



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 PM UTC

PDB ID : 4O3W / pdb_00004o3w
Title : Crystal structure of the vaccine antigen Transferrin Binding Protein B (TbpB) mutant Tyr-63-Ala from Actinobacillus suis H57
Authors : Calmettes, C.; Yu, R.H.; Schryvers, A.B.; Moraes, T.F.
Deposited on : 2013-12-18
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

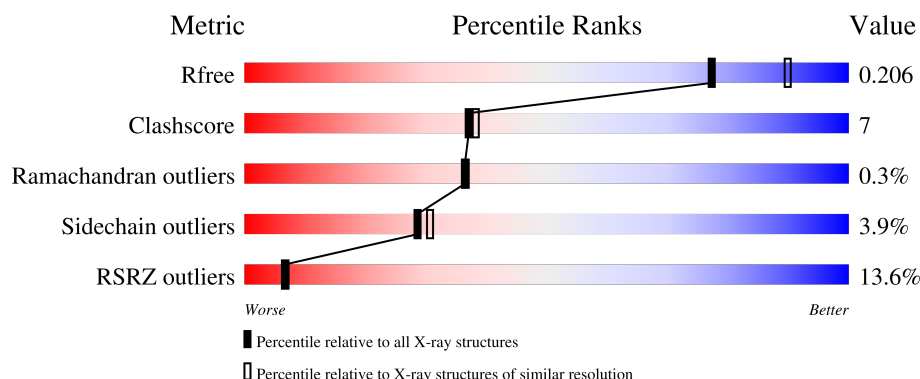
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	572	
1	B	572	

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	601	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9062 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	546	Total	C	N	O	S	0	2	0
			4259	2663	736	852	8			
1	B	535	Total	C	N	O	S	0	2	0
			4171	2610	720	833	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP Q83UA7
A	7	SER	-	expression tag	UNP Q83UA7
A	63	ALA	PHE	engineered mutation	UNP Q83UA7
B	6	GLY	-	expression tag	UNP Q83UA7
B	7	SER	-	expression tag	UNP Q83UA7
B	63	ALA	PHE	engineered mutation	UNP Q83UA7

- Molecule 2 is GLYCEROL (CCD ID: 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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

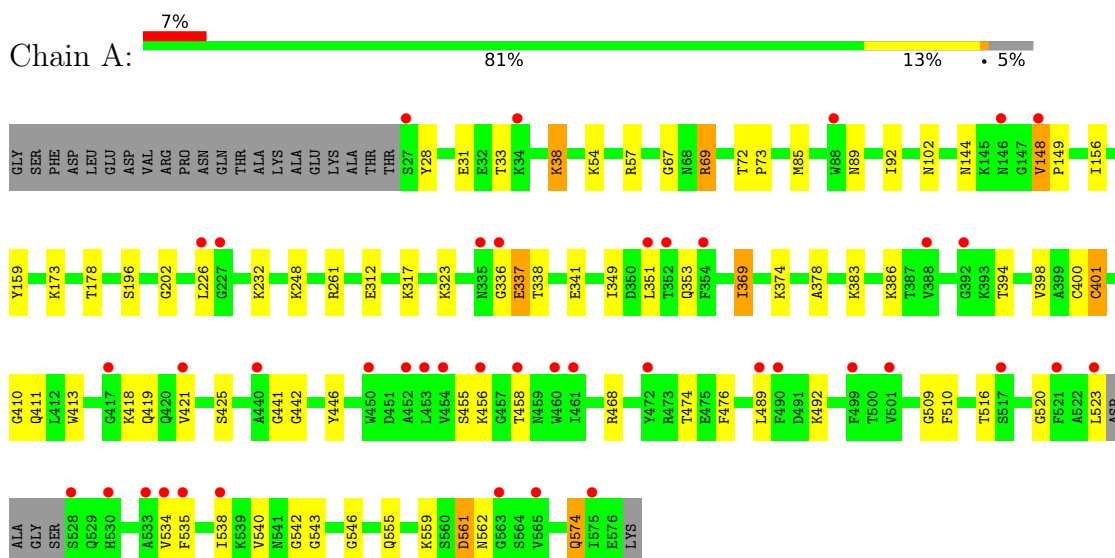
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	345	Total	O	0	0
			345	345		
4	B	264	Total	O	0	0
			264	264		

