



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:45 PM UTC

PDB ID : 4O4U / pdb_00004o4u
Title : Crystal structure of the vaccine antigen Transferrin Binding Protein B (TbpB) mutant Trp-176-Ala from Haemophilus parasuis Hp5
Authors : Calmettes, C.; Yu, R.H.; Schryvers, A.B.; Moraes, T.F.
Deposited on : 2013-12-19
Resolution : 2.64 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

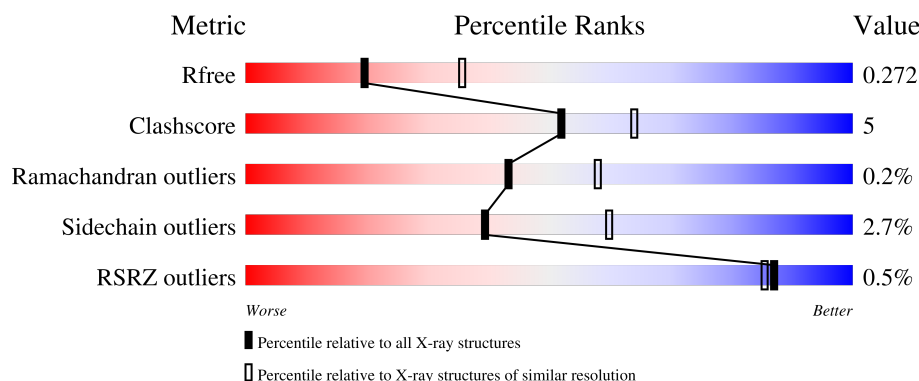
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

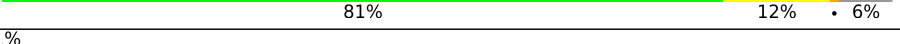
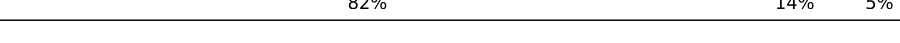
The reported resolution of this entry is 2.64 Å.

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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	532	 81% 13% • 5%
1	B	532	 80% 13% • 6%
1	C	532	 81% 12% • 6%
1	D	532	 82% 14% 5%

2 Entry composition [i](#)

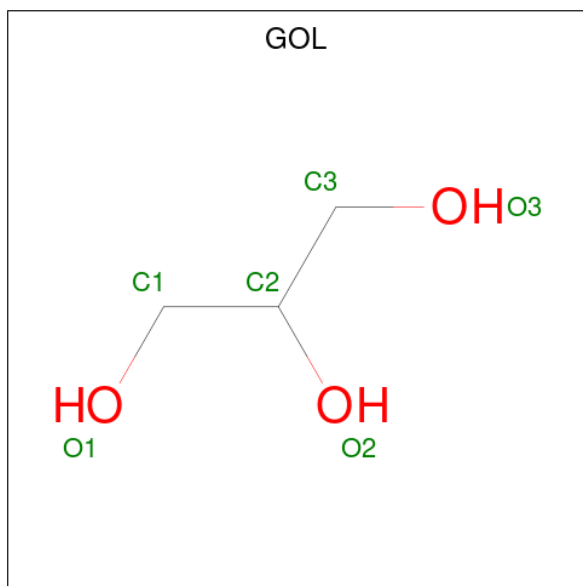
There are 3 unique types of molecules in this entry. The entry contains 15892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TbpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3912	2465	655	782	10			
1	B	500	Total	C	N	O	S	0	0	0
			3871	2441	644	776	10			
1	C	499	Total	C	N	O	S	0	0	0
			3861	2434	643	774	10			
1	D	507	Total	C	N	O	S	0	2	0
			3944	2487	659	788	10			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

