Full wwPDB X-ray Structure Validation Report

Jun 23, 2024 – 02:51 AM EDT

PDB ID	:	6NCW
Title	:	Crystal structure of a GH2 beta-galacturonidase from Eisenbergiella tayi bound to glycerol
Authors	:	Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-12-12
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

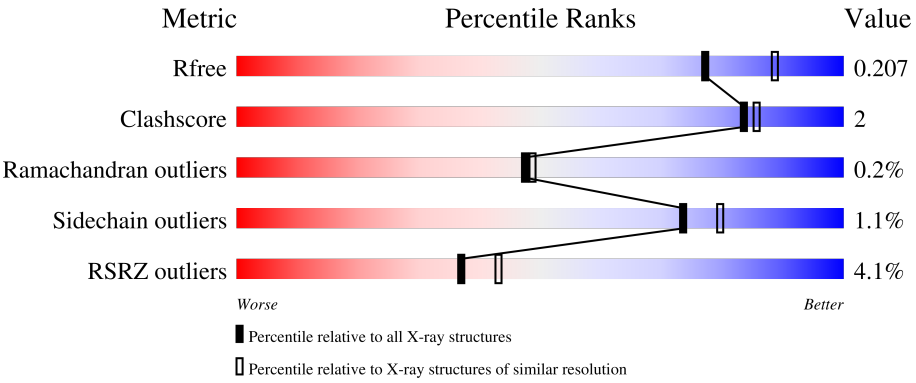
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	574	5% 89% 9% ·
1	B	574	4% 90% 7% ·
1	C	574	2% 91% 6% ·
1	D	574	5% 91% 6% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19641 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 Beta-galacturonidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	1	0
			4540	2889	771	858	22			
1	B	560	Total	C	N	O	S	0	0	0
			4512	2866	769	855	22			
1	C	559	Total	C	N	O	S	0	1	0
			4510	2866	769	853	22			
1	D	560	Total	C	N	O	S	0	0	0
			4529	2882	770	855	22			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLU	-	expression tag	UNP A0A1E3AEY6
A	561	ASN	-	expression tag	UNP A0A1E3AEY6
A	562	LEU	-	expression tag	UNP A0A1E3AEY6
A	563	TYR	-	expression tag	UNP A0A1E3AEY6
A	564	PHE	-	expression tag	UNP A0A1E3AEY6
A	565	GLN	-	expression tag	UNP A0A1E3AEY6
A	566	SER	-	expression tag	UNP A0A1E3AEY6
A	567	GLY	-	expression tag	UNP A0A1E3AEY6
A	568	SER	-	expression tag	UNP A0A1E3AEY6
A	569	HIS	-	expression tag	UNP A0A1E3AEY6
A	570	HIS	-	expression tag	UNP A0A1E3AEY6
A	571	HIS	-	expression tag	UNP A0A1E3AEY6
A	572	HIS	-	expression tag	UNP A0A1E3AEY6
A	573	HIS	-	expression tag	UNP A0A1E3AEY6
A	574	HIS	-	expression tag	UNP A0A1E3AEY6
B	560	GLU	-	expression tag	UNP A0A1E3AEY6
B	561	ASN	-	expression tag	UNP A0A1E3AEY6
B	562	LEU	-	expression tag	UNP A0A1E3AEY6
B	563	TYR	-	expression tag	UNP A0A1E3AEY6
B	564	PHE	-	expression tag	UNP A0A1E3AEY6
B	565	GLN	-	expression tag	UNP A0A1E3AEY6