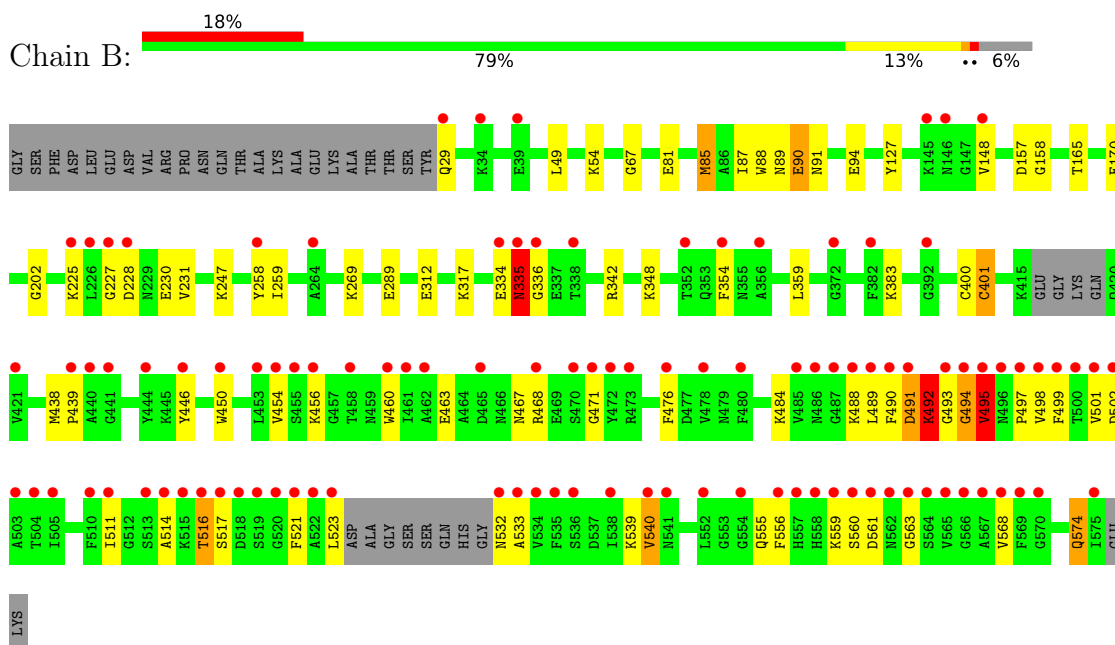
3 Residue-property plots [i](#)

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



• Molecule 1: Transferrin binding protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.81Å 74.51Å 106.60Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	46.28 – 2.10 46.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.4 (46.28-2.10) 91.4 (46.28-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.190 , 0.205 0.193 , 0.206	Depositor DCC
R_{free} test set	1851 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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, SO4

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	0.51	0/4342	0.79	2/5839 (0.0%)
1	B	0.48	0/4251	0.83	7/5718 (0.1%)
All	All	0.49	0/8593	0.81	9/11557 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	492	LYS	N-CA-C	8.72	123.28	111.24
1	B	494	GLY	CA-C-N	5.82	132.18	121.70
1	B	494	GLY	C-N-CA	5.82	132.18	121.70
1	B	336	GLY	N-CA-C	-5.51	105.20	112.81
1	B	335	ASN	CA-C-N	5.35	128.26	122.69
1	B	335	ASN	C-N-CA	5.35	128.26	122.69
1	B	491	ASP	N-CA-C	5.32	117.81	107.71
1	A	546	GLY	CA-C-N	5.08	125.11	119.32
1	A	546	GLY	C-N-CA	5.08	125.11	119.32

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	4259	0	4134	50	0
1	B	4171	0	4053	70	0
2	A	12	0	16	2	0
2	B	6	0	8	7	0
3	B	5	0	0	1	0
4	A	345	0	0	13	0
4	B	264	0	0	5	0
All	All	9062	0	8211	119	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 7.

