



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 3SQL / pdb\_00003sql  
Title : Crystal Structure of Glycoside Hydrolase from Synechococcus  
Authors : Kim, Y.; Chhor, G.; Bearden, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2011-07-05  
Resolution : 2.25 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>.

---

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

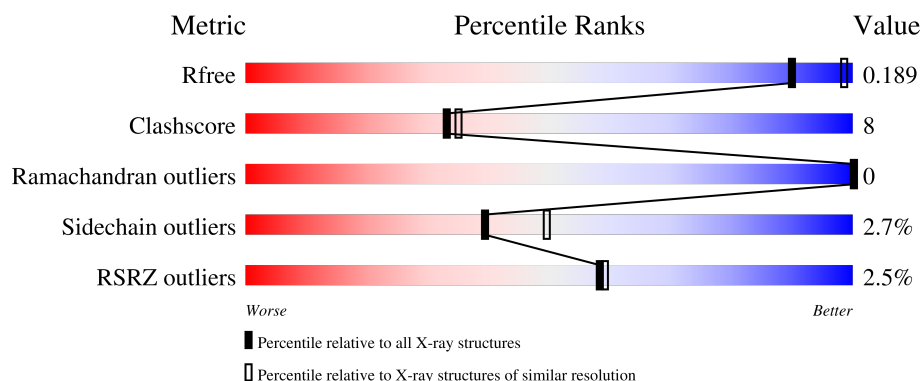
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	535	
1	B	535	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	A	548	-	-	X	-
2	ACY	B	545	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8907 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.

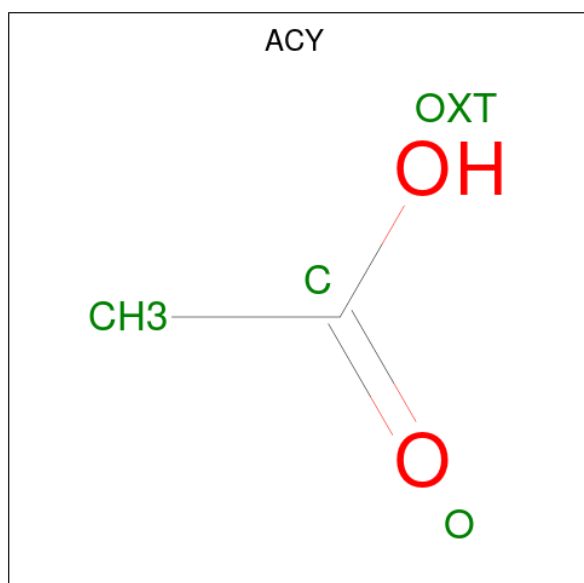
- Molecule 1 is a protein called Glycosyl hydrolase family 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	Se	0	16	0
			4179	2676	718	772	3	10			
1	B	521	Total	C	N	O	S	Se	0	13	0
			4121	2643	700	764	3	11			

There are 6 discrepancies between the modelled and reference sequences:

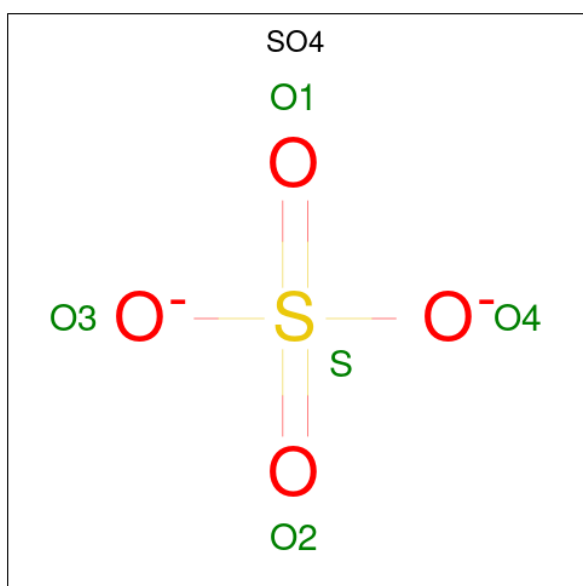
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B1XLD2
A	-1	ASN	-	expression tag	UNP B1XLD2
A	0	ALA	-	expression tag	UNP B1XLD2
B	-2	SER	-	expression tag	UNP B1XLD2
B	-1	ASN	-	expression tag	UNP B1XLD2
B	0	ALA	-	expression tag	UNP B1XLD2