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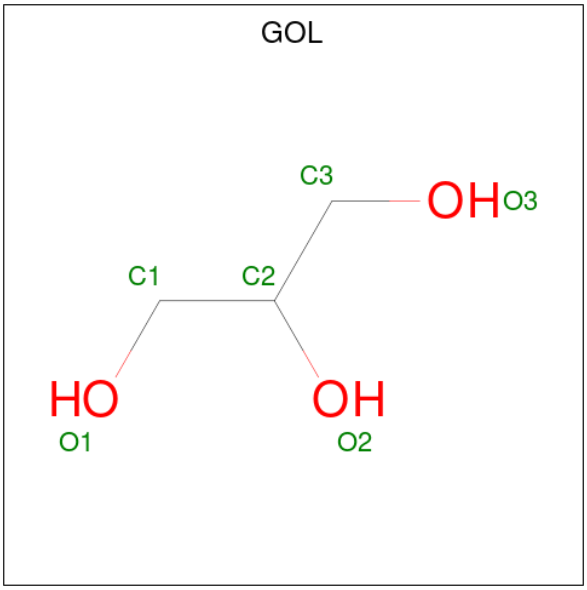
Chain	Residue	Modelled	Actual	Comment	Reference
B	566	SER	-	expression tag	UNP A0A1E3AEY6
B	567	GLY	-	expression tag	UNP A0A1E3AEY6
B	568	SER	-	expression tag	UNP A0A1E3AEY6
B	569	HIS	-	expression tag	UNP A0A1E3AEY6
B	570	HIS	-	expression tag	UNP A0A1E3AEY6
B	571	HIS	-	expression tag	UNP A0A1E3AEY6
B	572	HIS	-	expression tag	UNP A0A1E3AEY6
B	573	HIS	-	expression tag	UNP A0A1E3AEY6
B	574	HIS	-	expression tag	UNP A0A1E3AEY6
C	560	GLU	-	expression tag	UNP A0A1E3AEY6
C	561	ASN	-	expression tag	UNP A0A1E3AEY6
C	562	LEU	-	expression tag	UNP A0A1E3AEY6
C	563	TYR	-	expression tag	UNP A0A1E3AEY6
C	564	PHE	-	expression tag	UNP A0A1E3AEY6
C	565	GLN	-	expression tag	UNP A0A1E3AEY6
C	566	SER	-	expression tag	UNP A0A1E3AEY6
C	567	GLY	-	expression tag	UNP A0A1E3AEY6
C	568	SER	-	expression tag	UNP A0A1E3AEY6
C	569	HIS	-	expression tag	UNP A0A1E3AEY6
C	570	HIS	-	expression tag	UNP A0A1E3AEY6
C	571	HIS	-	expression tag	UNP A0A1E3AEY6
C	572	HIS	-	expression tag	UNP A0A1E3AEY6
C	573	HIS	-	expression tag	UNP A0A1E3AEY6
C	574	HIS	-	expression tag	UNP A0A1E3AEY6
D	560	GLU	-	expression tag	UNP A0A1E3AEY6
D	561	ASN	-	expression tag	UNP A0A1E3AEY6
D	562	LEU	-	expression tag	UNP A0A1E3AEY6
D	563	TYR	-	expression tag	UNP A0A1E3AEY6
D	564	PHE	-	expression tag	UNP A0A1E3AEY6
D	565	GLN	-	expression tag	UNP A0A1E3AEY6
D	566	SER	-	expression tag	UNP A0A1E3AEY6
D	567	GLY	-	expression tag	UNP A0A1E3AEY6
D	568	SER	-	expression tag	UNP A0A1E3AEY6
D	569	HIS	-	expression tag	UNP A0A1E3AEY6
D	570	HIS	-	expression tag	UNP A0A1E3AEY6
D	571	HIS	-	expression tag	UNP A0A1E3AEY6
D	572	HIS	-	expression tag	UNP A0A1E3AEY6
D	573	HIS	-	expression tag	UNP A0A1E3AEY6
D	574	HIS	-	expression tag	UNP A0A1E3AEY6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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

- Molecule 4 is water.

