



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:12 pm BST

PDB ID : 4BB7  
Title : Crystal structure of the yeast Rsc2 BAH domain  
Authors : Chambers, A.L.; Pearl, L.H.; Oliver, A.W.; Downs, J.A.  
Deposited on : 2012-09-20  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



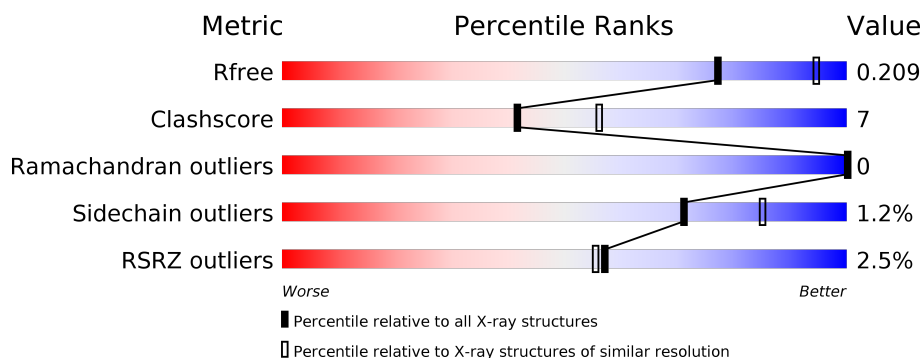
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	258	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>9%</div> </div> </div>
1	B	258	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>9%</div> </div> </div>
1	C	258	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	D	258	<div> <div></div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8175 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 CHROMATIN STRUCTURE-REMODELING COMPLEX SUBUNIT RSC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	3	0	0
			1893	1205	337	340	11			
1	B	234	Total	C	N	O	S	0	0	0
			1881	1200	331	339	11			
1	C	234	Total	C	N	O	S	0	0	0
			1893	1207	336	339	11			
1	D	235	Total	C	N	O	S	9	1	0
			1913	1218	340	344	11			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	384	MET	-	expression tag	UNP Q06488
A	385	HIS	-	expression tag	UNP Q06488
A	386	HIS	-	expression tag	UNP Q06488
A	387	HIS	-	expression tag	UNP Q06488
A	388	HIS	-	expression tag	UNP Q06488
A	389	HIS	-	expression tag	UNP Q06488
A	390	HIS	-	expression tag	UNP Q06488
A	391	LEU	-	expression tag	UNP Q06488
A	392	GLU	-	expression tag	UNP Q06488
A	393	VAL	-	expression tag	UNP Q06488
A	394	LEU	-	expression tag	UNP Q06488
A	395	PHE	-	expression tag	UNP Q06488
A	396	GLN	-	expression tag	UNP Q06488
A	397	GLY	-	expression tag	UNP Q06488
A	398	PRO	-	expression tag	UNP Q06488
A	399	HIS	-	expression tag	UNP Q06488
A	400	MET	-	expression tag	UNP Q06488
B	384	MET	-	expression tag	UNP Q06488
B	385	HIS	-	expression tag	UNP Q06488
B	386	HIS	-	expression tag	UNP Q06488