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



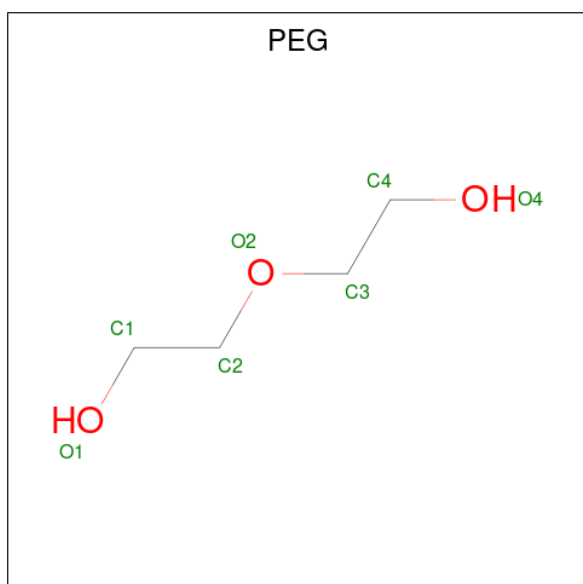
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

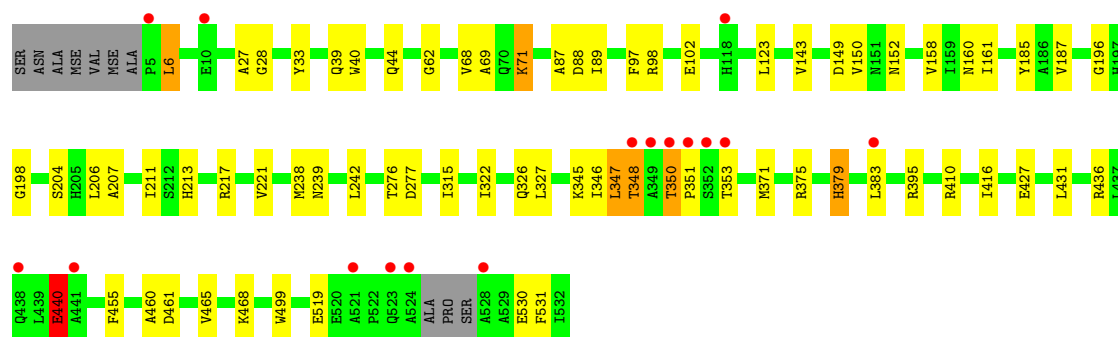
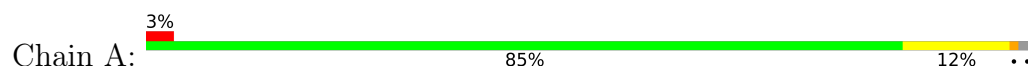
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	288	Total	O	0	0
			288	288		
6	B	241	Total	O	0	0
			241	241		

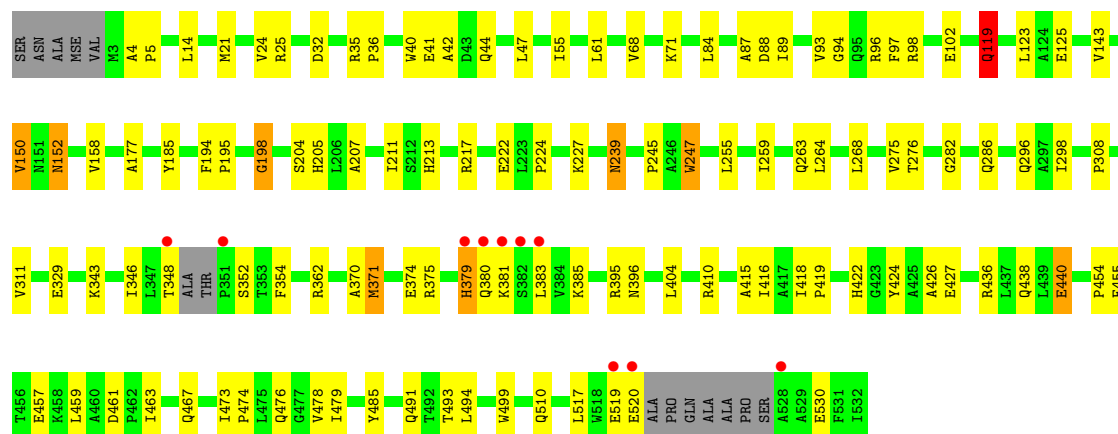
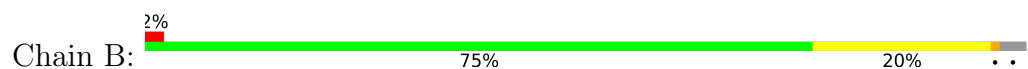
### 3 Residue-property plots [i](#)