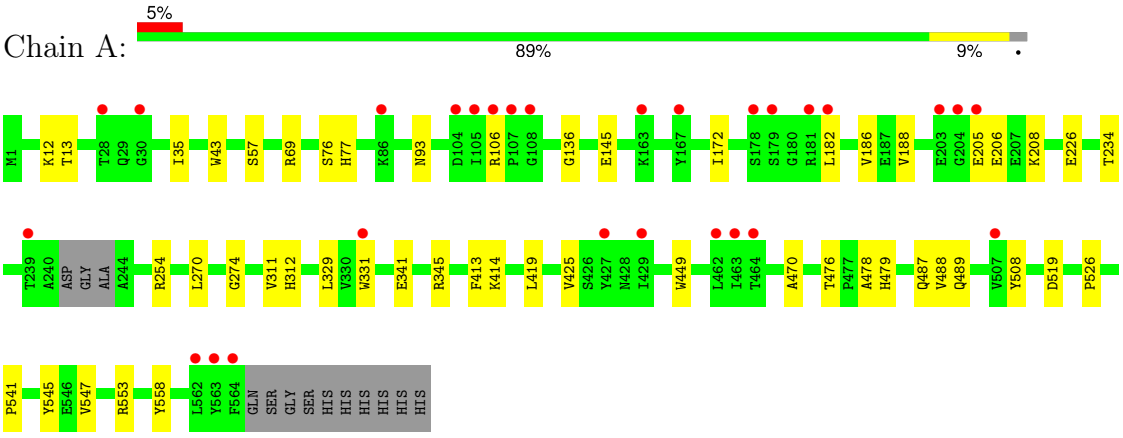
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	376	Total O 376 376	0	0
4	B	363	Total O 363 363	0	0
4	C	381	Total O 381 381	0	0
4	D	366	Total O 366 366	0	0

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.

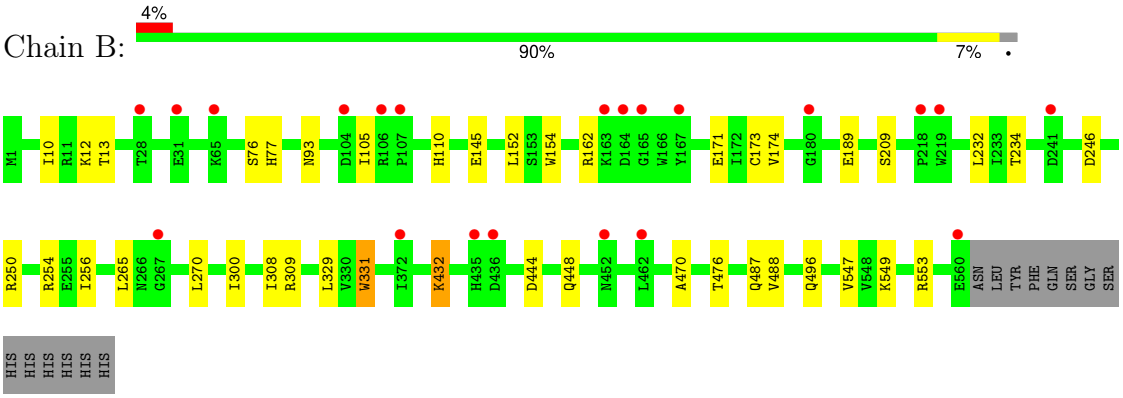
• Molecule 1: Beta-galacturonidase

Chain A:



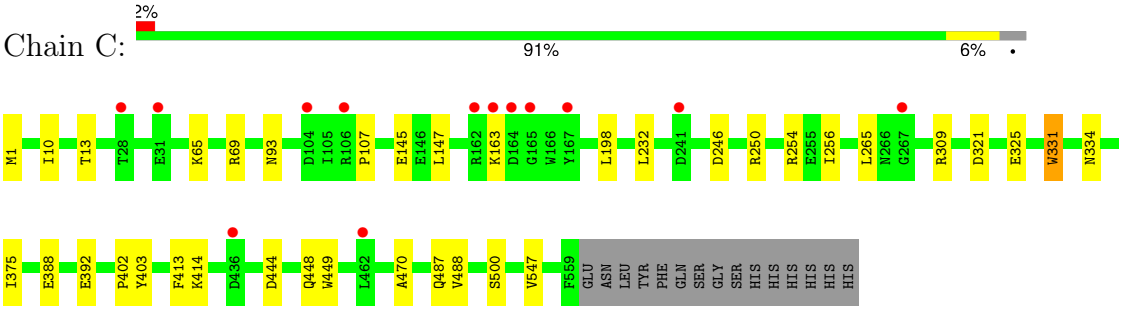
• Molecule 1: Beta-galacturonidase

Chain B:



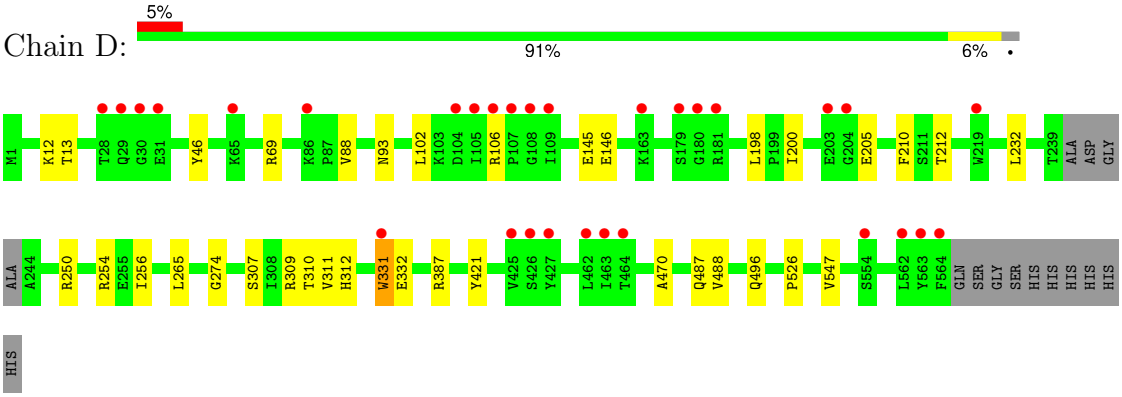
• Molecule 1: Beta-galacturonidase

Chain C:



• Molecule 1: Beta-galacturonidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.93Å 87.68Å 124.38Å 93.29° 101.55° 90.37°	Depositor
Resolution (Å)	29.54 – 2.10 29.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.54-2.10) 97.6 (29.54-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.165 , 0.208 0.165 , 0.207	Depositor DCC
R_{free} test set	2012 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19641	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, 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	0.44	0/4667	0.60	0/6333
1	B	0.43	0/4635	0.59	0/6291
1	C	0.43	0/4633	0.59	0/6289
1	D	0.44	0/4653	0.59	0/6314
All	All	0.44	0/18588	0.59	0/25227

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

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	4540	0	4340	25	0
1	B	4512	0	4312	23	0
1	C	4510	0	4314	19	0
1	D	4529	0	4329	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	32	0	0
3	C	12	0	16	0	0
3	D	12	0	16	0	0
4	A	376	0	0	3	0
4	B	363	0	0	1	0
4	C	381	0	0	0	0
4	D	366	0	0	3	0
All	All	19641	0	17375	84	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 2.

