



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:06 AM UTC

PDB ID : 4TVS / pdb_00004tvs
Title : LAP1(aa356-583), H.sapiens, bound to VHH-BS1
Authors : Sosa, B.A.; Schwartz, T.U.
Deposited on : 2014-06-27
Resolution : 1.60 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

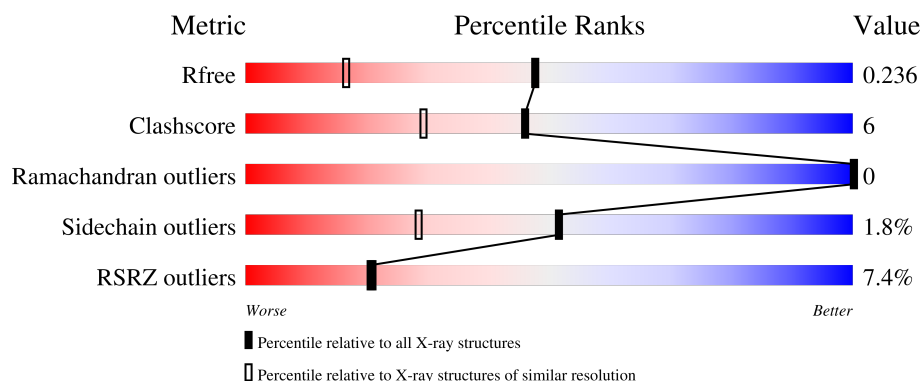
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

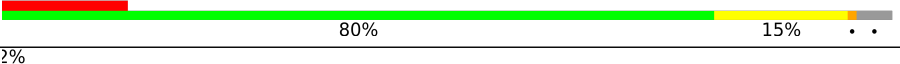
The reported resolution of this entry is 1.60 Å.

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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	231	
1	B	231	
2	a	134	
2	b	134	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6162 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 Torsin-1A-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1793	1125	314	349	5			
1	B	222	Total	C	N	O	S	0	0	0
			1769	1107	312	345	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	GLY	-	expression tag	UNP Q5JTV8
A	354	PRO	-	expression tag	UNP Q5JTV8
A	355	GLY	-	expression tag	UNP Q5JTV8
B	353	GLY	-	expression tag	UNP Q5JTV8
B	354	PRO	-	expression tag	UNP Q5JTV8
B	355	GLY	-	expression tag	UNP Q5JTV8

- Molecule 2 is a protein called VHH Domain BS-1.

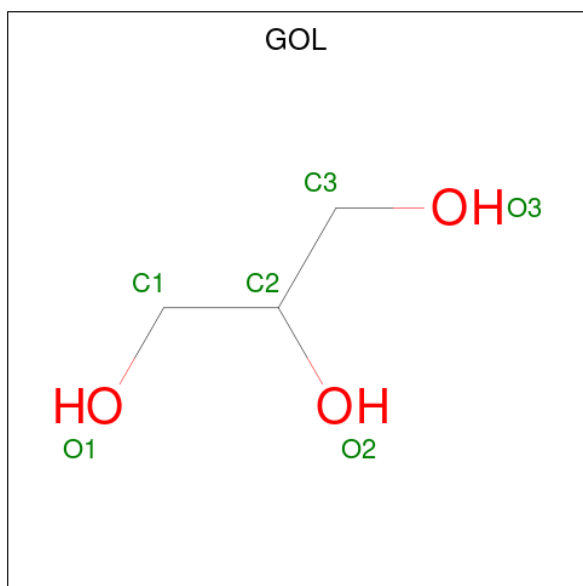
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	128	Total	C	N	O	S	0	1	0
			983	613	173	193	4			
2	b	128	Total	C	N	O	S	0	0	0
			975	608	170	193	4			

- 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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	C	O	0	0
			6	3	3		
4	a	1	Total	C	O	0	0
			6	3	3		
4	b	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	b	1	Total	C	O	0	0
			6	3	3		