All (119) 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:81:GLU:HG2	4:B:925:HOH:O	1.59	1.03
1:B:494:GLY:HA2	1:B:495:VAL:HG22	1.49	0.94
1:B:89:ASN:HB2	2:B:601:GOL:H31	1.53	0.88
1:B:54:LYS:HZ3	1:B:158:GLY:H	1.20	0.85
1:B:88:TRP:H	2:B:601:GOL:H2	1.45	0.82
1:B:81:GLU:CG	4:B:925:HOH:O	2.22	0.82
1:B:87:ILE:HB	2:B:601:GOL:H32	1.60	0.82
1:A:54:LYS:HG2	4:A:888:HOH:O	1.81	0.80
1:A:28:TYR:HB3	1:A:574:GLN:HG2	1.70	0.74
1:B:225:LYS:HZ2	1:B:228:ASP:HA	1.55	0.72
1:B:67:GLY:HA2	1:B:148:VAL:HG11	1.78	0.66
1:B:334:GLU:O	1:B:334:GLU:HG2	1.95	0.66
1:B:490:PHE:CG	1:B:491:ASP:N	2.64	0.66
1:B:334:GLU:O	1:B:335:ASN:ND2	2.29	0.65
1:B:335:ASN:HD22	1:B:335:ASN:C	2.05	0.65
1:B:490:PHE:CD1	1:B:491:ASP:N	2.65	0.64
1:B:148:VAL:HA	4:B:955:HOH:O	1.97	0.64
1:B:54:LYS:NZ	1:B:158:GLY:H	1.97	0.61
1:A:57:ARG:NE	4:A:964:HOH:O	2.22	0.61
1:B:484:LYS:NZ	1:B:502:ASP:OD1	2.33	0.61
1:A:57:ARG:HB2	4:A:964:HOH:O	2.00	0.61
1:A:69:ARG:HG3	1:A:69:ARG:HH21	1.65	0.61
1:A:323:LYS:NZ	4:A:1031:HOH:O	2.33	0.60
1:A:349:ILE:HD11	1:A:555:GLN:HG3	1.83	0.59
1:B:471:GLY:HA2	1:B:492:LYS:HG2	1.84	0.59
1:A:232:LYS:NZ	4:A:962:HOH:O	2.36	0.58
1:A:57:ARG:CD	4:A:964:HOH:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HE2	1:B:157:ASP:OD2	2.05	0.57
1:B:89:ASN:CB	2:B:601:GOL:H31	2.31	0.57
1:B:446:TYR:HB2	1:B:476:PHE:HB2	1.87	0.57
1:A:69:ARG:HH21	1:A:69:ARG:CG	2.17	0.56
1:B:258:TYR:HD1	3:B:602:SO4:O4	1.89	0.56
1:B:460:TRP:HZ2	1:B:491:ASP:HB2	1.70	0.56
1:B:354:PHE:HB2	1:B:559:LYS:HB2	1.89	0.55
1:A:89:ASN:HA	2:A:602:GOL:H31	1.89	0.54
1:A:54:LYS:HE2	4:A:888:HOH:O	2.07	0.54
1:A:561:ASP:OD1	1:A:561:ASP:N	2.39	0.54
1:A:178:THR:OG1	1:B:334:GLU:OE1	2.21	0.53
1:A:351:LEU:HG	1:A:425:SER:HA	1.91	0.53
1:A:72:THR:HG22	1:A:73:PRO:O	2.09	0.53
1:B:383:LYS:NZ	1:B:463:GLU:HG2	2.25	0.52
1:A:369:ILE:HD13	1:A:374[A]:LYS:HG2	1.91	0.52
1:A:57:ARG:HD3	4:A:964:HOH:O	2.10	0.51
1:B:54:LYS:HD2	1:B:158:GLY:O	2.09	0.51
1:A:337:GLU:HG2	1:A:338:THR:HG23	1.93	0.51
1:A:336:GLY:HA2	1:A:338:THR:N	2.26	0.51
1:A:144:ASN:OD1	1:A:148:VAL:HG13	2.11	0.51
1:B:460:TRP:CZ2	1:B:491:ASP:HB2	2.45	0.51
1:B:560:SER:OG	1:B:561:ASP:N	2.44	0.51
1:B:467:ASN:HB3	1:B:471:GLY:HA3	1.94	0.50
1:B:511:ILE:HD11	1:B:539:LYS:HE2	1.94	0.50
1:B:468:ARG:HH12	1:B:574:GLN:HE22	1.59	0.50
1:B:89:ASN:H	2:B:601:GOL:H31	1.77	0.49
1:A:474:THR:HG22	1:A:489:LEU:HG	1.95	0.49
1:B:231:VAL:HG22	1:B:259:ILE:HD13	1.94	0.49
1:A:89:ASN:N	2:A:601:GOL:O2	2.46	0.49
1:B:490:PHE:HZ	1:B:493:GLY:H	1.59	0.49
1:A:456:LYS:O	1:A:562:ASN:ND2	2.46	0.49
1:B:460:TRP:HZ2	1:B:491:ASP:CG	2.21	0.48
1:B:454:VAL:HB	1:B:460:TRP:HB3	1.96	0.48
1:B:490:PHE:HZ	1:B:493:GLY:N	2.11	0.48
1:B:225:LYS:HD2	1:B:230:GLU:HG2	1.96	0.47
1:A:378:ALA:O	1:A:386:LYS:NZ	2.39	0.47
