Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 05:32 AM EDT

PDB ID	:	3PQU
Title	:	The crystal structures of porcine pathogen AsH57_TbpB
Authors	:	Calmettes, C.; Moraes, T.F.
Deposited on	:	2010-11-26
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 (i) 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 (i)) were used in the production of this report:

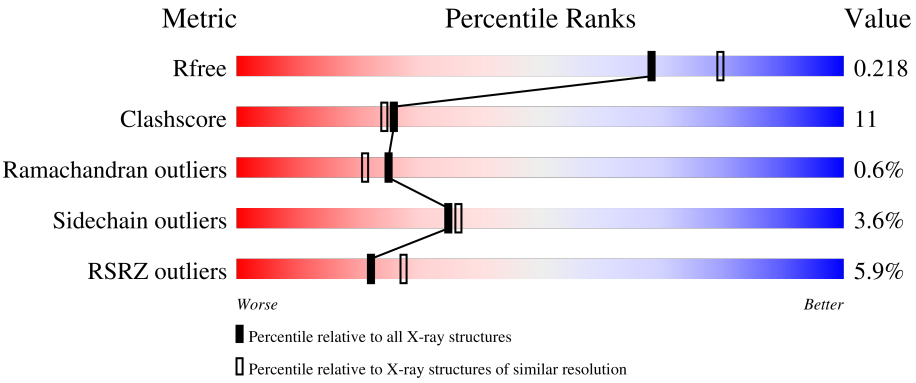
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	570	4% 81% 14%
1	B	570	7% 74% 19% 5%

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	GOL	B	3968	-	-	X	-

2 Entry composition (i)

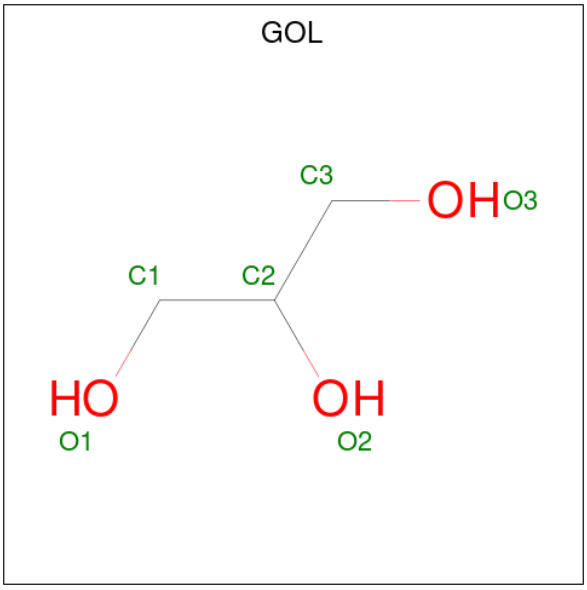
There are 3 unique types of molecules in this entry. The entry contains 9509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transferrin binding protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	4	9	0
			4312	2702	741	861	8			
1	B	540	Total	C	N	O	S	0	12	0
			4277	2688	731	850	8			

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

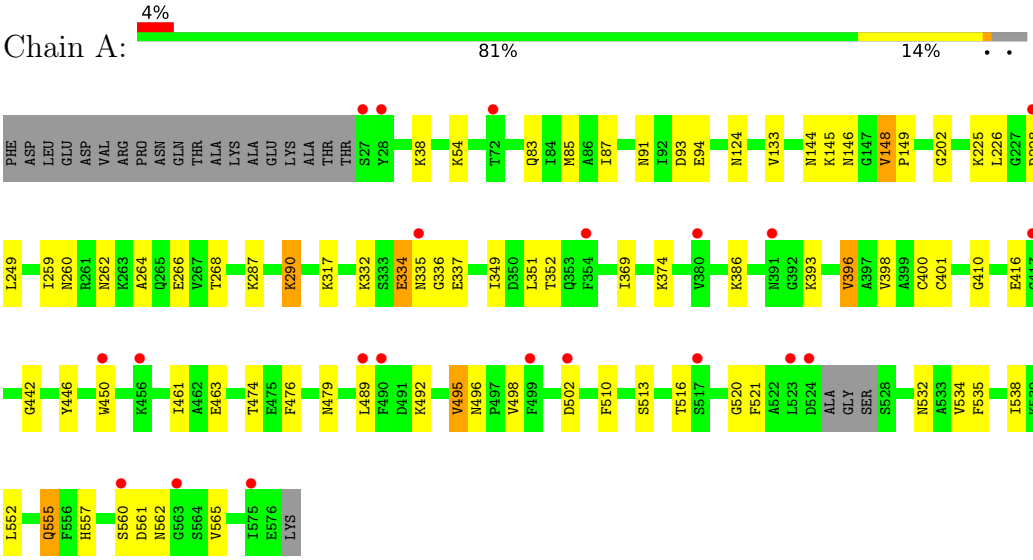
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	472	Total O 472 472	0	0
3	B	418	Total O 418 418	0	0

