



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:36 AM EDT

PDB ID : 3RSY  
Title : Cellobiose phosphorylase from *Cellulomonas uda* in complex with sulfate and glycerol  
Authors : Van Hoorebeke, A.; Stout, J.; Soetaert, W.; Van Beeumen, J.; Desmet, T.; Savvides, S.  
Deposited on : 2011-05-02  
Resolution : 1.81 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

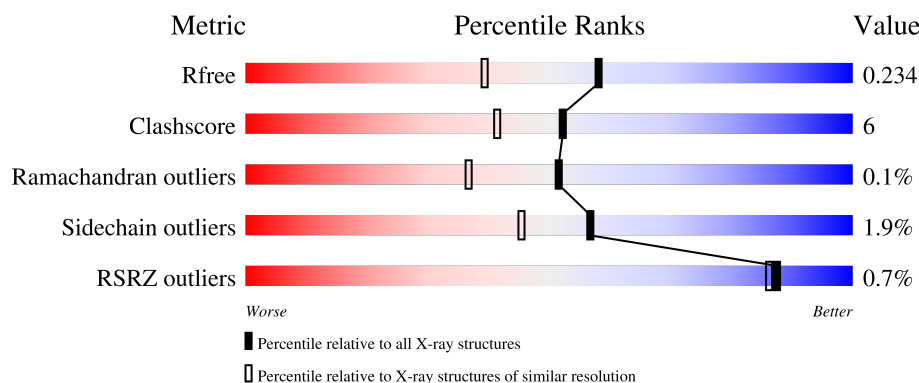
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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  $\geq 3$ , 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	822	
1	B	822	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26742 atoms, of which 12183 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 Cellobiose phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	822	Total	C	H	N	O	S	14	11	0
			12576	4114	6075	1113	1257	17			
1	B	822	Total	C	H	N	O	S	14	12	0
			12568	4105	6076	1110	1260	17			

- 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	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		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

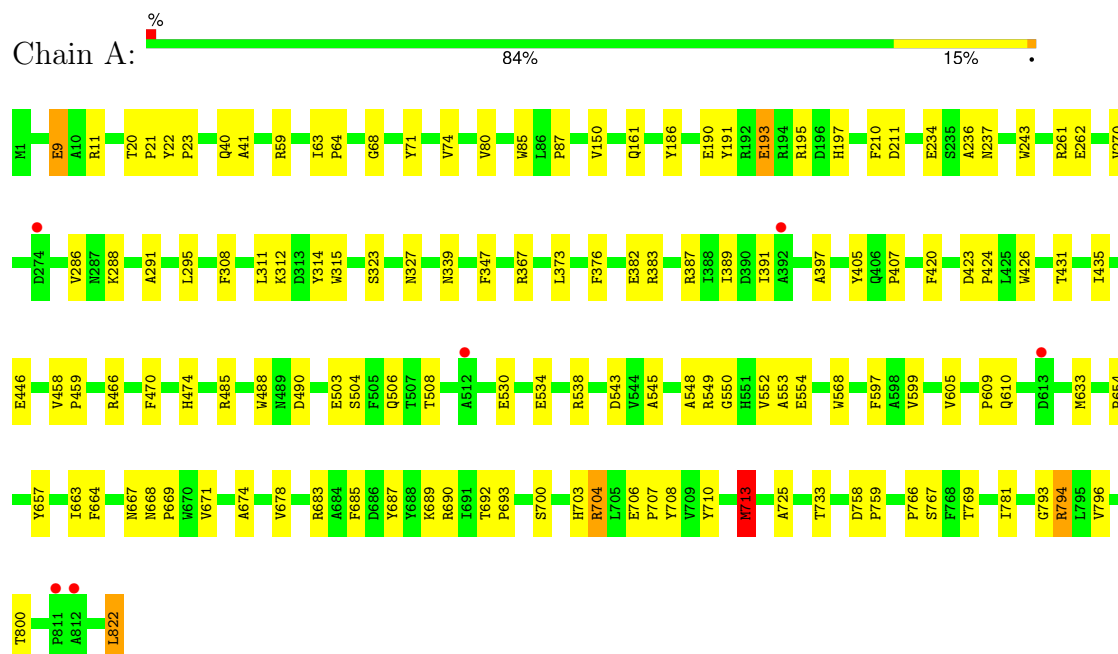
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	795	Total	O	0	0
			795	795		
4	B	727	Total	O	0	0
			727	727		

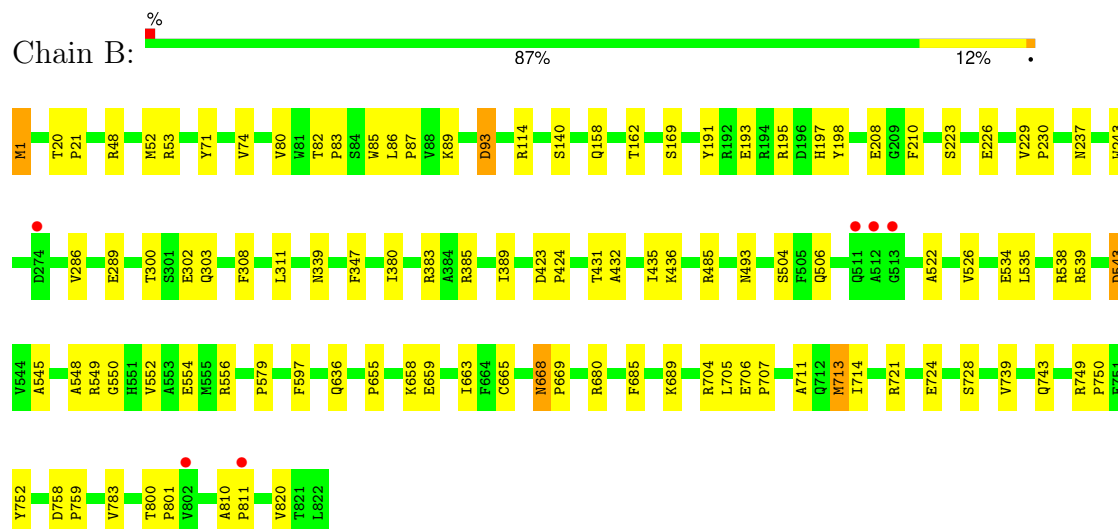
### 3 Residue-property plots [i](#)

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: Cellobiose phosphorylase



#### • Molecule 1: Cellobiose phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.10Å 103.78Å 99.15Å 90.00° 96.57° 90.00°	Depositor
Resolution (Å)	19.98 – 1.81 19.98 – 1.81	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.98-1.81) 94.6 (19.98-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.202 , 0.238 0.199 , 0.234	Depositor DCC
$R_{free}$ test set	7440 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.83	3/6687 (0.0%)	0.85	3/9117 (0.0%)
