



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:16 PM UTC

PDB ID : 3M46 / pdb_00003m46
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 : 4-5-2 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

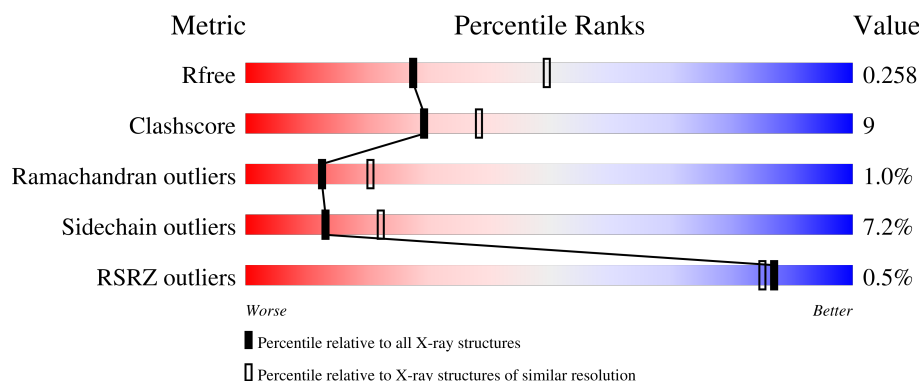
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 $\leq 5\%$. 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	666	% 75% 20% ..
1	B	666	73% 22% ..

2 Entry composition

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

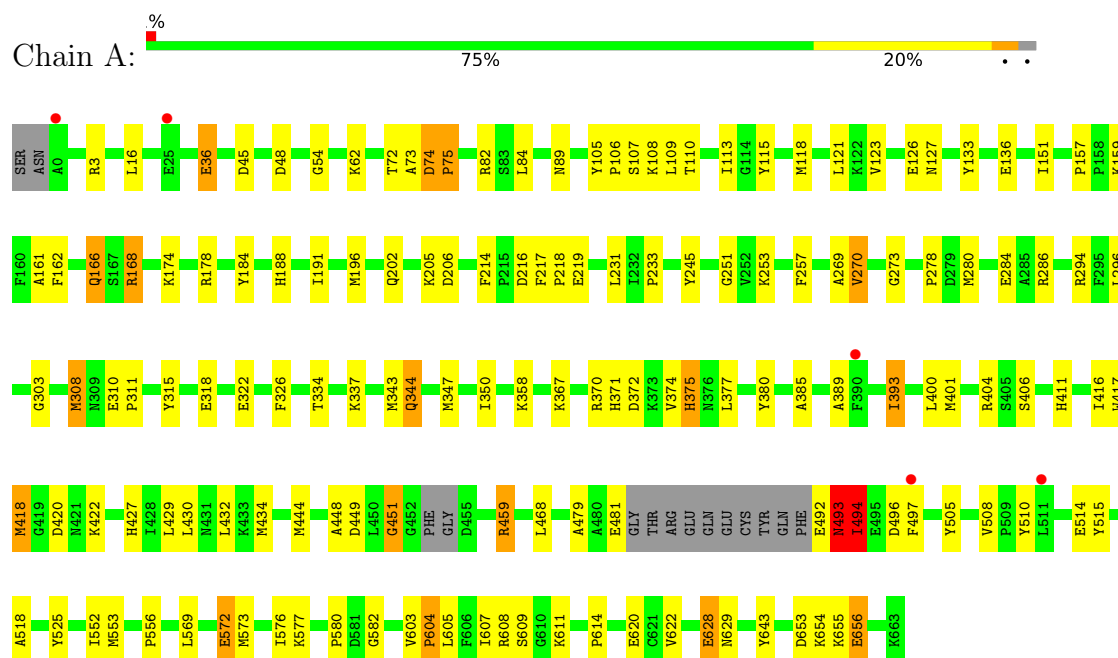
- Molecule 3 is water.