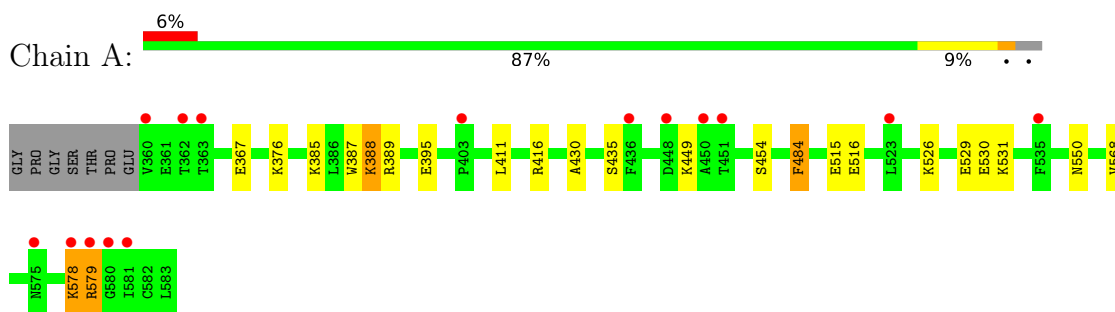
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	0
			216	216		
5	B	137	Total	O	0	0
			137	137		
5	a	139	Total	O	0	0
			139	139		
5	b	121	Total	O	0	0
			121	121		

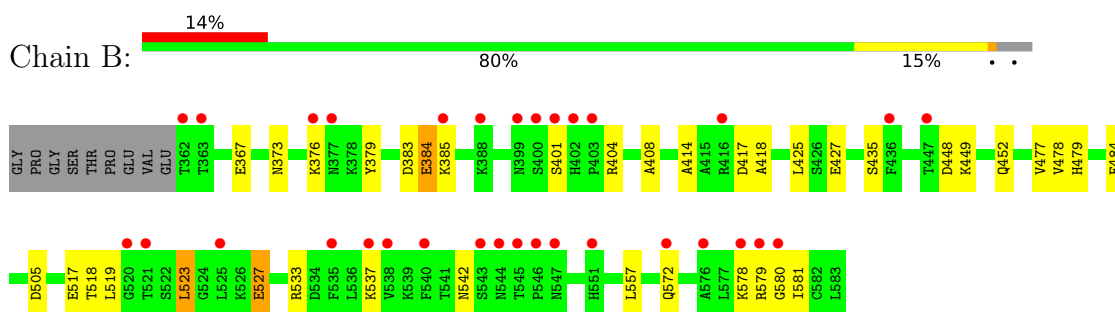
3 Residue-property plots [i](#)

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.

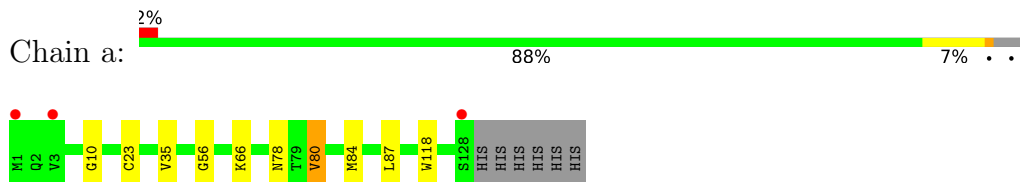
• Molecule 1: Torsin-1A-interacting protein 1



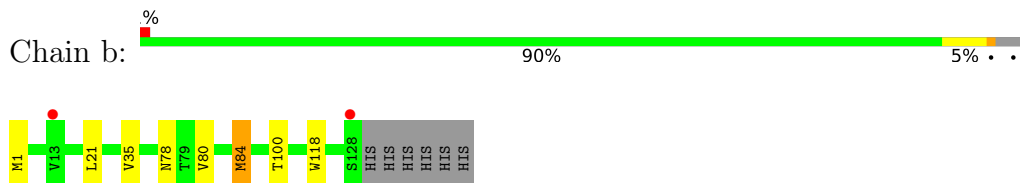
• Molecule 1: Torsin-1A-interacting protein 1