1	B	0.79	1/6692 (0.0%)	0.84	5/9124 (0.1%)
All	All	0.81	4/13379 (0.0%)	0.85	8/18241 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	TRP	NE1-CE2	-6.45	1.29	1.37
1	A	568	TRP	NE1-CE2	-5.29	1.30	1.37
1	A	243	TRP	NE1-CE2	-5.15	1.30	1.37
1	A	315	TRP	NE1-CE2	-5.03	1.31	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	543	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	48	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	543	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	543	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	713	MET	CG-SD-CE	-5.17	91.92	100.20
1	A	704	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	114	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	6501	6075	6087	82	0
1	B	6492	6076	6085	58	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	12	16	16	3	0
3	B	12	16	16	1	0
4	A	795	0	0	13	0
4	B	727	0	0	8	0
All	All	14559	12183	12204	140	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 6.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TRP:O	3:A:826:GOL:H12	1.44	1.14
1:B:71:TYR:CE2	1:B:87:PRO:HG3	2.03	0.94
1:A:490:ASP:H	3:A:826:GOL:H32	1.41	0.85
1:A:504:SER:O	1:A:508:THR:HG23	1.78	0.83
1:B:302:GLU:HA	4:B:1218:HOH:O	1.80	0.81
1:A:690:ARG:HA	4:A:1479:HOH:O	1.81	0.79
1:A:488:TRP:O	3:A:826:GOL:C1	2.29	0.76
1:B:347:PHE:HE2	1:B:383:ARG:NH1	1.86	0.74
1:A:503:GLU:HB3	1:A:508:THR:HG21	1.69	0.73
1:B:52:MET:HE3	4:B:1716:HOH:O	1.90	0.72
1:A:382[B]:GLU:OE2	4:A:1191:HOH:O	2.09	0.69
1:A:71:TYR:CE2	1:A:87:PRO:HG3	2.30	0.65
1:A:389:ILE:HD12	1:A:446:GLU:HG2	1.79	0.64
1:A:191:TYR:CE2	1:A:286:VAL:HG12	2.33	0.64
1:A:530:GLU:HG3	4:A:1221:HOH:O	1.99	0.61
1:B:191:TYR:CE2	1:B:286[B]:VAL:HG22	2.35	0.61
1:A:458:VAL:HB	1:A:459[B]:PRO:HD2	1.82	0.61
1:B:721:ARG:O	1:B:724:GLU:HG3	2.01	0.61
1:A:767:SER:HB2	4:A:1824:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HB	1:B:21[B]:PRO:HD2	1.84	0.59
1:A:548:ALA:O	1:A:552:VAL:HG23	2.03	0.59