1:B:91:ASN:ND2	1:B:94:GLU:HB2	2.31	0.46
1:B:501:VAL:HG12	1:B:514:ALA:HB2	1.98	0.46
1:A:31:GLU:HG3	1:A:33:THR:HG23	1.98	0.46
1:B:247:LYS:NZ	4:B:875:HOH:O	2.47	0.46
1:A:561:ASP:HA	1:A:562:ASN:HA	1.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HB2	1:B:523:LEU:HD21	1.97	0.46
1:A:173:LYS:HD3	1:A:341:GLU:HB2	1.97	0.45
1:B:87:ILE:HG22	2:B:601:GOL:H11	1.97	0.45
1:B:516:THR:HG22	1:B:517:SER:H	1.81	0.45
1:A:148:VAL:HA	4:A:1029:HOH:O	2.17	0.45
1:B:227:GLY:HA3	4:B:962:HOH:O	2.17	0.45
1:A:418:LYS:HA	1:A:419:GLN:HA	1.59	0.45
1:B:335:ASN:ND2	1:B:335:ASN:C	2.73	0.45
1:B:488:LYS:HB3	1:B:497:PRO:HB3	1.98	0.45
1:A:413:TRP:CD1	1:A:421:VAL:HG13	2.52	0.45
1:B:29:GLN:O	1:B:574:GLN:HG3	2.17	0.45
1:A:492:LYS:HB2	1:A:492:LYS:HE3	1.67	0.45
1:A:57:ARG:HD2	1:A:156:ILE:O	2.17	0.44
1:A:67:GLY:HA2	1:A:148:VAL:HG21	1.98	0.44
1:B:85:MET:HE2	1:B:85:MET:HB2	1.87	0.44
1:B:540:VAL:HB	1:B:556:PHE:HB3	1.99	0.44
1:B:269:LYS:HD2	1:B:289:GLU:HG3	2.00	0.44
1:A:226:LEU:O	1:A:261:ARG:HA	2.18	0.44
1:B:456:LYS:HG2	1:B:563:GLY:HA2	1.99	0.44
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.81	0.43
1:A:510:PHE:CZ	1:A:542:GLY:HA3	2.53	0.43
1:B:498:VAL:HG23	1:B:499:PHE:HD1	1.83	0.43
1:A:535:PHE:CD1	1:A:538:ILE:HD11	2.53	0.43
1:A:400:CYS:HA	1:A:401:CYS:HA	1.84	0.43
1:B:456:LYS:NZ	1:B:533:ALA:HA	2.33	0.43
1:A:102:ASN:ND2	4:A:875:HOH:O	2.36	0.43
1:B:90:GLU:H	1:B:90:GLU:HG2	1.54	0.43
1:A:383:LYS:NZ	4:A:1023:HOH:O	2.51	0.42
1:A:441:GLY:HA2	1:A:442:GLY:HA2	1.82	0.42
1:B:460:TRP:HZ2	1:B:491:ASP:CB	2.30	0.42
1:A:38:LYS:HB2	1:A:38:LYS:HE2	1.84	0.42
1:B:348:LYS:HB2	1:B:359:LEU:HD21	2.01	0.42
1:B:521:PHE:O	1:B:532:ASN:HB2	2.20	0.42
1:A:148:VAL:HA	1:A:149:PRO:HD3	1.89	0.41
1:B:127:TYR:O	1:B:165:THR:HG22	2.19	0.41
1:B:438:MET:HA	1:B:439:PRO:HD3	1.87	0.41
1:B:450:TRP:CE3	1:B:489:LEU:HD23	2.55	0.41
1:B:488:LYS:HG2	1:B:497:PRO:HG3	2.02	0.41
1:B:400:CYS:HA	1:B:401:CYS:HA	1.87	0.41
1:B:456:LYS:HB2	1:B:523:LEU:HD11	2.02	0.41
1:A:446:TYR:HB2	1:A:476:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:VAL:O	1:A:410:GLY:HA3	2.21	0.41
1:B:490:PHE:CZ	1:B:492:LYS:N	2.89	0.41
1:A:248:LYS:HE2	4:A:980:HOH:O	2.20	0.41
1:A:57:ARG:NH2	4:A:805:HOH:O	2.50	0.40
1:B:170:GLU:HG2	1:B:342:ARG:HG3	2.03	0.40
1:A:509:GLY:HA2	1:A:543:GLY:HA2	2.03	0.40
1:A:54:LYS:HG3	1:A:159:TYR:CE1	2.57	0.40
1:A:520:GLY:HA3	1:A:534:VAL:HG22	2.04	0.40
1:B:450:TRP:HB2	1:B:568:VAL:O	2.21	0.40
1:B:89:ASN:H	2:B:601:GOL:C3	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	544/572 (95%)	521 (96%)	22 (4%)	1 (0%)	43	44
1	B	531/572 (93%)	502 (94%)	27 (5%)	2 (0%)	30	28
All	All	1075/1144 (94%)	1023 (95%)	49 (5%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	VAL
1	A	202	GLY
1	B	202	GLY