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

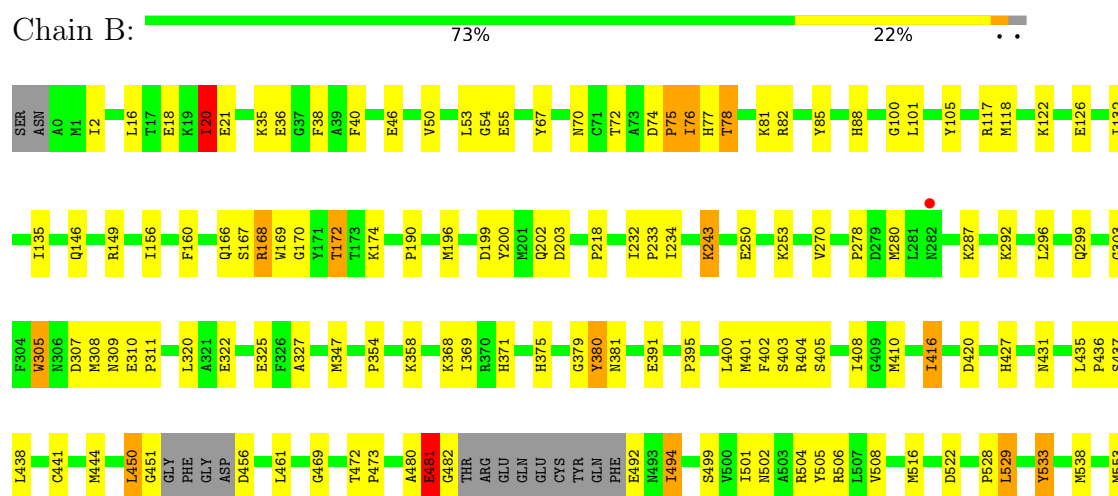
3 Residue-property plots

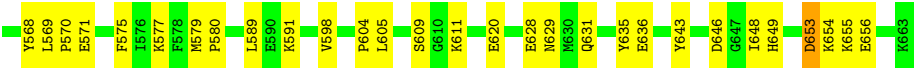
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

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 82.89 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.0 (82.89-2.66) 99.1 (82.89-2.66)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.95%)	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)	0.29 , 16.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.85	0/5486	1.01	6/7395 (0.1%)
1	B	0.87	2/5470 (0.0%)	1.03	9/7372 (0.1%)
All	All	0.86	2/10956 (0.0%)	1.02	15/14767 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	VAL	CA-CB	5.87	1.57	1.54
1	B	20	ILE	CA-CB	5.04	1.61	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASP	CA-C-N	7.07	128.68	119.84
1	A	74	ASP	C-N-CA	7.07	128.68	119.84
1	B	327	ALA	N-CA-C	-6.42	104.36	111.36
1	B	653	ASP	N-CA-C	6.27	118.12	111.28
1	A	126	GLU	N-CA-C	6.04	117.94	111.36
1	A	552	ILE	N-CA-C	5.94	117.47	108.80
1	B	105	TYR	CA-C-N	5.74	126.23	120.04
1	B	105	TYR	C-N-CA	5.74	126.23	120.04
1	B	533	TYR	CA-C-N	5.25	124.75	119.19
1	B	533	TYR	C-N-CA	5.25	124.75	119.19
1	A	494	ILE	N-CA-C	5.21	120.18	109.34
1	B	232	ILE	CA-C-N	5.18	124.94	119.76
1	B	232	ILE	C-N-CA	5.18	124.94	119.76
1	B	169	TRP	N-CA-C	-5.04	102.18	109.59
1	A	622	VAL	N-CA-C	5.03	115.75	110.62

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	92	0
1	B	5329	0	5121	91	0
2	B	6	0	8	0	0
3	A	24	0	0	0	0
3	B	28	0	0	0	0
All	All	10735	0	10251	180	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 9.