1:A:758:ASP:N	1:A:759[A]:PRO:HD3	2.20	0.57
3:B:826:GOL:H32	4:B:1125:HOH:O	2.04	0.57
1:A:191:TYR:CD2	1:A:286:VAL:HG12	2.40	0.57
1:B:545:ALA:O	1:B:549:ARG:HG3	2.06	0.56
1:A:431:THR:O	1:A:435:ILE:HG13	2.06	0.55
1:B:380:ILE:HD12	1:B:383:ARG:HB2	1.87	0.55
1:B:229:VAL:HB	1:B:230:PRO:HD3	1.89	0.54
1:A:609[A]:PRO:HG3	1:A:678:VAL:O	2.08	0.54
1:B:663:ILE:O	1:B:713:MET:HA	2.08	0.54
1:A:20:THR:HB	1:A:21[B]:PRO:HD2	1.89	0.54
1:A:534:GLU:O	1:A:538:ARG:HG3	2.08	0.53
1:B:191:TYR:CE2	1:B:286[A]:VAL:HG12	2.43	0.53
1:A:327:ASN:OD1	1:A:766[B]:PRO:HD2	2.08	0.53
1:A:683:ARG:HD2	1:A:687:TYR:CZ	2.44	0.53
1:A:186:TYR:CZ	1:A:288:LYS:HD3	2.44	0.53
1:B:485:ARG:HD2	1:B:506:GLN:O	2.08	0.53
1:A:685:PHE:O	1:A:689:LYS:HG3	2.09	0.52
1:A:470:PHE:O	1:A:474:HIS:HD2	1.92	0.52
1:B:534:GLU:O	1:B:538:ARG:HG3	2.10	0.52
1:B:191:TYR:CD2	1:B:286[A]:VAL:HG12	2.44	0.51
1:A:195:ARG:HD3	1:A:197:HIS:NE2	2.26	0.51
1:A:793:GLY:HA2	1:A:822:LEU:HB3	1.92	0.51
1:A:796:VAL:HG13	1:A:800:THR:C	2.31	0.50
1:B:810:ALA:HB1	1:B:811[B]:PRO:HD2	1.93	0.50
1:A:21[B]:PRO:HG2	1:A:704:ARG:O	2.10	0.50
1:A:654:PRO:HG2	4:B:1089:HOH:O	2.10	0.50
1:A:74:VAL:O	1:A:80:VAL:HA	2.12	0.50
1:A:9:GLU:O	1:A:9:GLU:OE1	2.29	0.50
1:A:311:LEU:O	1:A:314:TYR:HB3	2.12	0.50
1:B:739:VAL:O	1:B:743:GLN:HB2	2.12	0.49
1:B:93:ASP:N	1:B:93:ASP:OD1	2.44	0.49
1:B:579:PRO:HD3	4:B:1780:HOH:O	2.13	0.49
1:A:633:MET:SD	1:A:671:VAL:HG11	2.52	0.49
1:A:713:MET:O	1:A:713:MET:HG3	2.11	0.49
1:B:685:PHE:O	1:B:689:LYS:HG3	2.12	0.49
1:A:40:GLN:O	1:A:41:ALA:HB3	2.12	0.49
1:B:300:THR:OG1	1:B:303:GLN:HG3	2.12	0.49
1:B:223:SER:OG	1:B:226:GLU:HG3	2.13	0.48
1:A:553:ALA:HB3	4:A:1325:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21[B]:PRO:HG2	1:B:704:ARG:O	2.14	0.48
1:A:68:GLY:HA3	4:A:1480:HOH:O	2.13	0.48
1:A:323:SER:HB3	4:A:1187:HOH:O	2.14	0.47
1:A:485:ARG:HD2	1:A:506:GLN:O	2.15	0.47
1:B:548:ALA:O	1:B:552:VAL:HG23	2.15	0.47
1:B:535:LEU:HD21	1:B:752:TYR:OH	2.14	0.47
1:A:599:VAL:CG1	1:A:674:ALA:HB1	2.45	0.47