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Chain	Residue	Modelled	Actual	Comment	Reference
B	387	HIS	-	expression tag	UNP Q06488
B	388	HIS	-	expression tag	UNP Q06488
B	389	HIS	-	expression tag	UNP Q06488
B	390	HIS	-	expression tag	UNP Q06488
B	391	LEU	-	expression tag	UNP Q06488
B	392	GLU	-	expression tag	UNP Q06488
B	393	VAL	-	expression tag	UNP Q06488
B	394	LEU	-	expression tag	UNP Q06488
B	395	PHE	-	expression tag	UNP Q06488
B	396	GLN	-	expression tag	UNP Q06488
B	397	GLY	-	expression tag	UNP Q06488
B	398	PRO	-	expression tag	UNP Q06488
B	399	HIS	-	expression tag	UNP Q06488
B	400	MET	-	expression tag	UNP Q06488
C	384	MET	-	expression tag	UNP Q06488
C	385	HIS	-	expression tag	UNP Q06488
C	386	HIS	-	expression tag	UNP Q06488
C	387	HIS	-	expression tag	UNP Q06488
C	388	HIS	-	expression tag	UNP Q06488
C	389	HIS	-	expression tag	UNP Q06488
C	390	HIS	-	expression tag	UNP Q06488
C	391	LEU	-	expression tag	UNP Q06488
C	392	GLU	-	expression tag	UNP Q06488
C	393	VAL	-	expression tag	UNP Q06488
C	394	LEU	-	expression tag	UNP Q06488
C	395	PHE	-	expression tag	UNP Q06488
C	396	GLN	-	expression tag	UNP Q06488
C	397	GLY	-	expression tag	UNP Q06488
C	398	PRO	-	expression tag	UNP Q06488
C	399	HIS	-	expression tag	UNP Q06488
C	400	MET	-	expression tag	UNP Q06488
D	384	MET	-	expression tag	UNP Q06488
D	385	HIS	-	expression tag	UNP Q06488
D	386	HIS	-	expression tag	UNP Q06488
D	387	HIS	-	expression tag	UNP Q06488
D	388	HIS	-	expression tag	UNP Q06488
D	389	HIS	-	expression tag	UNP Q06488
D	390	HIS	-	expression tag	UNP Q06488
D	391	LEU	-	expression tag	UNP Q06488
D	392	GLU	-	expression tag	UNP Q06488
D	393	VAL	-	expression tag	UNP Q06488
D	394	LEU	-	expression tag	UNP Q06488

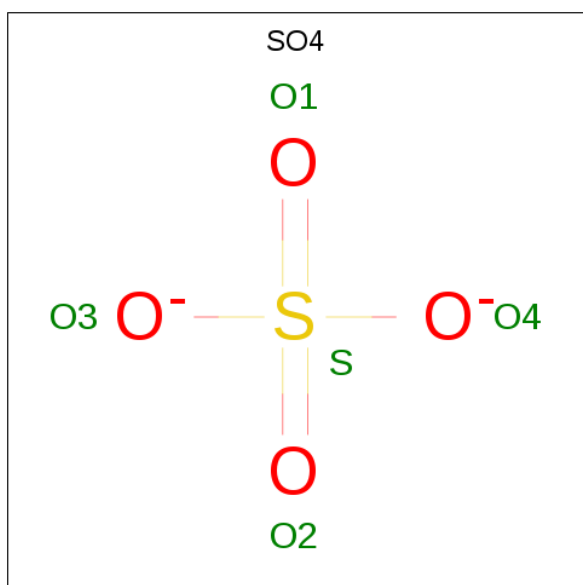
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Chain	Residue	Modelled	Actual	Comment	Reference
D	395	PHE	-	expression tag	UNP Q06488
D	396	GLN	-	expression tag	UNP Q06488
D	397	GLY	-	expression tag	UNP Q06488
D	398	PRO	-	expression tag	UNP Q06488
D	399	HIS	-	expression tag	UNP Q06488
D	400	MET	-	expression tag	UNP Q06488

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



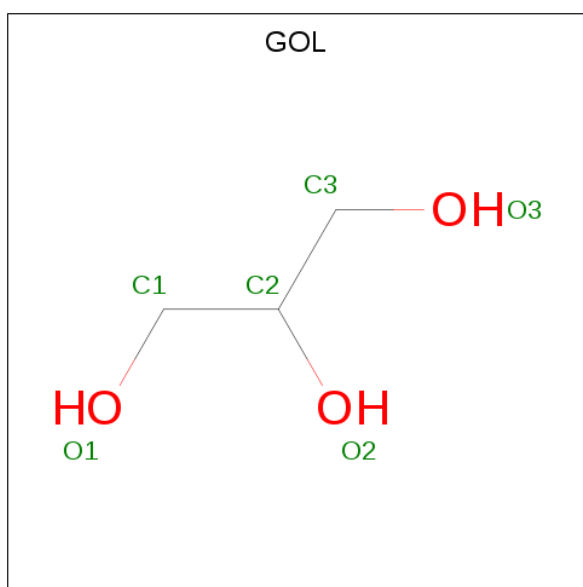
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0



- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Cl 3	0	0
3	A	2	Total 2	Cl 2	0	0
3	D	2	Total 2	Cl 2	0	0
3	C	1	Total 1	Cl 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	89	Total 89	O 89	0	0
5	C	172	Total 172	O 172	0	0
5	D	169	Total 169	O 169	0	0





• Molecule 1: CHROMATIN STRUCTURE-REMODELING COMPLEX SUBUNIT RSC2



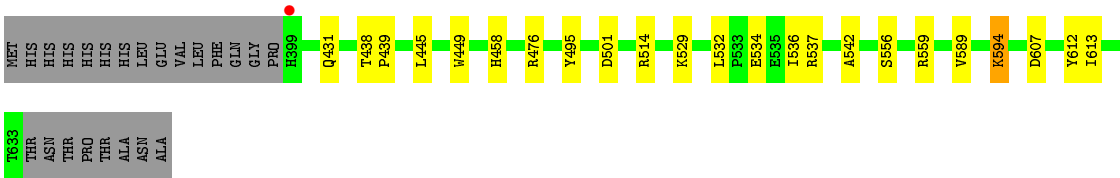


Chain D: 

82%

9%

9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.09 Å 64.07 Å 136.84 Å 90.00° 95.47° 90.00°	Depositor
Resolution (Å)	44.49 – 2.40 46.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.49-2.40) 98.6 (46.67-2.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.217 , 0.286 0.208 , 0.209	Depositor DCC
$R_{free}$ test set	2520 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4456e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: GOL, SO4, CL

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	0.23	0/1948	0.41	0/2653
1	B	0.24	0/1938	0.42	0/2641
1	C	0.28	0/1949	0.45	0/2655
1	D	0.27	0/1972	0.46	0/2685
All	All	0.26	0/7807	0.44	0/10634

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	1893	0	1820	34	0
1	B	1881	0	1797	40	0
1	C	1893	0	1832	19	0
1	D	1913	0	1853	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	1	0
4	D	6	0	8	0	0
5	A	111	0	0	4	0
5	B	89	0	0	0	0
5	C	172	0	0	2	0
5	D	169	0	0	2	0
All	All	8175	0	7310	105	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 7.