5.3.2 Protein sidechains ⓘ

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	453/471 (96%)	430 (95%)	23 (5%)	21	21
1	B	444/471 (94%)	432 (97%)	12 (3%)	39	45
All	All	897/942 (95%)	862 (96%)	35 (4%)	28	31

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

Mol	Chain	Res	Type
1	A	38	LYS
1	A	69	ARG
1	A	85	MET
1	A	92	ILE
1	A	148	VAL
1	A	196	SER
1	A	312	GLU
1	A	317	LYS
1	A	337	GLU
1	A	353	GLN
1	A	369	ILE
1	A	394	THR
1	A	401	CYS
1	A	411	GLN
1	A	455	SER
1	A	458	THR
1	A	468	ARG
1	A	516	THR
1	A	523	LEU
1	A	540	VAL
1	A	559	LYS
1	A	561	ASP
1	A	574	GLN
1	B	85	MET
1	B	90	GLU
1	B	312	GLU
1	B	317	LYS

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Mol	Chain	Res	Type
1	B	335	ASN
1	B	401	CYS
1	B	492	LYS
1	B	495	VAL
1	B	516	THR
1	B	540	VAL
1	B	555	GLN
1	B	574	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	220	HIS
1	A	246	ASN
1	A	381	ASN
1	A	414	GLN
1	A	529	GLN
1	B	29	GLN
1	B	102	ASN
1	B	229	ASN
1	B	335	ASN
1	B	391	ASN
1	B	414	GLN
1	B	443	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

