Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 05:26 AM EDT

PDB ID	:	3M46
Title	:	The crystal structure of the D73A mutant of glycoside HYDROLASE (FAMILY 31) from Ruminococcus obeum ATCC 29174
Authors	:	Tan, K.; Tesar, C.; Freeman, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-03-10
Resolution	:	2.66 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:

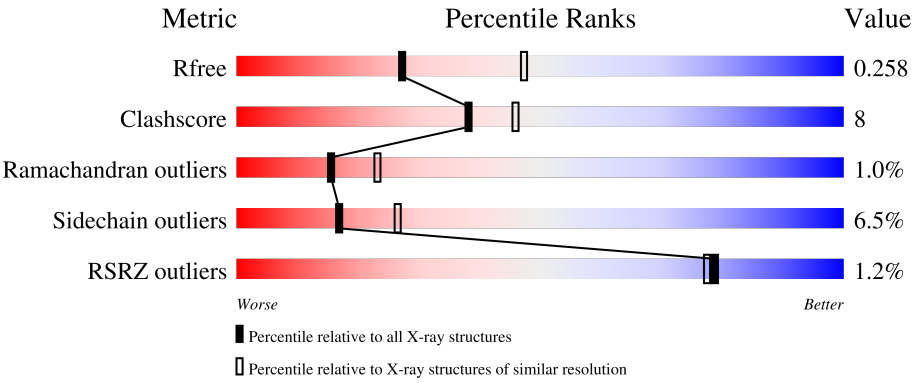
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	666	2% 77% 18%
1	B	666	% 77% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10735 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.

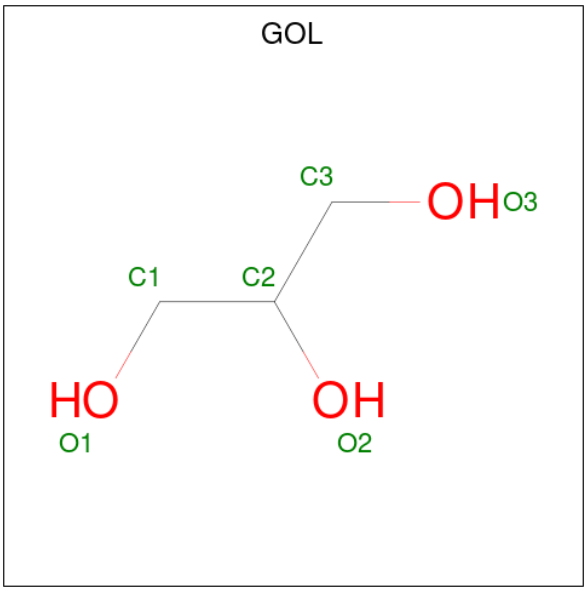
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	2	0
			5348	3431	877	1006	34			
1	B	651	Total	C	N	O	S	0	1	0
			5329	3423	874	998	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	73	ALA	ASP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	73	ALA	ASP	engineered mutation	UNP A5ZY13

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

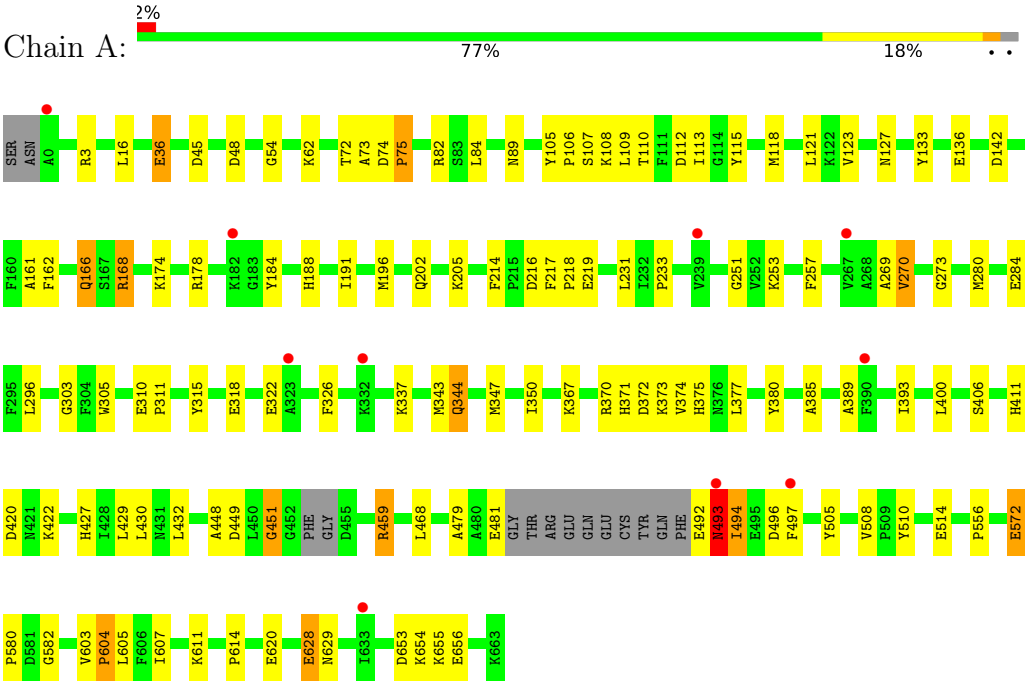
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	28	Total O 28 28	0	0