All (84) 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:C:488:VAL:HG13	1:C:547:VAL:HG21	1.66	0.75
1:B:10:ILE:HD12	1:B:246:ASP:HB3	1.72	0.71
1:C:13:THR:HG22	1:C:145:GLU:HG2	1.76	0.68
1:B:300:ILE:HG21	1:B:308:ILE:HD11	1.75	0.67
1:D:488:VAL:HG13	1:D:547:VAL:HG21	1.75	0.67
1:B:444:ASP:O	1:B:448:GLN:HG2	1.97	0.64
1:D:13:THR:HG22	1:D:145:GLU:HG2	1.81	0.63
1:B:300:ILE:HD13	1:B:308:ILE:HD11	1.82	0.62
1:B:488:VAL:HG13	1:B:547:VAL:HG21	1.81	0.61
1:A:519:ASP:HB3	4:A:973:HOH:O	2.01	0.61
1:B:232:LEU:HD23	1:B:250:ARG:HG2	1.81	0.61
1:A:476:THR:HG22	1:A:478:ALA:H	1.64	0.60
1:C:232:LEU:HD23	1:C:250:ARG:HG2	1.84	0.59
1:A:488:VAL:HG13	1:A:547:VAL:HG21	1.84	0.59
1:D:387:ARG:NH1	1:D:421:TYR:OH	2.36	0.59
1:A:13:THR:HG22	1:A:145:GLU:HG2	1.85	0.58
1:C:414:LYS:HG2	1:C:449:TRP:CG	2.39	0.58
1:A:172:ILE:HD12	1:A:186:VAL:HG11	1.88	0.56
1:D:232:LEU:HD23	1:D:250:ARG:HG2	1.88	0.56
1:C:444:ASP:O	1:C:448:GLN:HG2	2.07	0.55
1:B:270:LEU:HD21	1:B:329:LEU:HD13	1.90	0.54
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.74	0.52
1:B:162:ARG:HG2	1:B:162:ARG:NH1	2.25	0.52
1:C:321:ASP:O	1:C:325:GLU:HG3	2.10	0.52
1:D:256:ILE:HD11	1:D:265:LEU:HD13	1.90	0.52
1:B:171:GLU:OE1	1:B:209:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:HIS:ND1	1:A:489:GLN:OE1	2.39	0.50
1:D:88:VAL:HB	1:D:102:LEU:HD21	1.94	0.49
1:D:309:ARG:HG3	1:D:331:TRP:CD1	2.48	0.49
1:A:413:PHE:CE1	1:A:414:LYS:HD3	2.48	0.49
1:A:419:LEU:HD22	1:A:425:VAL:HG13	1.94	0.48
1:B:256:ILE:HD11	1:B:265:LEU:HD13	1.96	0.48
1:A:476:THR:HG23	4:D:1036:HOH:O	2.14	0.47
1:C:256:ILE:HD11	1:C:265:LEU:HD13	1.96	0.47
1:A:274:GLY:HA3	1:A:508:TYR:CD2	2.50	0.47
1:A:311:VAL:HA	1:A:312:HIS:HA	1.81	0.46
1:A:270:LEU:HD21	1:A:329:LEU:HD13	1.98	0.46
1:C:65:LYS:HG3	1:C:107:PRO:HB3	1.98	0.46
1:A:77:HIS:HB3	4:A:923:HOH:O	2.16	0.46
1:D:106:ARG:HG2	4:D:743:HOH:O	2.15	0.46
1:A:470:ALA:HB2	1:A:487:GLN:HB2	1.98	0.46
1:D:311:VAL:HA	1:D:312:HIS:HA	1.74	0.45
1:A:341:GLU:HG2	1:A:345:ARG:NH2	2.31	0.45
1:C:69:ARG:HB2	1:C:147:LEU:HD11	1.99	0.45
1:D:200:ILE:HD12	1:D:210:PHE:CD2	2.51	0.45