4 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	A	602	-	5,5,5	0.33	0	5,5,5	0.32	0
2	GOL	A	601	-	5,5,5	0.49	0	5,5,5	0.23	0
3	SO4	B	602	-	4,4,4	0.32	0	6,6,6	0.24	0
2	GOL	B	601	-	5,5,5	0.45	0	5,5,5	0.91	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	A	602	-	-	2/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	GOL	1	0
2	A	601	GOL	1	0
3	B	602	SO4	1	0
2	B	601	GOL	7	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, 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	546/572 (95%)	0.30	42 (7%)	19 21	13, 38, 81, 125	2 (0%)
1	B	535/572 (93%)	0.79	105 (19%)	3 3	18, 46, 109, 134	2 (0%)
All	All	1081/1144 (94%)	0.54	147 (13%)	7 7	13, 42, 94, 134	4 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	LEU	6.4
1	B	490	PHE	6.4
1	B	501	VAL	5.6
1	B	533	ALA	5.4
1	B	535	PHE	4.8
1	B	523	LEU	4.7
1	A	440	ALA	4.6
1	B	499	PHE	4.6
1	B	565	VAL	4.5
1	B	495	VAL	4.3
1	B	485	VAL	4.2
1	B	575	ILE	4.1
1	B	534	VAL	4.1
1	B	487	GLY	4.1
1	A	458	THR	4.0
1	B	498	VAL	3.9
1	B	521	PHE	3.9
1	B	564	SER	3.9
1	A	489	LEU	3.9
1	B	453	LEU	3.9
1	B	540	VAL	3.8
1	B	454	VAL	3.7
1	B	522	ALA	3.7
1	B	566	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	516	THR	3.6
1	B	462	ALA	3.6
1	B	421	VAL	3.6
1	A	563	GLY	3.6
1	A	460	TRP	3.5
1	B	505	ILE	3.5
1	B	560	SER	3.5
1	B	476	PHE	3.4
1	B	461	ILE	3.4
1	B	538	ILE	3.4
1	B	450	TRP	3.4
1	B	510	PHE	3.4
1	B	440	ALA	3.4
1	A	521	PHE	3.4
1	A	453	LEU	3.3
1	B	458	THR	3.2
1	B	500	THR	3.2
1	B	563	GLY	3.2
1	B	145	LYS	3.2
1	B	556	PHE	3.2
1	B	441	GLY	3.1
1	B	561	ASP	3.1
1	B	354	PHE	3.1
1	A	454	VAL	3.1
1	B	478	VAL	3.1
1	B	489	LEU	3.1
1	B	511	ILE	3.1
1	B	558	HIS	3.1
1	A	499	PHE	3.0
1	B	480	PHE	3.0
1	B	470	SER	3.0
1	B	336	GLY	2.9
1	B	567	ALA	2.9
1	B	569	PHE	2.9
1	B	519	SER	2.9
1	A	227	GLY	2.8
1	B	520	GLY	2.8
1	A	148	VAL	2.8
1	A	27	SER	2.8
1	B	472	TYR	2.8
1	B	497	PRO	2.8
1	B	494	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	452	ALA	2.7
1	A	352	THR	2.7
1	B	554	GLY	2.7
1	B	338	THR	2.7
1	A	421	VAL	2.7
1	A	461	ILE	2.7
1	A	528	SER	2.7
1	B	514	ALA	2.7
1	B	504	THR	2.7
1	B	455	SER	2.7
1	B	460	TRP	2.7
1	A	335	ASN	2.6
1	B	226	LEU	2.6
1	B	562	ASN	2.6
1	B	517	SER	2.6
1	B	225	LYS	2.6
1	B	471	GLY	2.6
1	A	535	PHE	2.6
1	B	465	ASP	2.6
1	B	502	ASP	2.6
1	B	334	GLU	2.6
1	B	552	LEU	2.6
1	B	570	GLY	2.5
1	B	496	ASN	2.5
1	B	491	ASP	2.5
1	A	533	ALA	2.5
1	B	356	ALA	2.5
1	A	226	LEU	2.5
1	A	354	PHE	2.5
1	B	493	GLY	2.5
1	A	530	HIS	2.5
1	B	503	ALA	2.5
1	B	148	VAL	2.5
1	A	517	SER	2.5
1	B	352	THR	2.5
1	A	456	LYS	2.5
1	B	34	LYS	2.4
1	B	227	GLY	2.4
1	B	382	PHE	2.4
1	B	456	LYS	2.4
1	B	446	TYR	2.3
1	B	264	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	486	ASN	2.3
1	B	513	SER	2.3
1	A	538	ILE	2.3
1	A	146	ASN	2.3
1	A	351	LEU	2.3
1	B	488	LYS	2.3
1	A	501	VAL	2.2
1	B	146	ASN	2.2
1	B	335	ASN	2.2
1	B	541	ASN	2.2
1	B	372	GLY	2.2
1	B	258	TYR	2.2
1	A	490	PHE	2.2
1	B	473	ARG	2.2
1	A	388	VAL	2.2
1	B	532	ASN	2.2
1	B	439	PRO	2.1
1	B	518	ASP	2.2
1	B	568	VAL	2.1
1	B	536	SER	2.1
1	A	34	LYS	2.1
1	B	559	LYS	2.1
1	B	228	ASP	2.1
1	A	392	GLY	2.1
1	B	392	GLY	2.1
1	A	472	TYR	2.1
1	B	444	TYR	2.1
1	B	29	GLN	2.1
1	A	88	TRP	2.1
1	B	557	HIS	2.1
1	A	417	GLY	2.1
1	B	515	LYS	2.1
1	A	534	VAL	2.1
1	A	565	VAL	2.1
1	A	450	TRP	2.1
1	B	39	GLU	2.0
1	B	468	ARG	2.0
1	A	575	ILE	2.0
1	A	336	GLY	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 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
3	SO4	B	602	5/5	0.60	0.13	94,96,129,180	0
2	GOL	B	601	6/6	0.79	0.14	45,46,59,60	0
2	GOL	A	602	6/6	0.79	0.13	57,60,63,76	0
2	GOL	A	601	6/6	0.87	0.15	38,47,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.