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.

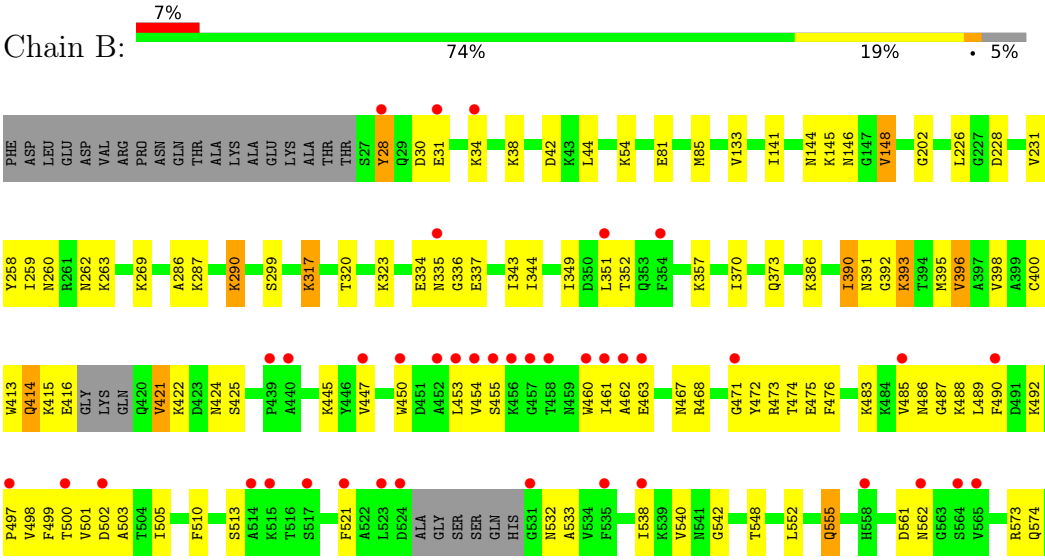
• Molecule 1: Transferrin binding protein B

Chain A:



• Molecule 1: Transferrin binding protein B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.67Å 74.47Å 106.40Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	44.76 – 2.10 46.25 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.76-2.10) 95.6 (46.25-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.172 , 0.218 0.173 , 0.218	Depositor DCC
R_{free} test set	6524 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9509	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% 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	0.43	0/4414	0.55	0/5936
1	B	0.41	0/4384	0.54	0/5894
All	All	0.42	0/8798	0.54	0/11830

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	GLU	Peptide

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	4312	0	4201	66	0
1	B	4277	0	4183	110	0
2	A	18	0	24	6	0
2	B	12	0	16	6	0
3	A	472	0	0	15	0
3	B	418	0	0	18	0
All	All	9509	0	8424	179	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 11.