1:B:210:PHE:O	1:B:237:ASN:HA	2.14	0.47
1:A:545:ALA:O	1:A:549:ARG:HG3	2.15	0.46
1:A:794:ARG:HG3	1:A:794:ARG:HH11	1.80	0.46
1:B:347:PHE:CE2	1:B:383:ARG:NH1	2.75	0.46
1:A:470:PHE:O	1:A:474:HIS:CD2	2.67	0.46
1:A:261:ARG:HG3	1:A:262:GLU:N	2.28	0.46
1:B:432:ALA:O	1:B:436:LYS:HG3	2.16	0.46
1:B:758:ASP:N	1:B:759:PRO:HD3	2.30	0.46
1:B:749:ARG:HA	1:B:750[A]:PRO:HD3	1.78	0.45
1:B:158:GLN:O	1:B:162:THR:HG23	2.16	0.45
1:A:405:TYR:O	1:A:407[A]:PRO:HD3	2.16	0.45
1:B:658:LYS:HB3	1:B:659:GLU:OE1	2.16	0.45
1:B:385:ARG:O	1:B:389:ILE:HG12	2.18	0.44
1:B:550:GLY:O	1:B:554:GLU:HG3	2.17	0.44
1:A:68:GLY:HA3	4:A:1098:HOH:O	2.17	0.44
1:A:387:ARG:O	1:A:391:ILE:HG23	2.18	0.44
1:A:63:ILE:HA	1:A:64[B]:PRO:HA	1.77	0.44
1:A:367:ARG:HB2	1:A:426:TRP:CD1	2.53	0.43
1:A:664:PHE:HB2	1:A:667:ASN:ND2	2.32	0.43
1:B:705:LEU:HD13	1:B:728:SER:HB3	1.99	0.43
1:A:668:ASN:N	1:A:669:PRO:CD	2.81	0.43
1:A:663:ILE:O	1:A:713:MET:HA	2.19	0.43
1:A:692:THR:HA	1:A:693:PRO:HD3	1.91	0.43
1:B:665:CYS:SG	1:B:714:ILE:HD12	2.59	0.43
1:A:423:ASP:HB2	1:A:424:PRO:HD3	2.01	0.42
1:B:1:MET:N	4:B:1070:HOH:O	2.52	0.42
1:A:211:ASP:OD1	1:A:236:ALA:HB3	2.19	0.42
1:B:668:ASN:N	1:B:669:PRO:HD2	2.34	0.42
1:A:22:TYR:CD2	1:A:23:PRO:HD2	2.54	0.42
1:A:605:VAL:HG22	1:A:678:VAL:HG12	2.01	0.42
1:B:711:ALA:HA	1:B:728:SER:HA	2.02	0.42
1:A:161:GLN:HG2	4:A:1288:HOH:O	2.18	0.42
1:B:783:VAL:HG22	1:B:820:VAL:HB	2.01	0.42
1:B:198:TYR:CE2	1:B:286[B]:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PHE:CD1	1:A:420:PHE:N	2.88	0.42
1:B:74:VAL:O	1:B:80:VAL:HA	2.19	0.42
1:B:522:ALA:O	1:B:526:VAL:HG23	2.20	0.42
1:A:710:TYR:HB3	1:A:733:THR:HG21	2.01	0.42
1:B:195:ARG:HD3	1:B:197:HIS:NE2	2.34	0.42
1:B:800:THR:HA	1:B:801:PRO:HD3	1.81	0.42
1:A:59:ARG:HD3	4:A:887:HOH:O	2.20	0.41
1:A:657:TYR:HB3	1:B:169:SER:HB3	2.01	0.41
1:B:82:THR:HA	1:B:83[A]:PRO:HD3	1.87	0.41
1:A:197:HIS:HA	1:A:270:VAL:O	2.20	0.41
1:A:685:PHE:CE2	1:A:689:LYS:HD3	2.55	0.41
1:A:703:HIS:CE1	1:A:725:ALA:HB2	2.55	0.41