All (105) 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)
3:D:704:CL:CL	5:D:2164:HOH:O	2.38	0.77
1:A:490:ILE:HD12	1:A:500:PRO:HG3	1.67	0.74
1:B:558:ILE:HB	1:B:561:LEU:HD12	1.72	0.71
1:A:411:HIS:O	1:A:414:ASP:HB2	1.91	0.70
1:A:596:GLN:HG2	5:A:2094:HOH:O	1.91	0.69
1:A:435:LEU:HD23	1:A:445:LEU:HB3	1.75	0.68
1:B:460:VAL:HG12	1:B:589:VAL:HB	1.77	0.66
1:C:438:THR:HB	1:C:439:PRO:HD2	1.79	0.65
1:B:445:LEU:HD23	1:B:480:VAL:HG12	1.81	0.61
1:C:610:PRO:HG2	1:C:613:ILE:HD12	1.83	0.60
1:A:562:LEU:HD12	1:A:563:PRO:HD2	1.82	0.60
1:A:529:LYS:O	1:A:537:ARG:HG3	2.01	0.59
1:C:400:MET:HE1	1:C:403:VAL:HG12	1.85	0.59
1:C:440:ASP:OD2	1:C:442:LYS:HE2	2.02	0.58
1:B:549:ARG:HD2	1:B:631:THR:HB	1.85	0.58
1:B:458:HIS:O	1:B:589:VAL:HA	2.03	0.58
1:C:514:ARG:HG3	5:C:2091:HOH:O	2.04	0.57
1:A:558:ILE:HB	1:A:561:LEU:HD12	1.86	0.56
1:B:562:LEU:HD12	1:B:563:PRO:HD2	1.87	0.56
1:A:496:GLN:HG2	5:A:2050:HOH:O	2.05	0.55
1:A:601:GLY:HA2	5:A:2097:HOH:O	2.07	0.54
1:C:567:THR:HB	1:C:568:PRO:HD2	1.90	0.54
1:B:438:THR:HB	1:B:439:PRO:HD2	1.89	0.54
1:C:449:TRP:CZ2	1:C:476:ARG:HG3	2.43	0.54
1:B:616:PRO:O	1:B:617:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:TYR:HB3	1:B:555:PRO:HD2	1.91	0.52
1:B:463:LEU:HD21	1:B:604:ALA:HB2	1.92	0.52
1:B:532:LEU:HB3	1:B:536:ILE:HD11	1.91	0.52
1:D:501:ASP:HB3	1:D:542:ALA:HB3	1.93	0.51
1:C:557:PRO:HG3	5:C:2119:HOH:O	2.10	0.51
1:A:465:TYR:CZ	1:A:553:LYS:HE3	2.46	0.51
1:B:553:LYS:HD2	1:B:613:ILE:HD12	1.93	0.50
1:A:399:HIS:N	1:B:398:PRO:HB3	2.27	0.50
1:A:493:THR:O	1:A:497:ARG:HD3	2.11	0.50
1:B:614:ILE:HD13	1:B:620:PRO:HG3	1.93	0.50
1:D:438:THR:HB	1:D:439:PRO:HD2	1.94	0.50
1:B:445:LEU:C	1:B:445:LEU:HD12	2.31	0.49
1:A:463:LEU:HB3	1:A:553:LYS:HB3	1.93	0.49
1:D:534:GLU:HA	1:D:537:ARG:HG2	1.93	0.49
1:A:490:ILE:HG23	1:A:510:VAL:HG23	1.95	0.48
1:C:445:LEU:HD12	1:C:445:LEU:C	2.33	0.48
1:A:466:LYS:O	1:A:467:ASN:HB2	2.13	0.48
1:B:460:VAL:HG11	1:B:562:LEU:HD22	1.95	0.48
1:B:533:PRO:HD2	1:B:536:ILE:HD11	1.96	0.48
1:B:460:VAL:HG11	1:B:562:LEU:HD13	1.94	0.48
1:B:492:PHE:O	1:B:496:GLN:HG3	2.14	0.47
1:A:444:TRP:CE2	1:A:479:LEU:HD23	2.49	0.47
1:A:613:ILE:C	1:A:614:ILE:HD12	2.35	0.47
1:B:410:TYR:CD1	1:B:483:LEU:HD13	2.50	0.47
1:B:460:VAL:HG12	1:B:589:VAL:CG2	2.45	0.46
1:C:596:GLN:HG2	1:C:607:ASP:OD2	2.16	0.46
1:B:460:VAL:CG1	1:B:562:LEU:HD13	2.45	0.46
1:B:498:GLY:HA2	1:B:546:VAL:HG23	1.96	0.46
1:B:400:MET:HE1	1:B:403:VAL:HG12	1.98	0.46
1:B:459:ARG:HB3	1:B:461:ASP:OD1	2.15	0.46
1:D:529:LYS:O	1:D:537:ARG:HD3	2.16	0.46
1:A:478:HIS:HB3	1:A:482:ASN:HD22	1.81	0.45
1:C:463:LEU:HD21	1:C:604:ALA:HB2	1.98	0.45