All (179) 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:349:ILE:HD11	1:B:555:GLN:HG3	1.62	0.81
1:A:349:ILE:HD11	1:A:555:GLN:HG3	1.63	0.81
1:B:447:VAL:HG22	1:B:574:GLN:NE2	1.97	0.79
1:B:54[B]:LYS:HG3	3:B:751:HOH:O	1.83	0.78
1:A:87:ILE:HB	2:A:578:GOL:H2	1.66	0.76
1:B:548:THR:HG23	1:B:573:ARG:HH22	1.52	0.75
1:A:54[B]:LYS:HG3	3:A:878:HOH:O	1.87	0.74
1:B:81:GLU:OE1	2:B:3968:GOL:H2	1.88	0.73
1:B:413:TRP:CD1	1:B:421:VAL:HG23	2.25	0.72
1:B:450:TRP:CE3	1:B:489:LEU:HD23	2.27	0.69
1:A:520:GLY:HA3	1:A:534:VAL:HG22	1.76	0.67
1:B:494:GLY:HA2	1:B:495:VAL:HB	1.77	0.67
1:B:260:ASN:HB3	1:B:262:ASN:H	1.59	0.67
1:B:495:VAL:HG13	1:B:496:ASN:N	2.09	0.67
1:A:498:VAL:O	1:A:516:THR:HG22	1.95	0.67
2:A:578:GOL:H31	3:A:618:HOH:O	1.95	0.67
1:B:415:LYS:O	1:B:416:GLU:HB2	1.93	0.66
1:A:260:ASN:HB3	1:A:262:ASN:H	1.60	0.66
1:B:373:GLN:HB2	1:B:390[A]:ILE:HD11	1.76	0.65
1:A:416:GLU:O	1:A:416:GLU:HG3	1.97	0.65
1:B:532:ASN:CG	1:B:533:ALA:H	2.00	0.64
1:B:351:LEU:HG	1:B:425:SER:HA	1.79	0.63
1:B:299[B]:SER:HB3	1:B:320:THR:HA	1.79	0.63
1:B:258[B]:TYR:HD2	3:B:840:HOH:O	1.82	0.61
1:B:489:LEU:HB2	1:B:499:PHE:HB2	1.82	0.61
1:B:494:GLY:HA2	1:B:495:VAL:CB	2.30	0.61
1:A:474:THR:HG22	1:A:489:LEU:HG	1.83	0.60
1:B:393:LYS:HD2	1:B:393:LYS:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:CB	2:A:578:GOL:H2	2.31	0.59
1:B:287:LYS:HE3	3:B:908:HOH:O	2.02	0.59
1:B:453:LEU:HD21	1:B:455:SER:OG	2.03	0.59
1:A:144:ASN:OD1	1:A:148:VAL:HG13	2.02	0.58
1:A:38:LYS:HB3	1:A:38:LYS:NZ	2.18	0.58
1:B:38:LYS:NZ	1:B:38:LYS:HB3	2.18	0.58
1:A:498:VAL:HG13	1:A:521:PHE:CE1	2.38	0.58
1:A:495:VAL:HG23	1:A:496:ASN:H	1.69	0.58
1:B:395:MET:SD	1:B:414:GLN:HG2	2.43	0.58
1:B:252:SER:OG	1:B:269[B]:LYS:HE3	2.04	0.57
1:B:450:TRP:CD2	1:B:489:LEU:HD23	2.39	0.57
1:B:532:ASN:CG	1:B:533:ALA:N	2.56	0.57
1:A:93:ASP:HA	3:A:869:HOH:O	2.03	0.57
1:B:31:GLU:OE2	1:B:573:ARG:HB3	2.03	0.57
1:A:336:GLY:HA2	1:A:337:GLU:C	2.24	0.57
1:B:144:ASN:OD1	1:B:148:VAL:HG13	2.04	0.57
1:B:336:GLY:HA2	1:B:337:GLU:C	2.25	0.57
1:A:124[A]:ASN:HB3	2:A:3968:GOL:H11	1.87	0.57
1:B:487:GLY:O	1:B:500:THR:HA	2.06	0.56
1:B:28:TYR:O	1:B:468:ARG:NH2	2.39	0.56
1:B:486:ASN:HA	1:B:501:VAL:O	2.06	0.55