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: Glycosyl hydrolase family 3



#### • Molecule 1: Glycosyl hydrolase family 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.73Å 128.73Å 182.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.11 – 2.25 43.11 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.11-2.25) 98.0 (43.11-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_761)	Depositor
R, $R_{free}$	0.163 , 0.196 0.157 , 0.189	Depositor DCC
$R_{free}$ test set	3658 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: EDO, ACY, PEG, 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	0.61	2/4271 (0.0%)	0.90	14/5817 (0.2%)
1	B	0.63	1/4210 (0.0%)	0.91	18/5731 (0.3%)
All	All	0.62	3/8481 (0.0%)	0.91	32/11548 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	VAL	C-O	-5.28	1.18	1.24
1	A	410	ARG	C-O	-5.23	1.19	1.24
1	A	87	ALA	CA-CB	-5.03	1.44	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	GLY	N-CA-C	8.64	122.52	112.50
1	B	461	ASP	CA-C-N	7.26	127.42	119.87
1	B	461	ASP	C-N-CA	7.26	127.42	119.87
1	A	461	ASP	CA-C-N	7.22	126.86	119.56
1	A	461	ASP	C-N-CA	7.22	126.86	119.56
1	B	259	ILE	N-CA-C	6.35	116.39	110.42
1	B	143	VAL	CA-C-N	-6.10	114.37	122.85
1	B	143	VAL	C-N-CA	-6.10	114.37	122.85
1	A	143	VAL	CA-C-N	-6.00	113.89	122.77
1	A	143	VAL	C-N-CA	-6.00	113.89	122.77
1	B	185	TYR	CA-C-N	-5.83	114.74	122.85
1	B	185	TYR	C-N-CA	-5.83	114.74	122.85
1	A	185	TYR	CA-C-N	-5.80	114.78	122.85
1	A	185	TYR	C-N-CA	-5.80	114.78	122.85
1	B	158	VAL	N-CA-C	5.75	117.67	111.58
1	A	158	VAL	N-CA-C	5.72	117.64	111.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	GLU	CA-C-N	-5.68	114.06	122.41
1	B	440	GLU	C-N-CA	-5.68	114.06	122.41
1	A	440	GLU	CA-C-N	-5.61	115.05	122.85
1	A	440	GLU	C-N-CA	-5.61	115.05	122.85
1	B	247	TRP	N-CA-C	5.57	118.20	111.40
1	B	87	ALA	CA-C-N	-5.56	114.58	122.41
1	B	87	ALA	C-N-CA	-5.56	114.58	122.41
1	B	119	GLN	N-CA-C	5.48	117.29	111.32
1	A	531	PHE	N-CA-C	5.35	119.91	113.17
1	A	350	THR	N-CA-C	-5.24	103.43	109.93
1	B	485	TYR	N-CA-C	5.21	118.89	112.54
1	A	89	ILE	N-CA-C	5.20	111.77	106.21
1	A	206	LEU	N-CA-C	5.19	119.67	112.45
1	B	224	PRO	CA-C-N	-5.11	113.78	119.19
1	B	224	PRO	C-N-CA	-5.11	113.78	119.19
1	A	187	VAL	N-CA-C	-5.08	101.15	108.42

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	4179	0	4180	55	0
1	B	4121	0	4122	83	0
2	A	8	0	6	3	0
2	B	8	0	6	2	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
4	A	12	0	18	6	0
4	B	8	0	12	1	0
5	B	7	0	10	3	0
6	A	288	0	0	10	0
6	B	241	0	0	3	0
All	All	8907	0	8354	131	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 8.