• Molecule 2: VHH Domain BS-1



• Molecule 2: VHH Domain BS-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.79Å 74.02Å 85.42Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	66.07 – 1.60 66.07 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (66.07-1.60) 86.7 (66.07-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.181 , 0.229 0.191 , 0.236	Depositor DCC
R_{free} test set	2814 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	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	0.97	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 42.17 % 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 2.1199e-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, 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	1.10	3/1828 (0.2%)	1.04	0/2469
1	B	0.94	2/1800 (0.1%)	1.02	4/2431 (0.2%)
2	a	1.21	0/1008	1.04	1/1366 (0.1%)
2	b	1.15	1/997 (0.1%)	1.03	0/1352
All	All	1.08	6/5633 (0.1%)	1.03	5/7618 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	VAL	CA-CB	7.30	1.61	1.53
1	A	579	ARG	CB-CG	-5.71	1.35	1.52
1	A	430	ALA	CA-CB	5.52	1.62	1.53
1	A	484	PHE	N-CA	5.36	1.52	1.45
2	b	84	MET	SD-CE	-5.35	1.66	1.79
1	B	408	ALA	CA-CB	-5.32	1.46	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	SER	CA-C-N	5.55	131.42	121.76
1	B	401	SER	C-N-CA	5.55	131.42	121.76
1	B	572	GLN	CA-C-N	-5.36	114.73	120.03
1	B	572	GLN	C-N-CA	-5.36	114.73	120.03
2	a	56	GLY	N-CA-C	-5.33	108.28	115.21

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	1793	0	1770	22	0
1	B	1769	0	1746	30	0
2	a	983	0	941	6	0
2	b	975	0	928	5	0
3	B	5	0	0	1	0
4	a	12	0	15	1	0
4	b	12	0	16	1	0
5	A	216	0	0	11	0
5	B	137	0	0	0	0
5	a	139	0	0	1	0
5	b	121	0	0	0	0
All	All	6162	0	5416	63	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 6.