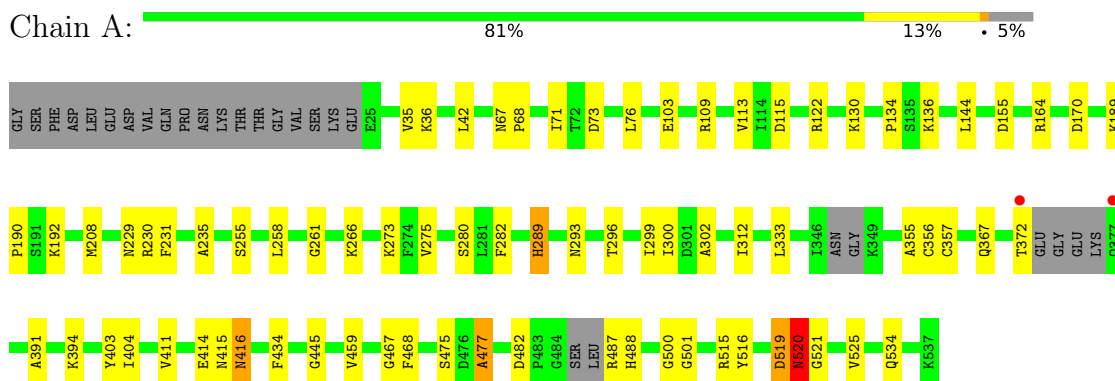
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total 79	O 79	0	0
3	B	91	Total 91	O 91	0	0
3	C	48	Total 48	O 48	0	0
3	D	80	Total 80	O 80	0	0

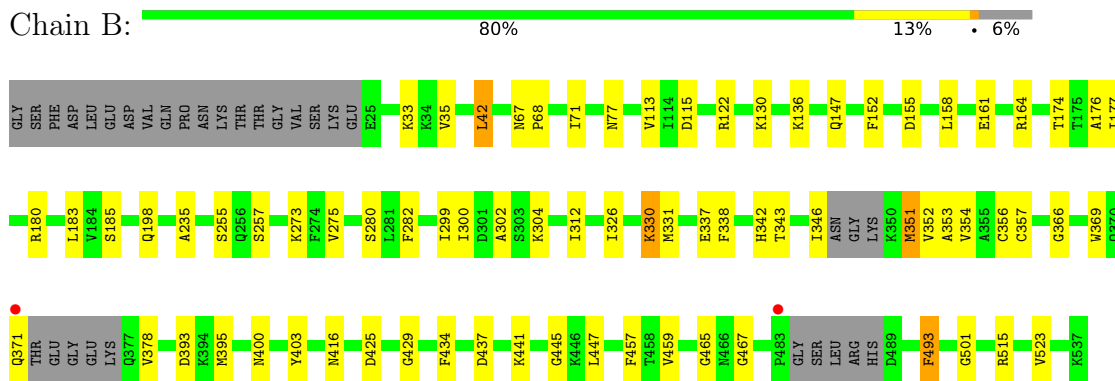
3 Residue-property plots

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.

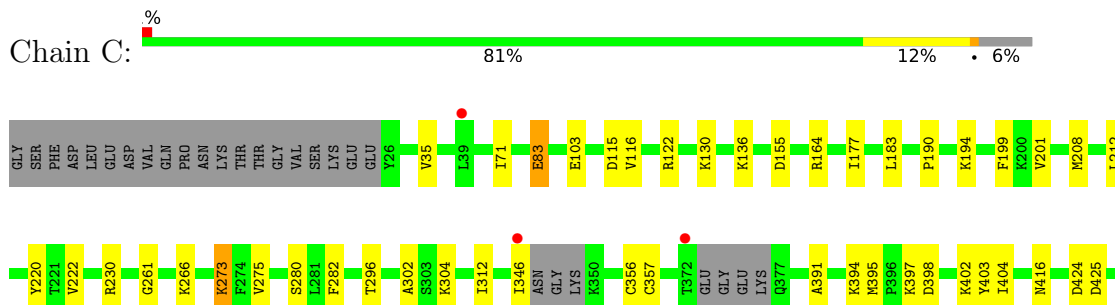
• Molecule 1: TbpB



• Molecule 1: TbpB

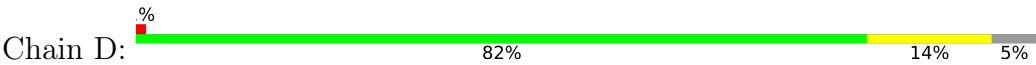


• Molecule 1: TbpB





● Molecule 1: TbpB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 135.70Å 103.96Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	48.39 – 2.64 48.39 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.39-2.64) 74.3 (48.39-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.214 , 0.266 0.218 , 0.272	Depositor DCC
R_{free} test set	2393 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15892	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.27	0/3987	0.71	1/5372 (0.0%)
1	B	0.28	0/3945	0.71	0/5317
1	C	0.26	0/3936	0.69	0/5308
1	D	0.27	0/4024	0.70	0/5424
All	All	0.27	0/15892	0.70	1/21421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	ALA	N-CA-C	-5.45	107.89	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3912	0	3795	40	0
1	B	3871	0	3752	43	0
1	C	3861	0	3734	37	0
1	D	3944	0	3828	39	0
2	D	6	0	8	1	0
3	A	79	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	91	0	0	2	0
3	C	48	0	0	1	0
3	D	80	0	0	1	0
All	All	15892	0	15117	157	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 5.