All (180) 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:A:343:MET:CE	1:A:347:MET:HE2	2.10	0.82
1:A:343:MET:HE2	1:A:347:MET:CE	2.09	0.81
1:A:343:MET:HE2	1:A:347:MET:HE2	1.63	0.78
1:B:553:MET:HE1	1:B:569:LEU:HD22	1.65	0.78
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:A:73:ALA:C	1:A:75:PRO:HD2	2.12	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:N	1:A:311:PRO:HA	2.06	0.70
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:418:MET:HE3	1:A:434:MET:HE1	1.75	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: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:B:234:ILE:HD11	1:B:307:ASP:CB	2.27	0.63
1:A:308:MET:HE2	1:A:404:ARG:NH1	2.13	0.62
1:B:553:MET:HE1	1:B:569:LEU:CD2	2.29	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
1:A:406:SER:HB3	1:A:416:ILE:HD11	1.83	0.61
1:A:343:MET:HE2	1:A:347:MET:HE3	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: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:B:643:TYR:CD2	1:B:643:TYR:C	2.80	0.58
1:A:628:GLU:HG3	1:A:629[B]:ASN:HD22	1.68	0.58
1:A:444:MET:HE2	1:A:525:TYR:HB2	1.85	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:A:401:MET:HE3	1:A:401:MET:HA	1.87	0.57
1:A:278:PRO:HG2	1:A:280:MET:HE2	1.85	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:B:278:PRO:HB2	1:B:280:MET:HE2	1.87	0.56
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:A:459:ARG:NH2	1:A:496:ASP:OD2	2.39	0.56
1:A:343:MET:CE	1:A:347:MET:CE	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:MET:HE3	1:B:402:PHE:H	1.73	0.53
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.43	0.53
1:B:577:LYS:HB3	1:B:579:MET:HE2	1.90	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:580:PRO:C	1:A:582:GLY:H	2.19	0.50
1:B:528:PRO:O	1:B:529:LEU:C	2.51	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
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:18:GLU:HG3	1:B:20:ILE:HG22	1.95	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: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:B:435:LEU:O	1:B:436:PRO:C	2.55	0.47
1:B:570:PRO:C	1:B:591:LYS:HG3	2.39	0.47
1:A:233:PRO:HD2	1:A:303:GLY:O	2.13	0.47
1:B:401:MET:HE3	1:B:402:PHE:N	2.29	0.47
1:A:553:MET:HE1	1:A:569:LEU:CD2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:C	1:A:605:LEU:HD12	2.40	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:206:ASP:O	1:A:245:TYR:OH	2.33	0.46
1:B:533:TYR:OH	1:B:571:GLU:OE2	2.23	0.46
1:A:343:MET:HE1	1:A:347:MET:HE2	1.91	0.45
1:B:605:LEU:C	1:B:605:LEU:HD12	2.41	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:B:250:GLU:OE1	1:B:292:LYS:NZ	2.44	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:444:MET:HE1	1:A:518:ALA:HB1	1.98	0.45
1:B:53:LEU:O	1:B:54:GLY:C	2.60	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:B:553:MET:CE	1:B:569:LEU:HD22	2.42	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:B:200:TYR:C	1:B:200:TYR:CD1	2.94	0.44
1:A:286:ARG:HG3	1:A:385:ALA:HB2	1.99	0.44
1:A:643:TYR:CD2	1:A:643:TYR:C	2.96	0.44
1:B:156:ILE:HG21	1:B:516:MET:HE1	2.00	0.43
1:A:326:PHE:HE2	1:A:343:MET:HA	1.83	0.43
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:B:202:GLN:O	1:B:203:ASP:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:436:PRO:HD2	2.34	0.43
1:A:505:TYR:HA	1:A:508:VAL:HG23	2.00	0.42
1:B:54:GLY:HA2	1:B:437:SER:C	2.44	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:A:608:ARG:O	1:A:609:SER:C	2.62	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:515:TYR:CD2	1:A:515:TYR:C	2.98	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:310:GLU:CD	1:B:404:ARG:HH11	2.22	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:A:553:MET:HE1	1:A:569:LEU:HD22	2.02	0.41
1:B:160:PHE:CD1	1:B:160:PHE:C	2.99	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: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:A:603:VAL:HA	1:A:604:PRO:HD3	1.61	0.40
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: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%)	10	17
1	B	646/666 (97%)	596 (92%)	45 (7%)	5 (1%)	16	27
All	All	1294/1332 (97%)	1200 (93%)	81 (6%)	13 (1%)	12	20

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%)	526 (93%)	37 (7%)	15	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	561/574 (98%)	517 (92%)	44 (8%)	11	20
All	All	1124/1148 (98%)	1043 (93%)	81 (7%)	13	22

All (81) 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	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	308	MET
1	A	334	THR
1	A	337	LYS
1	A	344	GLN
1	A	358	LYS
1	A	367	LYS
1	A	375	HIS
1	A	393	ILE
1	A	417	TRP
1	A	418	MET
1	A	427	HIS
1	A	430	LEU
1	A	432	LEU
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

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Mol	Chain	Res	Type
1	A	656	GLU
1	B	16	LEU
1	B	20	ILE
1	B	21	GLU
1	B	35	LYS
1	B	46	GLU
1	B	50	VAL
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	146	GLN
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	253	LYS
1	B	270	VAL
1	B	287	LYS
1	B	296	LEU
1	B	305	TRP
1	B	308	MET
1	B	320	LEU
1	B	354	PRO
1	B	358	LYS
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	450	LEU
1	B	481	GLU
1	B	492	GLU
1	B	494	ILE
1	B	611	LYS
1	B	629	ASN
1	B	631	GLN

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Mol	Chain	Res	Type
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 (17) 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	A	561	ASN
1	B	77	HIS
1	B	188	HIS
1	B	213	ASN
1	B	306	ASN
1	B	363	ASN
1	B	371	HIS
1	B	421	ASN
1	B	427	HIS
1	B	431	ASN
1	B	561	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.40	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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%)	-0.36	5 (0%)	82 79	18, 36, 52, 70	6 (0%)
1	B	651/666 (97%)	-0.41	1 (0%)	91 90	23, 35, 50, 60	2 (0%)
All	All	1303/1332 (97%)	-0.39	6 (0%)	87 85	18, 35, 51, 70	8 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	PHE	2.9
1	B	282	ASN	2.7
1	A	511	LEU	2.5
1	A	25	GLU	2.5
1	A	0	ALA	2.4
1	A	497	PHE	2.3

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	665	6/6	0.71	0.20	58,61,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.