All (63) 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:427:GLU:HG2	1:B:477:VAL:HG11	1.44	0.99
1:B:579:ARG:HG2	1:B:581:ILE:HG12	1.53	0.87
2:b:21:LEU:HG	2:b:84:MET:HE2	1.62	0.79
1:B:579:ARG:HG3	1:B:580:GLY:N	1.99	0.76
1:A:516:GLU:OE1	1:A:531:LYS:NZ	2.17	0.75
1:B:579:ARG:HG3	1:B:580:GLY:H	1.51	0.75
1:B:523:LEU:HD22	1:B:527:GLU:OE2	1.90	0.72
1:A:526:LYS:O	5:A:815:HOH:O	2.10	0.69
1:B:427:GLU:HG3	1:B:479:HIS:CE1	2.31	0.66
1:A:385:LYS:HB3	1:A:389:ARG:HE	1.61	0.65
1:A:416:ARG:NH1	5:A:697:HOH:O	2.32	0.63
2:a:84:MET:HE2	2:a:87:LEU:HD21	1.79	0.63
1:A:395:GLU:OE1	5:A:774:HOH:O	2.16	0.62
1:B:384:GLU:N	1:B:384:GLU:OE1	2.30	0.62
1:A:579:ARG:NH2	5:A:601:HOH:O	2.28	0.61
1:B:384:GLU:H	1:B:384:GLU:CD	2.08	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:NH1	5:A:601:HOH:O	2.26	0.59
1:B:533:ARG:HG2	1:B:537:LYS:HE3	1.84	0.59
1:A:416:ARG:HE	1:A:515:GLU:HA	1.67	0.58
1:A:416:ARG:HH11	1:A:515:GLU:HG2	1.67	0.58
1:A:530:GLU:HG3	5:A:815:HOH:O	2.02	0.58
1:A:550:ASN:HB2	5:A:728:HOH:O	2.03	0.58
1:A:376:LYS:HG2	1:A:387:TRP:CD2	2.40	0.56
1:B:427:GLU:HG3	1:B:479:HIS:NE2	2.21	0.55
1:B:383:ASP:OD1	1:B:384:GLU:N	2.41	0.53
1:B:373:ASN:CG	1:B:376:LYS:HZ2	2.18	0.52
1:A:385:LYS:HB3	1:A:389:ARG:NE	2.26	0.50
2:b:35:VAL:HG11	2:b:80:VAL:HG21	1.93	0.50
1:B:367:GLU:HG3	1:B:435:SER:OG	2.13	0.49
1:B:373:ASN:O	1:B:376:LYS:HG3	2.13	0.49
1:B:373:ASN:CB	1:B:376:LYS:HZ2	2.26	0.49
1:A:526:LYS:HE3	5:A:815:HOH:O	2.13	0.48
1:B:449:LYS:HG3	1:B:484:PHE:CE1	2.48	0.48
1:B:373:ASN:CA	1:B:376:LYS:HZ2	2.28	0.47
1:B:537:LYS:HA	1:B:557:LEU:HD21	1.96	0.46
2:b:118:TRP:CG	4:b:202:GOL:H32	2.50	0.46
1:B:373:ASN:CG	1:B:376:LYS:NZ	2.74	0.46
2:a:35:VAL:HG11	2:a:80:VAL:HG11	1.98	0.46
2:a:10:GLY:N	5:a:397:HOH:O	2.47	0.46
1:A:367:GLU:HG3	1:A:435:SER:OG	2.16	0.46
1:A:411:LEU:HD22	1:A:568:VAL:HG13	1.98	0.45
1:A:529:GLU:HB3	5:A:815:HOH:O	2.17	0.44
1:B:578:LYS:HD2	1:B:579:ARG:N	2.33	0.44
1:B:448:ASP:O	1:B:452:GLN:NE2	2.51	0.44
1:A:449:LYS:HG3	1:A:484:PHE:CE1	2.52	0.44
1:A:454:SER:HB2	5:A:618:HOH:O	2.17	0.44
1:A:578:LYS:NZ	5:A:605:HOH:O	2.51	0.43
1:A:385:LYS:HA	1:A:385:LYS:HD2	1.83	0.43
2:b:1:MET:HE3	2:b:1:MET:HB2	1.86	0.43
1:B:414:ALA:HB1	1:B:418:ALA:HB3	2.01	0.42
1:B:542:ASN:ND2	3:B:601:SO4:O4	2.52	0.42
1:B:417:ASP:OD2	1:B:518:THR:HB	2.20	0.42
1:B:404:ARG:HD2	1:B:505:ASP:HA	2.02	0.42
1:B:533:ARG:O	1:B:537:LYS:HG3	2.21	0.41
1:A:388:LYS:HB2	1:A:388:LYS:HE3	1.30	0.41
1:B:519:LEU:HA	1:B:519:LEU:HD23	1.84	0.41
2:a:35:VAL:HG11	2:a:80:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:118:TRP:CE3	4:a:202:GOL:H12	2.55	0.41
1:B:385:LYS:HA	1:B:385:LYS:HE3	2.02	0.41
2:a:23:CYS:HB3	2:a:80:VAL:HG13	2.02	0.41
1:B:579:ARG:CG	1:B:580:GLY:N	2.76	0.40
2:b:21:LEU:CG	2:b:84:MET:HE2	2.42	0.40
1:B:379:TYR:CD1	1:B:425:LEU:HD11	2.56	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	223/231 (96%)	219 (98%)	4 (2%)	0	100	100
1	B	220/231 (95%)	214 (97%)	6 (3%)	0	100	100
2	a	127/134 (95%)	126 (99%)	1 (1%)	0	100	100
2	b	126/134 (94%)	125 (99%)	1 (1%)	0	100	100
All	All	696/730 (95%)	684 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	199/203 (98%)	197 (99%)	2 (1%)	68	50
1	B	196/203 (97%)	192 (98%)	4 (2%)	48	24
2	a	103/108 (95%)	100 (97%)	3 (3%)	37	14
2	b	102/108 (94%)	100 (98%)	2 (2%)	48	24
All	All	600/622 (96%)	589 (98%)	11 (2%)	51	28