1:A:769:THR:HA	1:A:781:ILE:O	2.21	0.41
1:A:794:ARG:HG3	1:A:794:ARG:NH1	2.35	0.41
1:B:706:GLU:HA	1:B:707:PRO:HD3	1.92	0.41
1:B:191:TYR:CD2	1:B:286[B]:VAL:HG22	2.55	0.41
1:B:308:PHE:O	1:B:311:LEU:HB3	2.20	0.41
1:B:423:ASP:HB2	1:B:424:PRO:HD3	2.02	0.41
1:B:668:ASN:HB2	1:B:669:PRO:HD3	2.02	0.41
1:A:700:SER:HA	4:A:1412:HOH:O	2.20	0.41
1:B:431:THR:O	1:B:435:ILE:HG13	2.21	0.41
1:A:308:PHE:CE2	1:A:312:LYS:HE3	2.55	0.41
1:A:11[B]:ARG:HG3	4:A:1317:HOH:O	2.20	0.41
1:A:373:LEU:HA	1:A:376:PHE:CZ	2.55	0.41
1:A:347:PHE:HE2	1:A:383:ARG:HE	1.69	0.41
1:A:397:ALA:O	1:A:466:ARG:HD2	2.21	0.41
1:A:707:PRO:HD2	1:A:708:TYR:CD2	2.56	0.41
1:B:680:ARG:HB3	4:B:1090:HOH:O	2.20	0.41
1:A:291:ALA:O	1:A:295:LEU:HG	2.21	0.41
1:A:210:PHE:O	1:A:237:ASN:HA	2.21	0.40
1:A:9:GLU:OE1	1:A:9:GLU:C	2.58	0.40
1:A:190:GLU:O	1:A:193:GLU:HG3	2.21	0.40
1:A:550:GLY:O	1:A:554:GLU:HG3	2.21	0.40
1:A:706:GLU:HA	1:A:707:PRO:HD3	1.79	0.40
1:B:198:TYR:CE2	1:B:286[B]:VAL:CG1	3.04	0.40
1:A:610:GLN:HB2	4:A:1267:HOH:O	2.20	0.40
1:B:86:LEU:HD23	1:B:89:LYS:HG2	2.03	0.40
1:B:539:ARG:HA	4:B:1754:HOH:O	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	831/822 (101%)	788 (95%)	42 (5%)	1 (0%)	51	37
1	B	832/822 (101%)	793 (95%)	38 (5%)	1 (0%)	51	37
All	All	1663/1644 (101%)	1581 (95%)	80 (5%)	2 (0%)	51	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TRP
1	B	85	TRP

### 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	674/675 (100%)	665 (99%)	9 (1%)	69	61
1	B	678/675 (100%)	662 (98%)	16 (2%)	49	35
All	All	1352/1350 (100%)	1327 (98%)	25 (2%)	57	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	150	VAL
1	A	193	GLU
1	A	234	GLU

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Mol	Chain	Res	Type
1	A	339	ASN
1	A	597	PHE
1	A	713	MET
1	A	794	ARG
1	A	822	LEU
1	B	1	MET
1	B	53	ARG
1	B	93	ASP
1	B	140	SER
1	B	193	GLU
1	B	208	GLU
1	B	339	ASN
1	B	493	ASN
1	B	504	SER
1	B	543	ASP
1	B	556	ARG
1	B	597	PHE
1	B	636	GLN