All (131) 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:44[A]:GLN:HG2	6:A:707:HOH:O	1.76	0.84
1:B:463:ILE:HG22	1:B:467[B]:GLN:HE21	1.52	0.75
1:B:88:ASP:OD1	2:B:545:ACY:H3	1.87	0.75
1:B:123:LEU:HD21	1:B:371[B]:MSE:HE3	1.71	0.72
1:B:348:THR:HG22	1:B:348:THR:O	1.90	0.70
1:B:385:LYS:HB3	1:B:520:GLU:O	1.92	0.68
1:A:213:HIS:HB3	1:A:217:ARG:HG2	1.76	0.67
1:A:416:ILE:CD1	1:B:404:LEU:HD11	2.25	0.66
1:A:123:LEU:HD21	1:A:371[A]:MSE:HE3	1.78	0.66
1:A:465[A]:VAL:HG23	6:A:792:HOH:O	1.95	0.66
1:B:479:ILE:HD11	1:B:517:LEU:HD11	1.77	0.65
1:B:463:ILE:O	1:B:467[B]:GLN:HG3	1.97	0.65
1:A:468:LYS:HE3	6:A:746:HOH:O	1.96	0.64
1:B:42:ALA:N	5:B:542:PEG:H32	2.12	0.64
1:A:88:ASP:OD1	2:A:548:ACY:H3	1.98	0.64
4:A:550:EDO:H21	1:B:426:ALA:HB3	1.80	0.63
1:B:415:ALA:H	1:B:510:GLN:HE21	1.47	0.62
1:B:94:GLY:C	1:B:102[B]:GLU:HG2	2.23	0.62
1:B:40:TRP:O	5:B:542:PEG:H31	1.98	0.62
1:A:371[B]:MSE:HE3	1:A:375:ARG:HE	1.65	0.62
1:A:350:THR:OG1	1:A:351:PRO:HD2	2.00	0.62
1:A:211:ILE:HD12	1:A:242:LEU:HD13	1.82	0.61
1:A:239[A]:ASN:ND2	1:A:276:THR:HA	2.15	0.61
1:B:370:ALA:O	1:B:374[B]:GLU:HG3	2.02	0.60
1:A:350:THR:O	1:A:350:THR:HG23	2.02	0.60
1:A:28:GLY:HA3	1:A:62:GLY:O	2.03	0.59
1:B:473:ILE:HB	1:B:474:PRO:HD2	1.83	0.59
1:A:315:ILE:HD12	4:A:545:EDO:H22	1.85	0.59
1:B:24:VAL:HB	5:B:542:PEG:H11	1.83	0.58
1:B:467[B]:GLN:HG2	1:B:493:THR:HG21	1.86	0.57
1:A:44[B]:GLN:HG3	6:A:825:HOH:O	2.03	0.57
1:B:467[B]:GLN:HG2	1:B:493:THR:CG2	2.35	0.56
1:A:238:MSE:HE1	2:A:548:ACY:H2	1.88	0.56
1:A:239[A]:ASN:HD21	1:A:276:THR:HA	1.71	0.56
1:B:4:ALA:HB1	1:B:5:PRO:HD2	1.87	0.56
1:B:519:GLU:OE1	1:B:519:GLU:N	2.38	0.56
1:A:353:THR:HA	4:A:544:EDO:H22	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:CD1	4:A:545:EDO:H22	2.38	0.54
1:A:68:VAL:HG21	1:A:97:PHE:CD1	2.43	0.54
1:B:348:THR:O	1:B:348:THR:CG2	2.55	0.54
1:B:476:GLN:NE2	6:B:709:HOH:O	2.40	0.54
1:B:362:ARG:NH2	6:B:775:HOH:O	2.40	0.54
1:A:44[A]:GLN:NE2	6:A:825:HOH:O	2.40	0.53
1:A:213:HIS:HB3	1:A:217:ARG:CG	2.37	0.53
1:B:239[A]:ASN:OD1	1:B:276:THR:HA	2.08	0.53
1:A:346:ILE:HD12	1:A:346:ILE:C	2.34	0.53