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.

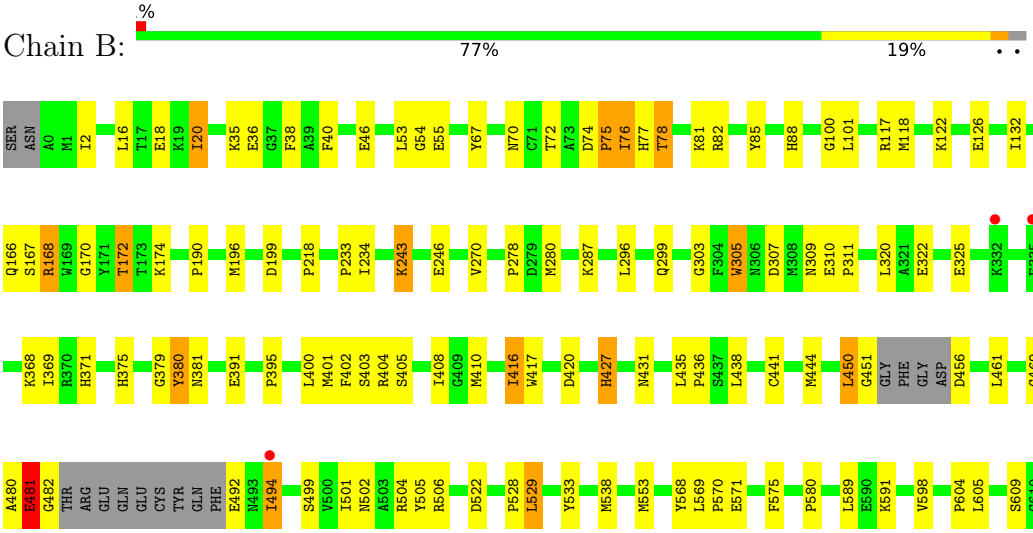
• Molecule 1: Uncharacterized protein

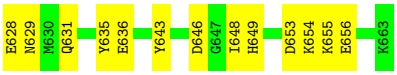
Chain A:



• Molecule 1: Uncharacterized protein

Chain B:




E628
N629
M630
Q631
Y635
E636
Y643
D646
Q647
I648
H649
D653
K654
K655
E656
K663

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.18Å 122.49Å 87.46Å 90.00° 108.60° 90.00°	Depositor
Resolution (Å)	82.89 – 2.66 49.26 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.0 (82.89-2.66) 99.0 (49.26-2.66)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.258 0.189 , 0.258	Depositor DCC
R_{free} test set	1825 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: 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	0.74	0/5486	0.77	1/7395 (0.0%)
1	B	0.75	1/5470 (0.0%)	0.77	0/7372
All	All	0.75	1/10956 (0.0%)	0.77	1/14767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	GLU	CG-CD	5.83	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	ASP	CB-CG-OD1	5.68	123.41	118.30