All (157) 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:D:227:ARG:NH1	1:D:232:THR:OG1	2.21	0.72
1:D:155:ASP:HB3	1:D:164:ARG:HH22	1.55	0.71
1:B:352:VAL:HG21	1:B:371:GLN:NE2	2.09	0.68
1:A:391:ALA:HB3	1:A:394:LYS:HB2	1.75	0.67
1:D:166:THR:H	2:D:601:GOL:H2	1.59	0.67
1:A:115:ASP:OD2	1:A:122:ARG:NH1	2.29	0.66
1:C:155:ASP:HB3	1:C:164:ARG:HH22	1.60	0.66
1:B:403:TYR:HB2	1:B:434:PHE:HB2	1.77	0.65
1:D:166:THR:HG22	1:D:176:ALA:HA	1.79	0.65
1:C:312:ILE:HG22	1:C:515:ARG:HH21	1.62	0.64
1:D:190:PRO:HB3	1:D:194:LYS:HE2	1.80	0.64
1:A:515:ARG:NH1	3:A:655:HOH:O	2.32	0.63
1:A:144:LEU:HD13	1:A:289:HIS:HD2	1.63	0.62
1:C:467:GLY:HA2	1:C:501:GLY:HA2	1.82	0.62
1:A:445:GLY:N	1:A:459:VAL:O	2.32	0.60
1:D:425:ASP:HB3	1:D:429:GLY:HA3	1.83	0.60
1:D:155:ASP:HB2	1:D:280:SER:HA	1.83	0.60
1:B:393:ASP:HB2	1:D:205:THR:HG22	1.84	0.59
1:B:400:ASN:ND2	1:B:437:ASP:OD1	2.31	0.59
1:D:95:GLU:HG2	1:D:117:TYR:HE2	1.67	0.59
1:B:77:ASN:ND2	3:B:690:HOH:O	2.36	0.58
1:A:403:TYR:HB2	1:A:434:PHE:HB2	1.86	0.57
1:C:403:TYR:HB2	1:C:434:PHE:HB2	1.86	0.57
1:B:331:MET:HE3	1:B:342:HIS:HB2	1.86	0.57
1:B:155:ASP:HB3	1:B:164:ARG:HH22	1.69	0.57
1:D:403:TYR:HB2	1:D:434:PHE:HB2	1.87	0.56
1:C:115:ASP:OD2	1:C:122:ARG:NH1	2.36	0.56
1:C:425:ASP:HB3	1:C:429:GLY:HA3	1.88	0.55
1:D:95:GLU:HG2	1:D:117:TYR:CE2	2.40	0.55
1:A:266:LYS:HB3	1:A:296:THR:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:PRO:HB3	1:C:194:LYS:HE2	1.88	0.55
1:D:498:VAL:HG22	1:D:514:PHE:HB3	1.90	0.54
1:A:333:LEU:HD22	1:A:355:ALA:HB2	1.89	0.54
1:C:445:GLY:N	1:C:459:VAL:O	2.39	0.54
1:A:71:ILE:HG21	1:A:130:LYS:HE2	1.89	0.53
1:B:147:GLN:NE2	1:B:198:GLN:OE1	2.41	0.53
1:B:177:ILE:HG23	1:B:183:LEU:HD13	1.91	0.53
1:D:122:ARG:NH1	3:D:707:HOH:O	2.35	0.53
1:A:468:PHE:CZ	1:A:500:GLY:HA3	2.44	0.52
1:C:273:LYS:HD3	1:C:282:PHE:HE1	1.75	0.52
1:B:330:LYS:H	1:B:330:LYS:HE2	1.74	0.52
1:A:467:GLY:HA2	1:A:501:GLY:HA2	1.91	0.52
1:D:467:GLY:HA2	1:D:501:GLY:HA2	1.92	0.51
1:B:312:ILE:HG22	1:B:515:ARG:HH21	1.74	0.51
1:B:337:GLU:HG3	1:B:338:PHE:H	1.76	0.51
1:C:275:VAL:HG22	1:C:282:PHE:HD1	1.76	0.51
1:A:144:LEU:HD13	1:A:289:HIS:CD2	2.46	0.51
1:B:467:GLY:HA2	1:B:501:GLY:HA2	1.92	0.51
1:D:152:PHE:CE2	1:D:185:SER:HB3	2.46	0.50
1:D:115:ASP:OD2	1:D:122:ARG:NH1	2.40	0.50
1:B:331:MET:HE1	1:B:353:ALA:HB3	1.94	0.50
1:B:416:ASN:OD1	1:B:416:ASN:N	2.45	0.50
1:B:352:VAL:HG21	1:B:371:GLN:CD	2.36	0.50
1:C:520:ASN:HA	1:C:522:SER:H	1.75	0.50