1:A:516:THR:HG21	3:A:892:HOH:O	2.05	0.55
2:B:3968:GOL:H31	3:B:904:HOH:O	2.06	0.55
1:A:149:PRO:HD3	3:A:827:HOH:O	2.06	0.55
1:B:454:VAL:HG21	1:B:521:PHE:HZ	1.72	0.54
1:A:535:PHE:HD2	3:A:892:HOH:O	1.91	0.54
1:A:54[B]:LYS:HE3	3:A:878:HOH:O	2.07	0.54
1:A:510:PHE:CZ	1:A:542:GLY:HA3	2.43	0.53
1:B:467:ASN:HB3	1:B:471:GLY:HA3	1.90	0.53
1:A:334:GLU:HG2	3:A:709:HOH:O	2.08	0.53
1:A:266[B]:GLU:HG2	3:A:851:HOH:O	2.09	0.53
1:A:336:GLY:HA2	1:A:337:GLU:HB2	1.91	0.53
1:A:418:LYS:HA	1:A:419:GLN:HB3	1.91	0.52
1:B:54[B]:LYS:HE3	3:B:751:HOH:O	2.09	0.52
1:B:336:GLY:HA2	1:B:337:GLU:HB2	1.90	0.52
1:B:474:THR:HA	1:B:488:LYS:O	2.09	0.52
1:A:332:LYS:CE	2:A:3968:GOL:H12	2.40	0.52
1:B:510:PHE:CZ	1:B:542:GLY:HA3	2.44	0.52
1:A:145:LYS:HG3	1:A:146:ASN:N	2.25	0.52
1:A:287:LYS:HD2	3:A:846:HOH:O	2.09	0.52
1:A:442:GLY:O	1:A:479:ASN:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:NE2	3:A:605:HOH:O	2.42	0.52
1:B:252:SER:CB	1:B:269[B]:LYS:HE3	2.41	0.51
1:B:498:VAL:HG13	1:B:521:PHE:CD2	2.45	0.51
1:A:560:SER:O	1:A:562:ASN:HA	2.10	0.51
1:B:145:LYS:HG3	1:B:146:ASN:N	2.26	0.51
1:B:287:LYS:HD2	3:B:967:HOH:O	2.10	0.51
1:B:416:GLU:O	1:B:422:LYS:HD2	2.11	0.50
1:A:144:ASN:CG	1:A:148:VAL:HG13	2.32	0.50
1:B:226:LEU:HD12	1:B:226:LEU:N	2.26	0.50
1:B:496:ASN:HB3	1:B:497:PRO:HD2	1.93	0.50
1:A:268:THR:HG22	3:B:809:HOH:O	2.12	0.50
1:A:513:SER:HA	1:A:538:ILE:O	2.12	0.49
1:B:513:SER:HA	1:B:538:ILE:O	2.11	0.49
1:A:446:TYR:HB2	1:A:476:PHE:HB2	1.95	0.49
1:A:374[B]:LYS:NZ	3:A:857:HOH:O	2.45	0.49
1:B:476:PHE:CE1	1:B:487:GLY:HA3	2.47	0.49
1:B:44:LEU:HB2	2:B:3968:GOL:O1	2.11	0.49
1:A:418:LYS:N	1:A:419:GLN:HA	2.28	0.48
1:B:475:GLU:O	1:B:487:GLY:HA2	2.13	0.48
1:A:226:LEU:N	1:A:226:LEU:HD12	2.28	0.48
1:B:561:ASP:HA	1:B:562:ASN:HA	1.53	0.48
1:B:450:TRP:CD1	1:B:474:THR:HG23	2.49	0.48
1:B:495:VAL:CG1	1:B:496:ASN:N	2.76	0.48
1:A:264:ALA:HB1	3:A:755:HOH:O	2.13	0.48
1:B:269[B]:LYS:NZ	3:B:884:HOH:O	2.45	0.48
1:B:337:GLU:OE2	1:B:337:GLU:HA	2.13	0.48
1:A:144:ASN:ND2	1:A:148:VAL:HG13	2.28	0.47
1:B:42:ASP:HB3	2:B:3968:GOL:O1	2.13	0.47
1:B:54[B]:LYS:HG2	3:B:877:HOH:O	2.14	0.47
1:B:146:ASN:ND2	3:B:988:HOH:O	2.46	0.47
1:B:393:LYS:HD2	1:B:393:LYS:N	2.28	0.47
1:B:496:ASN:HB3	1:B:497:PRO:CD	2.43	0.47