1:B:195:PRO:O	1:B:222:GLU:HB3	2.09	0.52
1:B:125[B]:GLU:HG3	1:B:177:ALA:HB1	1.91	0.52
1:B:467[B]:GLN:CG	1:B:493:THR:HG21	2.40	0.52
1:A:350:THR:O	1:A:350:THR:CG2	2.56	0.52
1:B:467[B]:GLN:NE2	1:B:493:THR:HG21	2.24	0.52
1:A:69:ALA:HB1	4:A:544:EDO:H11	1.92	0.51
1:A:436[A]:ARG:NH1	1:B:427:GLU:OE1	2.43	0.51
1:B:463:ILE:HG22	1:B:467[B]:GLN:NE2	2.22	0.51
1:A:436[B]:ARG:O	1:B:438:GLN:HG2	2.10	0.51
1:A:98[B]:ARG:NH2	6:A:783:HOH:O	2.44	0.51
1:B:227:LYS:HG2	1:B:268:LEU:HD22	1.92	0.51
1:A:436[A]:ARG:O	1:B:438:GLN:HG2	2.11	0.51
1:B:380:GLN:O	1:B:381:LYS:HB3	2.10	0.51
1:A:530:GLU:HA	1:B:455:PHE:CZ	2.46	0.50
1:A:345:LYS:O	1:A:348:THR:HB	2.11	0.50
1:B:371[A]:MSE:O	1:B:375:ARG:HG3	2.13	0.49
1:A:431:LEU:CD2	1:A:460:ALA:HB1	2.43	0.49
1:B:247:TRP:CE3	1:B:263:GLN:HG3	2.48	0.48
1:B:98[A]:ARG:HG2	1:B:98[A]:ARG:HH11	1.78	0.48
1:B:21:MSE:HE1	1:B:298:ILE:HG12	1.95	0.48
1:B:375:ARG:HE	1:B:375:ARG:HB3	1.51	0.48
1:B:308:PRO:HG2	1:B:311:VAL:HG22	1.96	0.48
1:B:286[B]:GLN:O	1:B:286[B]:GLN:HG2	2.13	0.47
4:A:545:EDO:H21	6:A:619:HOH:O	2.15	0.47
1:B:282:GLY:O	1:B:286[B]:GLN:HB3	2.15	0.47
1:B:84:LEU:HG	1:B:343:LYS:HE2	1.97	0.47
1:B:213:HIS:HB3	1:B:217:ARG:CG	2.45	0.47
1:A:379[B]:HIS:N	1:A:379[B]:HIS:CD2	2.83	0.47
1:B:418:ILE:HB	1:B:419:PRO:HD3	1.97	0.47
1:A:6:LEU:HD13	1:A:347:LEU:HD21	1.97	0.46
1:A:150:VAL:O	1:A:198:GLY:HA3	2.15	0.45
1:A:530:GLU:HG2	1:B:455:PHE:CD1	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:HIS:CE1	1:B:454:PRO:HB3	2.51	0.45
1:B:239[B]:ASN:HD21	1:B:264:LEU:HD22	1.81	0.45
1:B:204:SER:HA	1:B:207:ALA:O	2.16	0.45
1:B:371[B]:MSE:O	1:B:375:ARG:HG3	2.17	0.44
1:B:379:HIS:HD2	6:B:739:HOH:O	1.99	0.44
1:A:204:SER:HA	1:A:207:ALA:O	2.16	0.44
1:B:96:ARG:HD3	1:B:96:ARG:HA	1.75	0.44
1:B:150:VAL:O	1:B:198:GLY:HA3	2.17	0.44
1:A:102[B]:GLU:CG	6:A:622:HOH:O	2.66	0.44
1:B:32:ASP:OD1	1:B:44[A]:GLN:HG2	2.16	0.44
1:A:427:GLU:OE2	1:B:436:ARG:NH1	2.51	0.44
1:B:255:LEU:HB3	1:B:296:GLN:HG3	1.99	0.43
1:B:194:PHE:HD2	1:B:239[B]:ASN:HD22	1.65	0.43
1:B:379:HIS:CD2	1:B:379:HIS:N	2.87	0.43
1:B:98[B]:ARG:CZ	1:B:410:ARG:NH1	2.81	0.43