1:A:501:ASP:OD1	1:A:544:ILE:HD11	2.16	0.45
1:B:450:TYR:CE2	1:B:471:LYS:HB2	2.52	0.45
1:D:556:SER:HB3	1:D:559:ARG:HB3	1.98	0.45
1:A:440:ASP:OD2	1:A:442:LYS:HE2	2.16	0.45
1:A:400:MET:HE2	1:A:435:LEU:HB3	1.98	0.44
1:A:410:TYR:CD1	1:A:483:LEU:HD13	2.51	0.44
1:C:411:HIS:O	1:C:414:ASP:HB2	2.17	0.44
1:B:489:VAL:HG22	1:B:509:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:SER:OG	1:C:620:PRO:HD2	2.18	0.44
1:D:458:HIS:O	1:D:589:VAL:HA	2.17	0.44
1:A:516:ASN:HB3	1:A:521:ILE:H	1.83	0.44
1:C:456:THR:O	1:C:587:GLY:HA3	2.18	0.44
1:B:543:THR:O	1:B:545:PRO:HD3	2.19	0.43
1:D:431:GLN:HE22	1:D:532:LEU:HD22	1.83	0.43
1:A:624:GLN:O	1:A:632:ILE:HA	2.17	0.43
1:D:445:LEU:C	1:D:445:LEU:HD12	2.38	0.43
1:B:533:PRO:HD2	1:B:536:ILE:CD1	2.49	0.43
1:D:514:ARG:HD3	5:D:2090:HOH:O	2.17	0.43
1:A:399:HIS:N	1:B:398:PRO:CB	2.81	0.43
1:A:400:MET:CE	1:A:435:LEU:HB3	2.49	0.43
1:A:403:VAL:HG11	1:A:480:VAL:HB	2.01	0.43
1:B:460:VAL:HG12	1:B:589:VAL:CB	2.46	0.42
1:C:475:TYR:CE2	1:D:439:PRO:HG2	2.54	0.42
1:B:425:GLN:O	1:B:427:PRO:HD3	2.19	0.42
1:D:534:GLU:HA	1:D:537:ARG:CG	2.48	0.42
1:D:612:TYR:CD1	1:D:613:ILE:HG13	2.54	0.42
1:A:501:ASP:HB3	1:A:542:ALA:HB3	2.01	0.42
1:D:594:LYS:NZ	1:D:607:ASP:OD1	2.48	0.42
1:B:550:LYS:HG2	1:B:612:TYR:HA	2.01	0.42
1:A:403:VAL:HG21	1:A:435:LEU:HD22	2.02	0.42
1:B:554:TYR:CD1	1:B:554:TYR:N	2.87	0.42
1:C:437:LYS:HB2	1:C:437:LYS:HE3	1.84	0.42
1:B:400:MET:HG2	1:B:437:LYS:NZ	2.35	0.41
1:B:533:PRO:O	1:B:536:ILE:HG12	2.20	0.41
1:B:422:ASN:ND2	1:B:583:PRO:O	2.54	0.41
1:A:449:TRP:CZ2	1:A:476:ARG:HG3	2.56	0.41
1:A:420:ASN:HB2	1:A:428:ILE:HG13	2.03	0.41
1:A:538:ASP:HB3	1:D:536:ILE:HA	2.02	0.41
1:A:414:ASP:OD2	1:A:486:LYS:HE2	2.20	0.41
1:B:488:TYR:O	1:B:508:LEU:HD12	2.21	0.41
1:C:458:HIS:O	1:C:589:VAL:HA	2.21	0.41
1:C:449:TRP:CE2	1:C:476:ARG:HG3	2.57	0.40
1:A:480:VAL:HG22	5:A:2027:HOH:O	2.21	0.40
1:C:556:SER:HA	1:C:557:PRO:HD3	1.96	0.40
1:B:438:THR:HB	1:B:439:PRO:CD	2.52	0.40
1:D:449:TRP:CZ2	1:D:476:ARG:HG3	2.56	0.40
1:B:567:THR:HB	1:B:568:PRO:HD2	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	231/258 (90%)	223 (96%)	8 (4%)	0	100	100
1	B	230/258 (89%)	213 (93%)	17 (7%)	0	100	100
1	C	232/258 (90%)	227 (98%)	5 (2%)	0	100	100
1	D	234/258 (91%)	227 (97%)	7 (3%)	0	100	100
All	All	927/1032 (90%)	890 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	203/233 (87%)	201 (99%)	2 (1%)	76	88
1	B	201/233 (86%)	198 (98%)	3 (2%)	65	80
1	C	204/233 (88%)	201 (98%)	3 (2%)	65	80
1	D	207/233 (89%)	205 (99%)	2 (1%)	76	88
All	All	815/932 (87%)	805 (99%)	10 (1%)	71	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	414	ASP
1	A	594	LYS

