0	6,6,6	0.14	0
4	SO4	B	5	-	4,4,4	0.12	0	6,6,6	0.12	0
4	SO4	B	6	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	B	731	-	4,4,4	0.17	0	6,6,6	0.21	0
4	SO4	B	8	-	4,4,4	0.14	0	6,6,6	0.09	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	MPD	A	4984	-	-	0/5/5/5	0/0/0/0
4	SO4	A	7	-	-	0/0/0/0	0/0/0/0
4	SO4	A	731	-	-	0/0/0/0	0/0/0/0
4	SO4	A	732	-	-	0/0/0/0	0/0/0/0
4	SO4	B	5	-	-	0/0/0/0	0/0/0/0
4	SO4	B	6	-	-	0/0/0/0	0/0/0/0
4	SO4	B	731	-	-	0/0/0/0	0/0/0/0
4	SO4	B	8	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	238/298 (79%)	-0.19	0 100	100	33, 50, 65, 77	0
1	B	245/298 (82%)	-0.09	3 (1%) 75	79	27, 50, 73, 90	0
All	All	483/596 (81%)	-0.14	3 (0%) 86	89	27, 50, 69, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	THR	2.5
1	B	627	LEU	2.2
1	B	592	TRP	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
2	CA	A	4	1/1	0.18	6.79	36,36,36,36	0
2	CA	A	2	1/1	0.18	5.18	41,41,41,41	0
2	CA	B	1	1/1	0.16	4.49	43,43,43,43	0
3	MPD	A	4984	8/8	0.23	4.32	38,52,56,59	0
2	CA	B	4	1/1	0.16	2.90	28,28,28,28	0
2	CA	A	3	1/1	0.16	2.85	39,39,39,39	0
2	CA	B	2	1/1	0.15	2.64	27,27,27,27	0
2	CA	B	3	1/1	0.13	1.11	44,44,44,44	0
2	CA	A	1	1/1	0.11	-0.32	51,51,51,51	0
4	SO4	A	732	5/5	0.10	-0.87	76,77,81,91	0
4	SO4	A	731	5/5	0.11	-1.33	45,54,59,74	0
4	SO4	B	731	5/5	0.07	-2.55	52,54,63,77	0
4	SO4	B	6	5/5	0.10	-2.67	72,77,78,82	0
4	SO4	B	5	5/5	0.07	-2.73	61,63,79,80	0
4	SO4	A	7	5/5	0.08	-3.55	55,58,60,71	0
4	SO4	B	8	5/5	0.08	-	81,87,104,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.