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	5348	0	5122	81	0
1	B	5329	0	5121	81	0
2	B	6	0	8	0	0
3	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
All	All	10735	0	10251	159	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 (159) 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:B:481:GLU:HG3	1:B:482:GLY:H	1.32	0.94
1:B:234:ILE:HD11	1:B:307:ASP:HB2	1.52	0.91
1:B:481:GLU:HG3	1:B:482:GLY:N	1.87	0.90
1:B:494:ILE:H	1:B:494:ILE:HD13	1.38	0.89
1:A:115:TYR:OH	1:B:456:ASP:HB3	1.76	0.86
1:A:74:ASP:N	1:A:75:PRO:HD2	1.92	0.84
1:B:167:SER:O	1:B:168:ARG:HD3	1.79	0.83
1:A:492:GLU:O	1:A:497:PHE:HE1	1.62	0.82
1:B:380:TYR:HA	1:B:410:MET:HG3	1.66	0.77
1:A:389:ALA:O	1:A:393:ILE:HD12	1.84	0.76
1:B:655:LYS:HE2	1:B:656:GLU:OE2	1.86	0.74
1:B:218:PRO:HG3	1:B:299:GLN:HG2	1.70	0.73
1:A:492:GLU:O	1:A:497:PHE:CE1	2.43	0.71
1:B:170:GLY:O	1:B:172:THR:HG22	1.90	0.71
1:A:310:GLU:N	1:A:311:PRO:HA	2.06	0.70
1:A:73:ALA:C	1:A:75:PRO:HD2	2.12	0.69
1:B:420:ASP:O	1:B:451:GLY:HA3	1.93	0.69
1:B:75:PRO:O	1:B:420:ASP:HB2	1.92	0.68
1:A:74:ASP:N	1:A:75:PRO:CD	2.56	0.68
1:A:106:PRO:HB2	1:A:374:VAL:HA	1.76	0.68
1:A:168:ARG:HG3	1:A:479:ALA:O	1.94	0.68
1:A:318:GLU:O	1:A:322:GLU:HG3	1.94	0.67
1:B:77:HIS:ND1	1:B:420:ASP:HB3	2.09	0.67
1:A:343:MET:CE	1:A:347:MET:HE2	2.26	0.66
1:A:377:LEU:O	1:A:380:TYR:HB3	1.95	0.66
1:B:598:VAL:HG11	1:B:604:PRO:HG3	1.79	0.64
1:B:427:HIS:O	1:B:431:ASN:ND2	2.30	0.64
1:A:343:MET:CE	1:A:347:MET:CE	2.77	0.63
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.27	0.63
1:A:343:MET:HE1	1:A:347:MET:HE2	1.80	0.62
1:A:202:GLN:O	1:A:205:LYS:HE2	2.00	0.62
1:B:190:PRO:HB3	1:B:620:GLU:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:HB3	1:A:416:ILE:HD11	1.83	0.61
1:A:115:TYR:OH	1:B:456:ASP:CB	2.47	0.60
1:A:216:ASP:OD2	1:A:219:GLU:HB2	2.01	0.60
1:A:280:MET:O	1:A:286:ARG:HD3	2.01	0.60
1:A:343:MET:HE2	1:A:347:MET:CE	2.32	0.60
1:A:510:TYR:CE1	1:A:514:GLU:HG2	2.37	0.59
1:A:459:ARG:HD2	1:A:492:GLU:HB3	1.83	0.59
1:A:36:GLU:O	1:A:36:GLU:HG2	2.00	0.59
1:A:628:GLU:HG3	1:A:629[B]:ASN:HD22	1.68	0.58
1:B:310:GLU:N	1:B:311:PRO:HA	2.18	0.57
1:B:2:ILE:HG12	1:B:135:ILE:HG12	1.87	0.57
1:B:499:SER:OG	1:B:580:PRO:HA	2.05	0.57
1:A:344:GLN:HG3	1:B:347:MET:HB3	1.87	0.57
1:A:196:MET:SD	1:A:231:LEU:HD22	2.44	0.56
1:A:84:LEU:HD13	1:A:418:MET:CE	2.36	0.56
1:B:533:TYR:OH	1:B:571:GLU:OE2	2.23	0.56
1:B:553:MET:HE2	1:B:569:LEU:HD22	1.87	0.56
1:A:459:ARG:NH2	1:A:496:ASP:OD2	2.39	0.56
1:A:343:MET:HE1	1:A:347:MET:CE	2.37	0.55
1:A:343:MET:HE2	1:A:347:MET:HE3	1.88	0.55