1:D:12:LYS:HE3	1:D:146:GLU:OE2	2.17	0.45
1:A:76:SER:HA	1:A:77:HIS:HA	1.68	0.45
1:D:496:GLN:HG3	4:D:957:HOH:O	2.17	0.44
1:B:189:GLU:HG3	1:B:234:THR:HB	1.98	0.44
1:B:105:ILE:HD12	1:B:110:HIS:CE1	2.53	0.44
1:B:496:GLN:HG3	4:B:895:HOH:O	2.18	0.44
1:B:13:THR:HG22	1:B:145:GLU:HG2	2.00	0.43
1:A:541:PRO:HB3	1:A:545:TYR:CD2	2.53	0.43
1:D:198:LEU:HD21	1:D:212:THR:HG22	2.01	0.43
1:A:226:GLU:OE2	1:A:558:TYR:OH	2.15	0.43
1:A:414:LYS:HG2	1:A:449:TRP:CG	2.53	0.43
1:C:413:PHE:CE1	1:C:414:LYS:HD3	2.53	0.43
1:D:274:GLY:HA2	1:D:307:SER:O	2.18	0.43
1:C:388:GLU:O	1:C:392:GLU:HG3	2.19	0.43
1:C:488:VAL:HG13	1:C:547:VAL:CG2	2.43	0.43
1:D:310:THR:OG1	1:D:332:GLU:HA	2.19	0.43
1:A:43:TRP:CZ2	1:A:136:GLY:HA3	2.54	0.43
1:C:470:ALA:HB2	1:C:487:GLN:HB2	2.00	0.42
1:D:470:ALA:HB2	1:D:487:GLN:HB2	2.01	0.42
1:C:10:ILE:HD12	1:C:246:ASP:HB3	2.02	0.42
1:B:154:TRP:CE2	1:B:173:CYS:HB2	2.55	0.42
1:C:402:PRO:HG2	1:C:403:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:SER:HA	1:B:77:HIS:HA	1.71	0.41
1:A:188:VAL:HA	1:A:234:THR:O	2.20	0.41
1:B:309:ARG:HG3	1:B:331:TRP:CD1	2.55	0.41
1:C:331:TRP:CD1	1:C:331:TRP:C	2.93	0.41
1:D:69:ARG:HD3	1:D:145:GLU:OE1	2.20	0.41
1:B:470:ALA:HB2	1:B:487:GLN:HB2	2.03	0.41
1:B:549:LYS:HE3	1:B:553:ARG:HH21	1.85	0.41
1:A:206:GLU:OE1	1:A:208:LYS:HD3	2.20	0.41
1:B:432:LYS:HD2	1:B:432:LYS:HA	1.87	0.41
1:A:12:LYS:NZ	4:A:710:HOH:O	2.51	0.41
1:A:69:ARG:HD3	1:A:145:GLU:OE1	2.21	0.41
1:B:152:LEU:HD23	1:B:174:VAL:HG22	2.03	0.41
1:C:198:LEU:HD12	1:C:198:LEU:N	2.36	0.41
1:B:300:ILE:HD13	1:B:308:ILE:CD1	2.50	0.41
1:C:309:ARG:HG3	1:C:331:TRP:CD1	2.56	0.40
1:C:334:ASN:OD1	1:C:375:ILE:HA	2.21	0.40
1:A:526:PRO:HG3	1:D:526:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/574 (97%)	544 (98%)	13 (2%)	1 (0%)	47	49
1	B	558/574 (97%)	544 (98%)	13 (2%)	1 (0%)	47	49
1	C	558/574 (97%)	542 (97%)	15 (3%)	1 (0%)	47	49
1	D	556/574 (97%)	541 (97%)	14 (2%)	1 (0%)	47	49
All	All	2230/2296 (97%)	2171 (97%)	55 (2%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	B	93	ASN
1	C	93	ASN
1	D	93	ASN