1:B:476:PHE:HA	1:B:486:ASN:O	2.15	0.47
1:A:232:LYS:HE2	3:A:640:HOH:O	2.14	0.47
1:B:144:ASN:ND2	1:B:148:VAL:HG13	2.30	0.47
1:B:398:VAL:O	1:B:410:GLY:HA3	2.15	0.47
1:B:495:VAL:HG13	1:B:496:ASN:H	1.77	0.47
1:A:124[B]:ASN:HB2	2:A:3968:GOL:H11	1.97	0.47
1:B:413:TRP:HD1	1:B:421:VAL:HG23	1.76	0.47
1:A:337:GLU:OE2	1:A:337:GLU:HA	2.14	0.47
1:B:144:ASN:CG	1:B:148:VAL:HG13	2.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232[A]:LYS:HE3	3:B:744:HOH:O	2.14	0.47
1:B:258[B]:TYR:CE1	1:B:263:LYS:HD3	2.49	0.46
1:A:398:VAL:O	1:A:410:GLY:HA3	2.16	0.46
1:B:552:LEU:C	1:B:552:LEU:HD12	2.36	0.46
1:B:494:GLY:HA2	1:B:495:VAL:HG12	1.98	0.46
1:B:462:ALA:HA	1:B:472:TYR:CE2	2.50	0.46
1:B:473:ARG:HB2	1:B:490:PHE:HB2	1.98	0.46
1:B:81:GLU:HG2	3:B:932:HOH:O	2.15	0.46
1:B:494:GLY:HA2	1:B:495:VAL:CG1	2.46	0.46
2:B:578:GOL:H2	3:B:801:HOH:O	2.15	0.46
1:B:413:TRP:CD1	1:B:421:VAL:CG2	2.97	0.45
1:B:485:VAL:HB	1:B:503:ALA:HB3	1.97	0.45
1:B:474:THR:HG22	1:B:489:LEU:HG	1.97	0.45
1:A:521:PHE:N	1:A:532:ASN:HB3	2.32	0.45
1:B:447:VAL:HG22	1:B:574:GLN:CD	2.37	0.45
1:B:492:LYS:O	1:B:492:LYS:HG3	2.17	0.45
1:B:351:LEU:HB2	1:B:424:ASN:O	2.16	0.44
1:B:54[B]:LYS:NZ	3:B:803:HOH:O	2.49	0.44
1:B:461:ILE:HD13	1:B:463:GLU:CG	2.47	0.44
1:A:290:LYS:HE3	1:A:290:LYS:HB2	1.81	0.44
1:B:290:LYS:HE3	1:B:290:LYS:HB2	1.80	0.44
1:B:323:LYS:HE3	3:B:592:HOH:O	2.18	0.44
1:B:28:TYR:CE2	1:B:445:LYS:HE2	2.53	0.44
1:B:231:VAL:HG22	1:B:259:ILE:HD13	1.99	0.44
1:A:231:VAL:HG22	1:A:259:ILE:HD13	2.00	0.43
1:B:317:LYS:HD2	1:B:317:LYS:C	2.38	0.43
1:B:460:TRP:CD2	1:B:521:PHE:HE1	2.36	0.43
1:A:351:LEU:HG	1:A:425:SER:HA	2.00	0.43
1:B:81:GLU:CD	2:B:3968:GOL:H2	2.38	0.43
1:B:258[B]:TYR:CZ	1:B:263:LYS:HE2	2.54	0.43
1:B:287:LYS:CE	3:B:908:HOH:O	2.64	0.43
1:B:521:PHE:O	1:B:532:ASN:ND2	2.52	0.43
1:A:91:ASN:ND2	1:A:94:GLU:HG3	2.33	0.43
1:A:461:ILE:HD13	1:A:463:GLU:HG2	2.01	0.43
1:B:386:LYS:O	1:B:396:VAL:HA	2.19	0.43
1:A:461:ILE:HD13	1:A:463:GLU:CG	2.48	0.43
1:B:476:PHE:CD1	1:B:487:GLY:HA3	2.54	0.43
1:B:343:ILE:HG13	1:B:344:ILE:HG13	2.01	0.42
1:A:54[A]:LYS:HG2	3:A:878:HOH:O	2.18	0.42
1:A:450:TRP:CD2	1:A:489:LEU:HD23	2.54	0.42