1:A:494:ILE:O	1:A:494:ILE:HG13	2.07	0.54
1:A:174:LYS:O	1:A:178:ARG:HG3	2.08	0.54
1:B:643:TYR:CD2	1:B:643:TYR:C	2.80	0.54
1:B:190:PRO:HB2	1:B:505:TYR:CE1	2.42	0.54
1:A:371:HIS:HE1	1:A:375:HIS:ND1	2.06	0.53
1:A:468:LEU:HD13	1:A:556:PRO:HG3	1.88	0.53
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.43	0.53
1:A:113:ILE:HG23	1:A:121:LEU:HD13	1.91	0.53
1:B:646:ASP:OD2	1:B:649:HIS:ND1	2.39	0.52
1:B:278:PRO:HB2	1:B:280:MET:CE	2.38	0.52
1:A:420:ASP:O	1:A:451:GLY:HA3	2.09	0.52
1:B:100:GLY:O	1:B:101:LEU:HD23	2.10	0.52
1:B:77:HIS:CE1	1:B:420:ASP:HB3	2.45	0.51
1:A:217:PHE:HB3	1:A:218:PRO:HD3	1.92	0.51
1:A:168:ARG:HA	1:A:479:ALA:O	2.11	0.50
1:A:105:TYR:CE2	1:A:107:SER:HB3	2.46	0.50
1:A:16:LEU:HA	1:A:151:ILE:HA	1.93	0.50
1:B:303:GLY:HA2	1:B:400:LEU:O	2.10	0.50
1:A:110:THR:O	1:A:123:VAL:HA	2.12	0.50
1:A:654:LYS:HB3	1:A:656:GLU:HG2	1.93	0.49
1:A:494:ILE:HA	1:A:497:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PHE:O	1:B:122:LYS:HA	2.12	0.49
1:A:3:ARG:O	1:A:133:TYR:HA	2.12	0.49
1:B:401:MET:HE3	1:B:402:PHE:H	1.77	0.49
1:B:18:GLU:HG3	1:B:20:ILE:HG22	1.95	0.48
1:B:553:MET:CE	1:B:569:LEU:HD22	2.42	0.48
1:B:53:LEU:HA	1:B:88:HIS:O	2.13	0.48
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.94	0.48
1:B:444:MET:O	1:B:473:PRO:HG2	2.13	0.48
1:B:469:GLY:HA2	1:B:472:THR:OG1	2.13	0.48
1:A:370:ARG:NE	1:A:372:ASP:OD1	2.43	0.48
1:B:190:PRO:HB2	1:B:505:TYR:CD1	2.49	0.48
1:A:343:MET:CE	1:A:347:MET:HE3	2.43	0.47
1:A:418:MET:O	1:A:449:ASP:N	2.47	0.47
1:A:492:GLU:HG2	1:A:493:ASN:H	1.79	0.47
1:A:233:PRO:HD2	1:A:303:GLY:O	2.13	0.47
1:A:576:ILE:HG13	1:A:607:ILE:CD1	2.45	0.47
1:B:310:GLU:OE1	1:B:404:ARG:NH1	2.31	0.47
1:A:269:ALA:HA	1:A:273:GLY:O	2.15	0.46
1:A:166:GLN:NE2	1:A:184:TYR:OH	2.46	0.46
1:B:494:ILE:H	1:B:494:ILE:CD1	2.08	0.46
1:A:188:HIS:HD2	1:A:620:GLU:OE2	1.99	0.46
1:B:598:VAL:CG1	1:B:604:PRO:HG3	2.45	0.46
1:A:45:ASP:HB3	1:A:48:ASP:OD1	2.15	0.46
1:A:580:PRO:C	1:A:582:GLY:H	2.19	0.46
1:B:528:PRO:O	1:B:529:LEU:C	2.51	0.45
1:A:611:LYS:HA	1:A:611:LYS:HD2	1.78	0.45
1:B:36:GLU:OE2	1:B:36:GLU:HA	2.17	0.45
1:B:371:HIS:HE1	1:B:375:HIS:ND1	2.14	0.45
1:A:494:ILE:HA	1:A:497:PHE:CD1	2.51	0.45
1:B:371:HIS:CE1	1:B:375:HIS:ND1	2.84	0.45
1:B:78:THR:HG23	1:B:81:LYS:HG2	1.99	0.45
1:A:510:TYR:HB2	1:A:614:PRO:HD2	1.98	0.45
1:A:168:ARG:CD	1:A:481:GLU:HB2	2.47	0.45
1:A:315:TYR:HB3	1:A:350:ILE:HD12	1.98	0.45
1:A:628:GLU:CG	1:A:629[B]:ASN:HD22	2.30	0.44
1:A:572:GLU:HG3	1:A:573:MET:N	2.31	0.44
1:B:305:TRP:CD1	1:B:305:TRP:N	2.86	0.44