5.3.2 Protein sidechains (i)

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	490/499 (98%)	482 (98%)	8 (2%)	62	69
1	B	486/499 (97%)	481 (99%)	5 (1%)	76	82
1	C	486/499 (97%)	481 (99%)	5 (1%)	76	82
1	D	489/499 (98%)	485 (99%)	4 (1%)	81	86
All	All	1951/1996 (98%)	1929 (99%)	22 (1%)	73	79

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	57	SER
1	A	106	ARG
1	A	182	LEU
1	A	205	GLU
1	A	254	ARG
1	A	331	TRP
1	A	553	ARG
1	B	12	LYS
1	B	254	ARG
1	B	331	TRP
1	B	432	LYS
1	B	476	THR
1	C	1	MET
1	C	163	LYS
1	C	254	ARG
1	C	331	TRP
1	C	500	SER

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Mol	Chain	Res	Type
1	D	46	TYR
1	D	205	GLU
1	D	254	ARG
1	D	331	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	GOL	B	604	-	5,5,5	0.76	0	5,5,5	1.06	0
3	GOL	D	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.91	0
3	GOL	A	603	-	5,5,5	1.08	0	5,5,5	0.89	0
3	GOL	A	602	-	5,5,5	0.91	0	5,5,5	1.13	0
3	GOL	C	602	-	5,5,5	0.89	0	5,5,5	0.96	0
3	GOL	D	602	-	5,5,5	1.07	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	602	-	5,5,5	1.04	0	5,5,5	0.78	0
3	GOL	B	605	-	5,5,5	0.56	0	5,5,5	1.28	1 (20%)
3	GOL	B	603	-	5,5,5	1.21	0	5,5,5	0.97	0
3	GOL	C	603	-	5,5,5	0.89	0	5,5,5	1.05	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	B	604	-	-	2/4/4/4	-
3	GOL	D	603	-	-	1/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	D	602	-	-	0/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	B	605	-	-	0/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	C	603	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	GOL	C1-C2	2.33	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	605	GOL	C3-C2-C1	-2.20	103.71	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	B	602	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	603	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-O2
3	C	603	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	D	603	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	561/574 (97%)	-0.01	28 (4%)	28	34	16, 26, 47, 65	0
1	B	560/574 (97%)	-0.06	21 (3%)	40	46	17, 28, 43, 65	0
1	C	559/574 (97%)	-0.06	13 (2%)	60	65	17, 28, 44, 63	0
1	D	560/574 (97%)	0.04	30 (5%)	25	31	16, 27, 47, 66	0
All	All	2240/2296 (97%)	-0.02	92 (4%)	37	43	16, 27, 46, 66	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	TYR	5.5
1	D	563	TYR	4.8
1	A	107	PRO	4.0
1	D	106	ARG	3.9
1	D	107	PRO	3.8
1	A	462	LEU	3.7
1	D	180	GLY	3.6
1	D	462	LEU	3.6
1	B	164	ASP	3.5
1	D	427	TYR	3.5
1	B	163	LYS	3.3
1	C	28	THR	3.2
1	B	28	THR	3.2
1	C	31	GLU	3.1
1	B	165	GLY	3.1
1	A	181	ARG	3.1
1	A	564	PHE	3.1
1	A	204	GLY	3.0
1	A	105	ILE	3.0
1	D	163	LYS	3.0
1	D	181	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	562	LEU	3.0
1	D	564	PHE	2.9
1	D	30	GLY	2.9
1	D	463	ILE	2.9
1	B	241	ASP	2.8
1	D	179	SER	2.8
1	C	436	ASP	2.8
1	A	163	LYS	2.8
1	C	163	LYS	2.8
1	C	106	ARG	2.7
1	C	104	ASP	2.7
1	A	106	ARG	2.7
1	A	179	SER	2.7
1	A	182	LEU	2.7
1	C	267	GLY	2.7
1	B	107	PRO	2.7
1	C	241	ASP	2.6
1	B	31	GLU	2.6
1	B	104	ASP	2.6
1	D	104	ASP	2.6
1	A	463	ILE	2.6
1	A	562	LEU	2.6
1	A	427	TYR	2.5
1	D	464	THR	2.5
1	A	104	ASP	2.5
1	B	180	GLY	2.5
1	A	464	THR	2.5
1	B	462	LEU	2.5
1	B	560	GLU	2.5
1	D	426	SER	2.4
1	D	108	GLY	2.4
1	A	167	TYR	2.4
1	C	162	ARG	2.4
1	C	167	TYR	2.4
1	B	436	ASP	2.4
1	C	462	LEU	2.4
1	A	28	THR	2.4
1	B	167	TYR	2.4
1	D	204	GLY	2.4
1	B	452	ASN	2.3
1	C	165	GLY	2.3
1	D	28	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	2.3
1	A	507	VAL	2.3
1	B	219	TRP	2.3
1	B	218	PRO	2.3
1	B	435	HIS	2.2
1	A	30	GLY	2.2
1	A	331	TRP	2.2
1	B	372	ILE	2.2
1	A	203	GLU	2.2
1	B	106	ARG	2.2
1	A	205	GLU	2.2
1	A	239	THR	2.2
1	A	178	SER	2.2
1	D	554	SER	2.2
1	A	86	LYS	2.2
1	D	219	TRP	2.1
1	B	65	LYS	2.1
1	D	331	TRP	2.1
1	D	86	LYS	2.1
1	D	105	ILE	2.1
1	D	29	GLN	2.1
1	D	109	ILE	2.1
1	C	164	ASP	2.1
1	D	31	GLU	2.0
1	D	65	LYS	2.0
1	A	108	GLY	2.0
1	D	203	GLU	2.0
1	A	429	ILE	2.0
1	D	425	VAL	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	603	6/6	0.89	0.13	35,37,39,40	0
3	GOL	D	603	6/6	0.89	0.14	29,34,36,36	0
3	GOL	B	603	6/6	0.92	0.14	31,34,35,35	0
3	GOL	D	602	6/6	0.93	0.16	22,23,24,25	0
3	GOL	B	605	6/6	0.94	0.15	28,29,35,48	0
3	GOL	A	602	6/6	0.94	0.10	32,35,40,40	0
3	GOL	B	604	6/6	0.96	0.08	35,36,39,43	0
3	GOL	B	602	6/6	0.97	0.14	20,22,25,25	0
3	GOL	A	603	6/6	0.97	0.15	21,22,24,24	0
3	GOL	C	602	6/6	0.97	0.13	19,23,26,28	0
2	CL	A	601	1/1	0.99	0.11	21,21,21,21	0
2	CL	C	601	1/1	1.00	0.09	22,22,22,22	0
2	CL	D	601	1/1	1.00	0.09	19,19,19,19	0
2	CL	B	601	1/1	1.00	0.08	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.