1:A:312:ILE:HG22	1:A:515:ARG:HH21	1.76	0.50
1:B:71:ILE:HG21	1:B:130:LYS:HE2	1.94	0.50
1:B:326:ILE:HG21	1:B:351:MET:HG2	1.93	0.50
1:B:180:ARG:NE	3:B:611:HOH:O	2.44	0.49
1:D:411:VAL:HG11	1:D:491:VAL:HG21	1.94	0.49
1:C:404:ILE:HG12	1:C:534:GLN:HG3	1.95	0.49
1:B:152:PHE:CE2	1:B:185:SER:HB3	2.48	0.49
1:A:155:ASP:HB2	1:A:280:SER:HA	1.95	0.49
1:C:520:ASN:HA	1:C:522:SER:N	2.29	0.48
1:C:391:ALA:HB3	1:C:394:LYS:HB2	1.95	0.48
1:D:404:ILE:HG12	1:D:534:GLN:HG3	1.96	0.48
1:D:71:ILE:HG21	1:D:130:LYS:HE2	1.96	0.47
1:D:275:VAL:HG22	1:D:282:PHE:HD1	1.79	0.47
1:C:428:ALA:HB1	1:C:451:ASN:HA	1.97	0.47
1:C:520:ASN:N	1:C:521:GLY:HA3	2.28	0.47
1:A:404:ILE:HG12	1:A:534:GLN:HG3	1.97	0.47
1:D:356:CYS:HA	1:D:357:CYS:HA	1.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ASP:O	1:D:249:ASN:ND2	2.48	0.47
1:D:360:LEU:O	1:D:364:LYS:NZ	2.47	0.47
1:D:424:ASP:OD1	1:D:424:ASP:N	2.44	0.47
1:B:425:ASP:HB3	1:B:429:GLY:HA3	1.97	0.46
1:B:136:LYS:HE3	1:B:302:ALA:HB3	1.96	0.46
1:C:122:ARG:NH1	3:C:607:HOH:O	2.34	0.46
1:D:83:GLU:H	1:D:83:GLU:CD	2.22	0.46
1:C:266:LYS:HB3	1:C:296:THR:HG21	1.97	0.46
1:A:356:CYS:HA	1:A:357:CYS:HA	1.74	0.46
1:B:115:ASP:OD2	1:B:122:ARG:NH1	2.38	0.46
1:B:445:GLY:N	1:B:459:VAL:O	2.47	0.46
1:B:447:LEU:HB2	1:B:457:PHE:HB2	1.97	0.46
1:D:155:ASP:O	1:D:164:ARG:NH1	2.48	0.46
1:D:266:LYS:HB3	1:D:296:THR:HG21	1.97	0.46
1:C:424:ASP:OD1	1:C:424:ASP:N	2.41	0.46
1:D:208:MET:HE1	1:D:231:PHE:CD2	2.51	0.46
1:C:395:MET:HE2	1:C:465:GLY:O	2.15	0.46
1:C:201:VAL:HG22	1:C:208:MET:HG3	1.98	0.45
1:A:273:LYS:HD2	1:A:282:PHE:HE1	1.82	0.45
1:A:275:VAL:HG22	1:A:282:PHE:HD1	1.81	0.45
1:B:42:LEU:HD12	1:B:257:SER:OG	2.16	0.45
1:C:416:ASN:OD1	1:C:416:ASN:N	2.50	0.45
1:C:449:ASP:HB2	1:C:456:VAL:HG11	1.97	0.45
1:B:155:ASP:HB2	1:B:280:SER:HA	1.99	0.45
1:B:337:GLU:HG3	1:B:338:PHE:N	2.32	0.45
1:A:487:ARG:HG2	1:A:488:HIS:H	1.81	0.45
1:B:369:TRP:HB2	1:B:378:VAL:HG13	1.98	0.45
1:B:299:ILE:HG13	1:B:300:ILE:HG13	2.00	0.44
1:B:457:PHE:HE1	1:B:493:PHE:HE2	1.64	0.44
1:D:273:LYS:HD2	1:D:282:PHE:HE1	1.82	0.44
1:D:266:LYS:HD3	1:D:296:THR:HG21	2.00	0.44
1:A:475:SER:C	1:A:477:ALA:H	2.26	0.44
1:B:158:LEU:HD21	1:B:180:ARG:HD3	1.99	0.44
1:A:134:PRO:HB2	1:A:229:ASN:ND2	2.32	0.44
1:C:177:ILE:HG23	1:C:183:LEU:HD13	1.98	0.44
1:A:73:ASP:OD1	1:A:130:LYS:NZ	2.51	0.43
1:B:275:VAL:HG22	1:B:282:PHE:HD1	1.84	0.43
1:A:76:LEU:HD22	1:A:109:ARG:HG2	2.00	0.43
1:A:235:ALA:HB3	1:A:255:SER:HB3	2.01	0.43