1:A:160:ASN:CG	1:A:161:ILE:H	2.26	0.43
1:A:39:GLN:HG2	1:A:40:TRP:CD1	2.53	0.43
1:B:396:ASN:HB2	1:B:424:TYR:HB3	2.00	0.43
1:A:211:ILE:CD1	1:A:242:LEU:HD13	2.47	0.43
1:A:455:PHE:CZ	1:B:530:GLU:HA	2.54	0.43
1:B:89:ILE:HD12	1:B:93:VAL:HG22	2.00	0.43
1:B:211:ILE:O	1:B:245:PRO:HD2	2.18	0.43
1:B:418:ILE:O	1:B:422:HIS:HD2	2.02	0.43
1:A:416:ILE:HD12	1:B:404:LEU:HD11	1.99	0.43
2:A:548:ACY:H1	6:A:750:HOH:O	2.19	0.42
1:B:36:PRO:HD2	1:B:41:GLU:OE1	2.19	0.42
1:B:68:VAL:HG21	1:B:97:PHE:CD1	2.54	0.42
1:B:354:PHE:CD2	1:B:354:PHE:C	2.97	0.42
1:A:27:ALA:O	1:A:71:LYS:HD3	2.20	0.42
1:B:25:ARG:NH1	1:B:61:LEU:HD23	2.35	0.42
1:A:322:ILE:HA	1:A:327:LEU:O	2.20	0.42
1:A:379[A]:HIS:HA	1:A:499:TRP:CZ3	2.55	0.42
1:A:395[B]:ARG:NH2	1:A:427:GLU:OE1	2.50	0.42
1:B:275:VAL:HG12	1:B:276:THR:O	2.19	0.42
1:A:33:TYR:OH	4:B:546:EDO:H11	2.20	0.41
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.70	0.41
1:A:152:ASN:ND2	1:A:221:VAL:HG11	2.35	0.41
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.89	0.41
1:A:44[A]:GLN:CG	6:A:707:HOH:O	2.52	0.41
1:A:440:GLU:H	1:A:440:GLU:HG3	1.51	0.41
1:B:255:LEU:HB3	1:B:296:GLN:CG	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:GLN:HA	1:B:491:GLN:OE1	2.21	0.41
1:A:239[A]:ASN:O	1:A:277:ASP:HB2	2.21	0.41
1:B:14:LEU:HD13	1:B:329:GLU:HG3	2.03	0.41
1:B:35:ARG:HA	1:B:36:PRO:HD3	1.97	0.41
1:B:88:ASP:CG	2:B:545:ACY:H3	2.45	0.41
1:B:152:ASN:H	1:B:152:ASN:ND2	2.19	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.91	0.41
1:A:149:ASP:OD1	1:A:196:GLY:HA2	2.20	0.40
1:B:119:GLN:OE1	1:B:375:ARG:NH2	2.53	0.40
1:B:152:ASN:C	1:B:152:ASN:HD22	2.29	0.40
1:B:478:VAL:O	1:B:499:TRP:HA	2.21	0.40
1:B:493:THR:O	1:B:494:LEU:HD23	2.22	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	537/535 (100%)	528 (98%)	9 (2%)	0	100	100
1	B	528/535 (99%)	516 (98%)	12 (2%)	0	100	100
All	All	1065/1070 (100%)	1044 (98%)	21 (2%)	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	440/420 (105%)	430 (98%)	10 (2%)	44	55
1	B	435/420 (104%)	419 (96%)	16 (4%)	30	37
All	All	875/840 (104%)	849 (97%)	26 (3%)	39	45