1	B	655	PRO
1	B	668	ASN
1	B	713	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	414	ASN
1	A	474	HIS
1	A	578	ASN
1	A	760	GLN
1	B	578	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	823	-	4,4,4	0.27	0	6,6,6	0.33	0
3	GOL	B	825	-	5,5,5	0.15	0	5,5,5	0.94	0
2	SO4	B	824	-	4,4,4	0.32	0	6,6,6	0.58	0
3	GOL	B	826	-	5,5,5	0.57	0	5,5,5	0.67	0
2	SO4	A	824	-	4,4,4	0.31	0	6,6,6	0.47	0
3	GOL	A	825	-	5,5,5	0.24	0	5,5,5	0.44	0
2	SO4	B	823	-	4,4,4	0.19	0	6,6,6	0.28	0
3	GOL	A	826	-	5,5,5	0.70	0	5,5,5	0.80	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	GOL	A	826	-	-	2/4/4/4	-
3	GOL	A	825	-	-	2/4/4/4	-
3	GOL	B	825	-	-	2/4/4/4	-
3	GOL	B	826	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	826	GOL	C1-C2-C3-O3
3	B	825	GOL	O1-C1-C2-C3
3	B	826	GOL	O1-C1-C2-C3
3	A	826	GOL	O2-C2-C3-O3
3	B	825	GOL	O1-C1-C2-O2
3	A	825	GOL	O1-C1-C2-C3
3	A	825	GOL	O1-C1-C2-O2
3	B	826	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	826	GOL	1	0
3	A	826	GOL	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	822/822 (100%)	-0.16	6 (0%) 87 86	10, 17, 28, 38	0
1	B	822/822 (100%)	-0.16	6 (0%) 87 86	10, 18, 28, 41	1 (0%)
All	All	1644/1644 (100%)	-0.16	12 (0%) 87 86	10, 17, 28, 41	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ALA	3.5
1	B	802	VAL	3.5
1	B	274	ASP	3.1
1	A	812	ALA	2.6
1	B	512	ALA	2.6
1	B	811[A]	PRO	2.5
1	A	274	ASP	2.4
1	A	392	ALA	2.4
1	A	613	ASP	2.3
1	B	511	GLN	2.1
1	B	513	GLY	2.1
1	A	811	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 monosaccharides 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
2	SO4	A	824	5/5	0.81	0.14	32,32,52,76	0
3	GOL	A	826	6/6	0.81	0.18	16,34,48,57	0
2	SO4	B	824	5/5	0.83	0.15	33,39,45,79	0
3	GOL	B	826	6/6	0.87	0.14	20,34,43,51	0
3	GOL	A	825	6/6	0.89	0.17	20,29,39,41	0
3	GOL	B	825	6/6	0.93	0.11	17,31,50,50	0
2	SO4	B	823	5/5	0.96	0.09	40,42,50,52	0
2	SO4	A	823	5/5	0.97	0.14	37,37,42,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.