1:A:36:LYS:HE3	1:A:36:LYS:HB2	1.75	0.43
1:A:411:VAL:HG13	1:A:525:VAL:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASP:HB2	1:C:280:SER:HA	2.00	0.43
1:B:235:ALA:HB3	1:B:255:SER:HB3	2.00	0.43
1:C:230:ARG:HA	1:C:261:GLY:HA2	2.01	0.43
1:A:134:PRO:HB2	1:A:229:ASN:HD21	1.84	0.42
1:C:356:CYS:HA	1:C:357:CYS:HA	1.71	0.42
1:B:33:LYS:H	1:B:33:LYS:HG2	1.60	0.42
1:C:71:ILE:HG21	1:C:130:LYS:HE2	2.00	0.42
1:B:354:VAL:O	1:B:366:GLY:HA3	2.18	0.42
1:C:498:VAL:HG22	1:C:514:PHE:HB3	2.01	0.42
1:D:432:THR:HG22	1:D:447:LEU:HG	2.02	0.42
1:D:134:PRO:HG3	1:D:316:THR:HG23	2.02	0.42
1:B:174:THR:HG22	1:B:176:ALA:H	1.85	0.42
1:A:155:ASP:O	1:A:164:ARG:NH1	2.51	0.42
1:A:230:ARG:HA	1:A:261:GLY:HA2	2.02	0.42
1:A:170:ASP:O	1:A:192:LYS:HG3	2.20	0.42
1:A:519:ASP:N	1:A:519:ASP:OD1	2.53	0.42
1:C:474:THR:O	1:C:475:SER:HB2	2.20	0.42
1:D:349:LYS:N	1:D:370:GLN:HE21	2.18	0.42
1:B:343:THR:HG22	1:B:352:VAL:HG22	2.01	0.41
1:C:136:LYS:HE3	1:C:302:ALA:HB3	2.01	0.41
1:D:253:VAL:HG21	1:D:278:ASP:OD2	2.20	0.41
1:A:208:MET:HE1	1:A:231:PHE:CD2	2.55	0.41
1:A:299:ILE:HG13	1:A:300:ILE:HG13	2.02	0.41
1:A:520:ASN:HA	1:A:521:GLY:HA2	1.70	0.41
1:B:67:ASN:HA	1:B:68:PRO:HD3	1.85	0.41
1:B:395:MET:HE2	1:B:465:GLY:O	2.20	0.41
1:D:53:VAL:HA	1:D:54:PRO:HD3	1.93	0.41
1:C:212:LEU:HB2	1:C:220:TYR:HB2	2.02	0.41
1:A:414:GLU:HB3	1:A:415:ASN:H	1.55	0.41
1:D:189:LYS:HA	1:D:190:PRO:HD3	1.93	0.41
1:B:356:CYS:HA	1:B:357:CYS:HA	1.74	0.41
1:C:456:VAL:HG23	1:C:457:PHE:CD2	2.56	0.41
1:A:136:LYS:HE2	1:A:302:ALA:HB3	2.03	0.41
1:A:67:ASN:HA	1:A:68:PRO:HD3	1.89	0.41
1:A:416:ASN:HB2	3:A:673:HOH:O	2.21	0.41
1:B:441:LYS:HD3	1:B:441:LYS:HA	1.91	0.41
1:C:83:GLU:CD	1:C:83:GLU:H	2.28	0.41
1:D:456:VAL:HG23	1:D:457:PHE:CD2	2.56	0.41
1:A:293:ASN:HB3	1:C:397:LYS:HD3	2.03	0.40
1:C:402:LYS:NZ	1:C:435:ASP:OD1	2.42	0.40
1:D:67:ASN:HA	1:D:68:PRO:HD3	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:TYR:CD1	1:D:189:LYS:HE2	2.56	0.40
1:A:189:LYS:HA	1:A:190:PRO:HD3	1.86	0.40
1:B:161:GLU:OE1	1:B:161:GLU:N	2.47	0.40
1:C:199:PHE:HE1	1:C:222:VAL:HG21	1.86	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	497/532 (93%)	476 (96%)	20 (4%)	1 (0%)	43	58
1	B	492/532 (92%)	478 (97%)	14 (3%)	0	100	100
1	C	491/532 (92%)	471 (96%)	18 (4%)	2 (0%)	30	42
1	D	503/532 (94%)	487 (97%)	16 (3%)	0	100	100
All	All	1983/2128 (93%)	1912 (96%)	68 (3%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	C	517	GLN
1	C	475	SER