1:B:141[A]:ILE:HG22	3:B:861:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:CYS:HA	1:B:401:CYS:HA	1.86	0.42
1:A:369:ILE:HD13	1:A:374[A]:LYS:HG2	2.02	0.42
1:A:148:VAL:HA	1:A:149:PRO:HD3	1.84	0.41
1:A:249:LEU:C	1:A:249:LEU:HD12	2.39	0.41
1:A:393:LYS:HE3	1:A:393:LYS:HB2	1.94	0.41
1:A:561:ASP:HA	1:A:562:ASN:HA	1.63	0.41
1:B:286:ALA:HB3	1:B:299[B]:SER:OG	2.20	0.41
1:B:461:ILE:HD13	1:B:463:GLU:HG2	2.01	0.41
1:A:336:GLY:HA2	1:A:337:GLU:CB	2.50	0.41
1:A:400:CYS:HA	1:A:401:CYS:HA	1.86	0.41
1:B:334:GLU:HG2	3:B:712:HOH:O	2.19	0.41
1:B:336:GLY:CA	1:B:337:GLU:C	2.89	0.41
1:A:336:GLY:CA	1:A:337:GLU:C	2.89	0.41
1:B:453:LEU:HD23	1:B:453:LEU:O	2.20	0.41
1:A:386:LYS:O	1:A:396:VAL:HA	2.20	0.41
1:B:483:LYS:HD2	1:B:505:ILE:O	2.20	0.41
1:B:494:GLY:CA	1:B:495:VAL:HG12	2.51	0.41
1:B:28:TYR:CZ	1:B:445:LYS:HG2	2.56	0.41
1:B:532:ASN:ND2	1:B:533:ALA:H	2.18	0.41
1:A:552:LEU:HD12	1:A:552:LEU:C	2.41	0.40
1:A:557:HIS:HA	1:A:565:VAL:O	2.21	0.40
1:A:498:VAL:HG13	1:A:521:PHE:CD1	2.56	0.40
1:B:252:SER:HB3	1:B:269[B]:LYS:HE3	2.04	0.40
1:B:370:ILE:HB	1:B:390[B]:ILE:CD1	2.50	0.40
1:A:225:LYS:HE2	1:A:225:LYS:HB3	1.92	0.40
1:B:453:LEU:HD23	1:B:453:LEU:C	2.42	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	552/570 (97%)	529 (96%)	21 (4%)	2 (0%)	34	32
1	B	546/570 (96%)	518 (95%)	23 (4%)	5 (1%)	17	12
All	All	1098/1140 (96%)	1047 (95%)	44 (4%)	7 (1%)	25	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	B	495	VAL
1	B	391	ASN
1	B	30	ASP
1	B	335	ASN
1	A	202	GLY
1	B	202	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	462/471 (98%)	448 (97%)	14 (3%)	41	44
1	B	459/471 (98%)	438 (95%)	21 (5%)	27	26
All	All	921/942 (98%)	886 (96%)	35 (4%)	35	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	MET
1	A	133[A]	VAL
1	A	133[B]	VAL
1	A	148	VAL
1	A	228	ASP
1	A	290	LYS
1	A	317	LYS
1	A	352	THR
1	A	396	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	LYS
1	A	495	VAL
1	A	502	ASP
1	A	540	VAL
1	A	555	GLN
1	B	28	TYR
1	B	34	LYS
1	B	85	MET
1	B	133[A]	VAL
1	B	133[B]	VAL
1	B	148	VAL
1	B	228	ASP
1	B	290	LYS
1	B	317	LYS
1	B	352	THR
1	B	357	LYS
1	B	390[A]	ILE
1	B	390[B]	ILE
1	B	393	LYS
1	B	396	VAL
1	B	414	GLN
1	B	421	VAL
1	B	495	VAL
1	B	502	ASP
1	B	540	VAL
1	B	555	GLN