1:A:157:PRO:HB2	1:A:161:ALA:HB3	1.99	0.44
1:A:418:MET:O	1:A:448:ALA:HA	2.18	0.44
1:A:286:ARG:HG3	1:A:385:ALA:HB2	1.99	0.44
1:A:326:PHE:HE2	1:A:343:MET:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASN:HB2	1:B:379:GLY:HA2	2.01	0.43
1:B:77:HIS:HE1	1:B:85:TYR:OH	2.02	0.43
1:B:481:GLU:CG	1:B:482:GLY:N	2.69	0.43
1:A:576:ILE:HG13	1:A:607:ILE:HD12	2.01	0.43
1:B:74:ASP:HA	1:B:75:PRO:HD3	1.74	0.43
1:A:36:GLU:O	1:A:36:GLU:CG	2.67	0.43
1:B:494:ILE:HD13	1:B:494:ILE:N	2.20	0.43
1:A:251:GLY:HA3	1:A:257:PHE:CE2	2.54	0.43
1:B:67:TYR:CD2	1:B:67:TYR:N	2.87	0.43
1:B:416:ILE:O	1:B:416:ILE:HG13	2.18	0.43
1:B:435:LEU:O	1:B:436:PRO:C	2.55	0.43
1:B:435:LEU:N	1:B:436:PRO:HD2	2.34	0.43
1:B:570:PRO:C	1:B:591:LYS:HG3	2.39	0.43
1:A:505:TYR:HA	1:A:508:VAL:HG23	2.00	0.42
1:B:408:ILE:HD11	1:B:441:CYS:HB3	2.00	0.42
1:B:609:SER:HA	1:B:635:TYR:CE2	2.53	0.42
1:B:280:MET:O	1:B:381:ASN:HB3	2.19	0.42
1:B:480:ALA:O	1:B:481:GLU:HB3	2.19	0.42
1:A:422:LYS:HD3	1:A:422:LYS:HA	1.90	0.42
1:A:174:LYS:HG3	1:A:214:PHE:CE1	2.55	0.42
1:A:577:LYS:HA	1:A:603:VAL:O	2.19	0.42
1:B:646:ASP:O	1:B:648:ILE:HD12	2.19	0.42
1:A:159:LYS:O	1:A:162:PHE:HB2	2.19	0.42
1:A:605:LEU:C	1:A:605:LEU:HD12	2.40	0.42
1:B:243:LYS:HE2	1:B:243:LYS:HB3	1.97	0.42
1:B:538:MET:HG2	1:B:568:TYR:CZ	2.54	0.41
1:A:196:MET:HB2	1:A:233:PRO:HA	2.03	0.41
1:B:502:ASN:O	1:B:506:ARG:HG3	2.20	0.41
1:B:70:ASN:O	1:B:72:THR:HG23	2.20	0.41
1:B:76:ILE:H	1:B:76:ILE:HG12	1.75	0.41
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.93	0.41
1:B:450:LEU:HD21	1:B:461:LEU:HG	2.01	0.41
1:B:196:MET:HB2	1:B:233:PRO:HA	2.01	0.41
1:B:391:GLU:O	1:B:395:PRO:HG3	2.21	0.41
1:A:303:GLY:HA2	1:A:400:LEU:O	2.20	0.41
1:B:605:LEU:C	1:B:605:LEU:HD12	2.41	0.41
1:A:429:LEU:HA	1:A:429:LEU:HD12	1.80	0.41
1:B:501:ILE:O	1:B:504:ARG:HB3	2.21	0.41
1:B:172:THR:HB	1:B:199:ASP:HB3	2.03	0.40
1:B:401:MET:HE3	1:B:402:PHE:N	2.36	0.40
1:A:603:VAL:HA	1:A:604:PRO:HD3	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLU:O	1:B:325:GLU:HB3	2.21	0.40
1:B:575:PHE:HB2	1:B:589:LEU:HD12	2.03	0.40
1:B:53:LEU:O	1:B:54:GLY:C	2.60	0.40
1:B:604:PRO:O	1:B:605:LEU:HB3	2.22	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	648/666 (97%)	604 (93%)	36 (6%)	8 (1%)	13	19
1	B	646/666 (97%)	596 (92%)	45 (7%)	5 (1%)	19	29
All	All	1294/1332 (97%)	1200 (93%)	81 (6%)	13 (1%)	15	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	PRO
1	A	411	HIS
1	A	451	GLY
1	B	481	GLU
1	B	628	GLU
1	B	522	ASP
1	A	493	ASN
1	B	529	LEU
1	A	604	PRO
1	B	75	PRO
1	A	191	ILE
1	A	270	VAL
1	A	54	GLY