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	417/440 (95%)	404 (97%)	13 (3%)	35	55
1	B	413/440 (94%)	403 (98%)	10 (2%)	43	64
1	C	412/440 (94%)	401 (97%)	11 (3%)	39	60
1	D	421/440 (96%)	410 (97%)	11 (3%)	40	61
All	All	1663/1760 (94%)	1618 (97%)	45 (3%)	39	60

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	42	LEU
1	A	103	GLU
1	A	113	VAL
1	A	258	LEU
1	A	289	HIS
1	A	367	GLN
1	A	372	THR
1	A	416	ASN
1	A	482	ASP
1	A	516	TYR
1	A	519	ASP
1	A	520	ASN
1	B	35	VAL
1	B	42	LEU
1	B	113	VAL
1	B	273	LYS
1	B	304	LYS
1	B	330	LYS
1	B	346	ILE
1	B	351	MET
1	B	493	PHE
1	B	523	VAL
1	C	35	VAL
1	C	83	GLU
1	C	103	GLU
1	C	116	VAL
1	C	273	LYS
1	C	304	LYS
1	C	346	ILE
1	C	398	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	490	ASN
1	C	515	ARG
1	C	517	GLN
1	D	35	VAL
1	D	37	GLU
1	D	39	LEU
1	D	42	LEU
1	D	113	VAL
1	D	213	SER
1	D	304	LYS
1	D	346	ILE
1	D	372	THR
1	D	486	LEU
1	D	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	B	256	GLN
1	B	386	GLN
1	C	415	ASN
1	C	517	GLN
1	D	159	ASN
1	D	400	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	D	601	-	5,5,5	0.35	0	5,5,5	0.27	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	D	601	-	-	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	D	601	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GOL	1	0

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	505/532 (94%)	-0.59	2 (0%) 88 87	13, 30, 66, 91	0
1	B	500/532 (93%)	-0.67	2 (0%) 88 87	7, 22, 60, 106	0
1	C	499/532 (93%)	-0.41	3 (0%) 85 83	10, 39, 80, 103	0
1	D	507/532 (95%)	-0.54	4 (0%) 82 80	9, 29, 65, 97	2 (0%)
All	All	2011/2128 (94%)	-0.55	11 (0%) 87 85	7, 30, 68, 106	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346	ILE	3.3
1	A	372	THR	3.2
1	C	39	LEU	2.8
1	C	372	THR	2.5
1	D	372	THR	2.5
1	B	483	PRO	2.5
1	A	377	GLN	2.4
1	D	346	ILE	2.3
1	B	371	GLN	2.3
1	D	167[A]	TYR	2.2
1	D	356	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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(Å ²)	Q<0.9
2	GOL	D	601	6/6	0.88	0.08	37,41,45,48	0

6.5 Other polymers

There are no such residues in this entry.