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Mol	Chain	Res	Type
1	B	437	LYS
1	B	594	LYS
1	B	628	GLU
1	C	594	LYS
1	C	595	MET
1	C	597	ARG
1	D	495	TYR
1	D	594	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	D	701	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	C	701	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	C	702	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	B	700	-	4,4,4	0.15	0	6,6,6	0.08	0
4	GOL	D	900	-	5,5,5	0.35	0	5,5,5	0.23	0
2	SO4	D	700	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	D	702	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	C	700	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	700	-	4,4,4	0.14	0	6,6,6	0.07	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
4	GOL	D	900	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	900	GOL	C1-C2-C3-O3
4	D	900	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	235/258 (91%)	0.29	9 (3%) 40 39	24, 33, 47, 56	1 (0%)
1	B	234/258 (90%)	0.25	11 (4%) 31 30	23, 32, 47, 57	0
1	C	234/258 (90%)	-0.05	2 (0%) 84 82	7, 16, 34, 49	0
1	D	235/258 (91%)	-0.12	1 (0%) 92 91	7, 15, 31, 46	2 (0%)
All	All	938/1032 (90%)	0.09	23 (2%) 57 55	7, 27, 43, 57	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	GLU	4.2
1	A	506	GLY	4.2
1	D	399	HIS	3.5
1	A	408	ILE	3.2
1	B	407	ASN	3.0
1	A	634	THR	2.9
1	A	400	MET	2.9
1	B	406	ASN	2.7
1	B	548	GLY	2.6
1	B	625	VAL	2.5
1	B	544	ILE	2.5
1	B	501	ASP	2.5
1	A	407	ASN	2.4
1	A	621	GLU	2.3
1	B	405	VAL	2.2
1	A	567	THR	2.2
1	A	401	ASP	2.2
1	C	407	ASN	2.2
1	C	501	ASP	2.2
1	B	633	THR	2.1
1	B	634	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	624	GLN	2.1
1	B	398	PRO	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	D	900	6/6	0.78	0.23	25,25,28,35	0
2	SO4	D	702	5/5	0.84	0.31	27,37,49,53	0
3	CL	D	704	1/1	0.88	0.11	49,49,49,49	0
2	SO4	D	701	5/5	0.89	0.19	20,23,41,44	0
3	CL	B	702	1/1	0.89	0.11	55,55,55,55	0
2	SO4	C	702	5/5	0.89	0.22	29,30,49,55	0
2	SO4	C	701	5/5	0.93	0.26	30,35,42,45	0
3	CL	B	701	1/1	0.93	0.20	44,44,44,44	0
3	CL	A	801	1/1	0.95	0.26	51,51,51,51	0
2	SO4	B	700	5/5	0.95	0.11	39,43,50,51	0
2	SO4	D	700	5/5	0.96	0.13	27,28,35,37	0
2	SO4	C	700	5/5	0.97	0.16	29,32,35,36	0
2	SO4	A	700	5/5	0.97	0.17	40,43,52,55	0
3	CL	B	703	1/1	0.98	0.13	27,27,27,27	0
3	CL	A	800	1/1	0.98	0.11	34,34,34,34	0
3	CL	D	703	1/1	0.99	0.15	14,14,14,14	0
3	CL	C	801	1/1	0.99	0.13	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.