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)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	578	-	5,5,5	0.36	0	5,5,5	0.28	0
2	GOL	A	3968	-	5,5,5	0.42	0	5,5,5	0.39	0
2	GOL	B	3968	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	A	578	-	5,5,5	0.45	0	5,5,5	0.17	0
2	GOL	A	579	-	5,5,5	0.36	0	5,5,5	0.44	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	578	-	-	2/4/4/4	-
2	GOL	A	3968	-	-	2/4/4/4	-
2	GOL	B	3968	-	-	2/4/4/4	-
2	GOL	A	578	-	-	0/4/4/4	-
2	GOL	A	579	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3968	GOL	O1-C1-C2-C3
2	B	3968	GOL	O1-C1-C2-C3
2	B	578	GOL	O1-C1-C2-C3
2	A	579	GOL	O1-C1-C2-O2
2	A	579	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	3968	GOL	O1-C1-C2-O2
2	B	3968	GOL	O1-C1-C2-O2
2	B	578	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	578	GOL	1	0
2	A	3968	GOL	3	0
2	B	3968	GOL	5	0
2	A	578	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	547/570 (95%)	-0.27	23 (4%)	36	42	10, 40, 105, 179	0
1	B	540/570 (94%)	-0.04	41 (7%)	13	18	13, 42, 125, 188	0
All	All	1087/1140 (95%)	-0.16	64 (5%)	22	27	10, 41, 113, 188	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	VAL	7.4
1	A	335	ASN	5.5
1	B	462	ALA	5.0
1	B	523	LEU	5.0
1	B	521	PHE	4.5
1	B	458	THR	4.4
1	B	440	ALA	4.4
1	B	453	LEU	4.3
1	B	354	PHE	4.2
1	B	335	ASN	4.2
1	A	354	PHE	4.2
1	A	563	GLY	4.2
1	B	460	TRP	4.1
1	A	523	LEU	4.1
1	A	419	GLN	4.0
1	B	457	GLY	4.0
1	B	485	VAL	3.8
1	B	452	ALA	3.8
1	B	524	ASP	3.8
1	B	565	VAL	3.7
1	B	351	LEU	3.5
1	B	490	PHE	3.4
1	B	439	PRO	3.3
1	B	558	HIS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	28	TYR	3.2
1	B	514	ALA	3.1
1	A	524	ASP	3.0
1	B	531	GLY	3.0
1	B	463	GLU	3.0
1	B	564	SER	2.9
1	B	450	TRP	2.8
1	B	461	ILE	2.8
1	B	34	LYS	2.8
1	A	27	SER	2.7
1	B	562	ASN	2.7
1	B	538	ILE	2.7
1	B	471	GLY	2.7
1	A	489	LEU	2.6
1	A	502	ASP	2.6
1	B	447	VAL	2.5
1	B	493	GLY	2.5
1	A	490	PHE	2.4
1	A	418	LYS	2.4
1	A	456	LYS	2.4
1	A	575	ILE	2.4
1	B	517	SER	2.3
1	A	391	ASN	2.3
1	B	535	PHE	2.3
1	A	72	THR	2.3
1	B	455	SER	2.3
1	B	502	ASP	2.2
1	A	380	VAL	2.2
1	A	450	TRP	2.1
1	A	28	TYR	2.1
1	A	228	ASP	2.1
1	A	560	SER	2.1
1	A	417	GLY	2.1
1	A	517	SER	2.1
1	B	500	THR	2.1
1	B	456	LYS	2.1
1	A	499	PHE	2.1
1	B	497	PRO	2.1
1	B	31	GLU	2.0
1	B	515	LYS	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
2	GOL	B	3968	6/6	0.79	0.17	58,83,86,89	0
2	GOL	A	579	6/6	0.82	0.21	60,81,89,97	0
2	GOL	A	578	6/6	0.90	0.11	38,59,61,65	0
2	GOL	A	3968	6/6	0.92	0.14	52,70,75,86	0
2	GOL	B	578	6/6	0.92	0.09	46,67,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.