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	71	LYS
1	A	326	GLN
1	A	347	LEU
1	A	348	THR
1	A	379[A]	HIS
1	A	379[B]	HIS
1	A	383	LEU
1	A	440	GLU
1	A	519	GLU
1	B	55	ILE
1	B	71	LYS
1	B	119	GLN
1	B	152	ASN
1	B	239[A]	ASN
1	B	239[B]	ASN
1	B	346	ILE
1	B	352	SER
1	B	371[A]	MSE
1	B	371[B]	MSE
1	B	379	HIS
1	B	383	LEU
1	B	395	ARG
1	B	416	ILE
1	B	440	GLU
1	B	457	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	249	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	263	GLN
1	A	266	HIS
1	A	380	GLN
1	A	447	GLN
1	A	476	GLN
1	A	523	GLN
1	B	152	ASN
1	B	219	ASN
1	B	344	GLN
1	B	379	HIS
1	B	380	GLN
1	B	447	GLN
1	B	510	GLN

### 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](#)

17 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	$\# Z  > 2$
3	SO4	A	549	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	546	-	3,3,3	0.56	0	2,2,2	0.23	0
2	ACY	B	541	-	3,3,3	0.85	0	3,3,3	0.69	0
3	SO4	B	544	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	542	-	4,4,4	0.25	0	6,6,6	0.05	0
2	ACY	A	548	-	3,3,3	0.77	0	3,3,3	0.95	0
3	SO4	A	543	-	4,4,4	0.24	0	6,6,6	0.08	0
4	EDO	A	550	-	3,3,3	0.43	0	2,2,2	0.43	0
4	EDO	A	545	-	3,3,3	0.47	0	2,2,2	0.13	0
4	EDO	B	548	-	3,3,3	0.44	0	2,2,2	0.41	0
2	ACY	B	545	-	3,3,3	0.88	0	3,3,3	0.67	0
3	SO4	B	547	-	4,4,4	0.24	0	6,6,6	0.07	0
5	PEG	B	542	-	6,6,6	0.53	0	5,5,5	0.48	0
4	EDO	A	544	-	3,3,3	0.77	0	2,2,2	0.92	0
3	SO4	B	533	-	4,4,4	0.24	0	6,6,6	0.08	0
2	ACY	A	541	-	3,3,3	0.76	0	3,3,3	0.93	0
3	SO4	A	547	-	4,4,4	0.26	0	6,6,6	0.13	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	EDO	B	546	-	-	1/1/1/1	-
4	EDO	A	550	-	-	0/1/1/1	-
4	EDO	A	545	-	-	0/1/1/1	-
4	EDO	B	548	-	-	0/1/1/1	-
5	PEG	B	542	-	-	2/4/4/4	-
4	EDO	A	544	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	542	PEG	O1-C1-C2-O2
4	B	546	EDO	O1-C1-C2-O2
5	B	542	PEG	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	546	EDO	1	0
2	A	548	ACY	3	0
4	A	550	EDO	1	0
4	A	545	EDO	3	0
2	B	545	ACY	2	0
5	B	542	PEG	3	0
4	A	544	EDO	2	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, 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	516/535 (96%)	-0.46	16 (3%)	51 51	16, 36, 63, 109	20 (3%)
1	B	511/535 (95%)	-0.43	10 (1%)	65 65	15, 40, 67, 131	15 (2%)
All	All	1027/1070 (95%)	-0.44	26 (2%)	58 59	15, 38, 65, 131	35 (3%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	PRO	7.4
1	A	351	PRO	6.8
1	A	350	THR	5.9
1	B	519	GLU	5.6
1	B	520	GLU	5.1
1	B	348	THR	4.7
1	B	383	LEU	4.5
1	B	379	HIS	4.4
1	A	352	SER	4.1
1	A	524	ALA	4.0
1	A	5	PRO	3.9
1	A	383	LEU	3.6
1	B	528	ALA	3.5
1	A	528	ALA	3.4
1	A	353	THR	3.1
1	A	521	ALA	3.0
1	A	349	ALA	3.0
1	A	10[A]	GLU	2.9
1	B	380	GLN	2.8
1	B	381	LYS	2.7
1	A	441	ALA	2.5
1	A	438[A]	GLN	2.4
1	A	118[A]	HIS	2.2
1	A	523	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	348	THR	2.1
1	B	382	SER	2.1

## 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, 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
5	PEG	B	542	7/7	0.78	0.23	46,63,75,76	0
3	SO4	A	549	5/5	0.83	0.15	165,165,166,167	0
4	EDO	A	544	4/4	0.84	0.24	53,59,61,63	0
2	ACY	A	548	4/4	0.86	0.17	49,54,55,56	0
4	EDO	B	546	4/4	0.86	0.19	57,58,61,63	0
3	SO4	B	547	5/5	0.86	0.18	142,143,143,146	0
3	SO4	A	547	5/5	0.88	0.17	131,134,134,135	0
3	SO4	A	543	5/5	0.89	0.18	151,152,153,154	0
4	EDO	B	548	4/4	0.89	0.17	61,68,73,77	0
3	SO4	B	533	5/5	0.89	0.16	140,141,142,142	0
4	EDO	A	550	4/4	0.90	0.20	85,86,87,88	0
2	ACY	B	545	4/4	0.90	0.16	44,58,60,64	0
4	EDO	A	545	4/4	0.92	0.14	38,42,43,48	0
3	SO4	A	542	5/5	0.94	0.16	132,132,135,135	0
3	SO4	B	544	5/5	0.94	0.14	125,126,128,130	0
2	ACY	A	541	4/4	0.97	0.09	33,34,36,37	0
2	ACY	B	541	4/4	0.98	0.06	26,31,32,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.