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	563/574 (98%)	529 (94%)	34 (6%)	19 30
1	B	561/574 (98%)	522 (93%)	39 (7%)	15 23
All	All	1124/1148 (98%)	1051 (94%)	73 (6%)	17 26

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	62	LYS
1	A	72	THR
1	A	82	ARG
1	A	89	ASN
1	A	108	LYS
1	A	118	MET
1	A	127	ASN
1	A	136	GLU
1	A	142	ASP
1	A	166	GLN
1	A	168	ARG
1	A	253	LYS
1	A	270	VAL
1	A	284	GLU
1	A	294	ARG
1	A	296	LEU
1	A	305	TRP
1	A	337	LYS
1	A	344	GLN
1	A	367	LYS
1	A	373	LYS
1	A	417	TRP
1	A	418	MET
1	A	427	HIS
1	A	430	LEU
1	A	432	LEU

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Mol	Chain	Res	Type
1	A	459	ARG
1	A	493	ASN
1	A	494	ILE
1	A	572	GLU
1	A	628	GLU
1	A	653	ASP
1	A	655	LYS
1	B	16	LEU
1	B	20	ILE
1	B	35	LYS
1	B	46	GLU
1	B	76	ILE
1	B	78	THR
1	B	82	ARG
1	B	117	ARG
1	B	118	MET
1	B	126	GLU
1	B	149	ARG
1	B	166	GLN
1	B	168	ARG
1	B	172	THR
1	B	174	LYS
1	B	243	LYS
1	B	270	VAL
1	B	287	LYS
1	B	296	LEU
1	B	305	TRP
1	B	320	LEU
1	B	368	LYS
1	B	369	ILE
1	B	380	TYR
1	B	403	SER
1	B	405	SER
1	B	416	ILE
1	B	417	TRP
1	B	427	HIS
1	B	450	LEU
1	B	481	GLU
1	B	492	GLU
1	B	494	ILE
1	B	611	LYS
1	B	629	ASN

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Mol	Chain	Res	Type
1	B	631	GLN
1	B	636	GLU
1	B	653	ASP
1	B	654	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	188	HIS
1	A	306	ASN
1	A	371	HIS
1	A	431	ASN
1	A	493	ASN
1	B	77	HIS
1	B	306	ASN
1	B	371	HIS
1	B	421	ASN
1	B	427	HIS
1	B	431	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	GOL	B	665	-	5,5,5	0.39	0	5,5,5	0.29	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
2	GOL	B	665	-	-	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
2	B	665	GOL	C1-C2-C3-O3
2	B	665	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	652/666 (97%)	-0.33	11 (1%) 70 67	26, 36, 52, 70	4 (0%)
1	B	651/666 (97%)	-0.41	4 (0%) 89 89	25, 35, 50, 60	1 (0%)
All	All	1303/1332 (97%)	-0.37	15 (1%) 79 77	25, 36, 51, 70	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	339	HIS	3.4
1	A	332	LYS	3.0
1	A	493	ASN	2.6
1	A	497	PHE	2.6
1	B	494	ILE	2.5
1	A	323	ALA	2.5
1	A	0	ALA	2.4
1	A	390	PHE	2.4
1	A	293	TYR	2.2
1	A	239	VAL	2.0
1	A	267	VAL	2.0
1	A	633	ILE	2.0
1	A	182	LYS	2.0
1	B	332	LYS	2.0
1	B	335	GLU	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	GOL	B	665	6/6	0.85	0.17	58,61,61,62	0

6.5 Other polymers

There are no such residues in this entry.