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	LYS
1	A	578	LYS
1	B	384	GLU
1	B	517	GLU
1	B	523	LEU
1	B	527	GLU
2	a	66	LYS
2	a	78	ASN
2	a	80	VAL
2	b	78	ASN
2	b	100	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	A	370	ASN
1	A	467	ASN
1	A	473	GLN
1	A	572	GLN
1	A	575	ASN
1	B	373	ASN
1	B	391	GLN
1	B	452	GLN
1	B	473	GLN
1	B	550	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
4	GOL	b	202	-	5,5,5	0.62	0	5,5,5	0.79	0
4	GOL	b	201	-	5,5,5	0.29	0	5,5,5	1.56	2 (40%)
3	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.35	0
4	GOL	a	201	-	5,5,5	0.71	0	5,5,5	2.26	2 (40%)
4	GOL	a	202	-	5,5,5	0.41	0	5,5,5	1.11	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
4	GOL	b	201	-	-	2/4/4/4	-
4	GOL	a	201	-	-	2/4/4/4	-
4	GOL	a	202	-	-	1/4/4/4	-
4	GOL	b	202	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	201	GOL	O2-C2-C1	4.05	125.93	109.18
4	b	201	GOL	O2-C2-C3	-2.29	99.70	109.18
4	b	201	GOL	C3-C2-C1	-2.18	103.82	111.80
4	a	201	GOL	C3-C2-C1	2.04	119.29	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	a	201	GOL	O1-C1-C2-C3
4	b	201	GOL	O1-C1-C2-C3
4	a	202	GOL	O1-C1-C2-C3
4	b	202	GOL	O1-C1-C2-C3
4	b	201	GOL	O1-C1-C2-O2
4	a	201	GOL	O2-C2-C3-O3
4	b	202	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	b	202	GOL	1	0
3	B	601	SO4	1	0
4	a	202	GOL	1	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	224/231 (96%)	0.66	15 (6%) 24 24	23, 34, 56, 80	1 (0%)
1	B	222/231 (96%)	1.05	32 (14%) 6 5	27, 44, 78, 106	0
2	a	128/134 (95%)	0.32	3 (2%) 61 64	18, 30, 48, 85	1 (0%)
2	b	128/134 (95%)	0.37	2 (1%) 70 74	23, 33, 50, 79	0
All	All	702/730 (96%)	0.67	52 (7%) 20 21	18, 35, 67, 106	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	THR	6.0
1	B	546	PRO	5.1
1	A	579	ARG	5.1
1	B	545	THR	4.8
1	B	403	PRO	4.2
1	A	360	VAL	4.2
2	a	1	MET	4.0
1	B	580	GLY	3.8
1	A	436[A]	PHE	3.7
1	B	540	PHE	3.5
1	B	543	SER	3.3
1	A	581	ILE	3.2
1	B	402	HIS	3.2
1	B	538	VAL	3.2
1	B	578	LYS	3.1
1	B	579	ARG	2.9
1	B	399	ASN	2.9
1	B	363	THR	2.8
1	B	521	THR	2.8
1	A	578	LYS	2.8
1	A	450	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	525	LEU	2.7
1	A	580	GLY	2.7
1	B	551	HIS	2.6
2	a	128	SER	2.5
1	B	544	ASN	2.5
1	A	575	ASN	2.5
2	b	13	VAL	2.5
1	B	401	SER	2.5
1	A	451	THR	2.4
1	B	388	LYS	2.3
1	A	403	PRO	2.3
1	B	436	PHE	2.3
1	A	448	ASP	2.3
1	B	520	GLY	2.3
2	a	3	VAL	2.3
1	B	385	LYS	2.2
1	A	363	THR	2.2
1	B	377	ASN	2.2
1	A	523	LEU	2.2
1	B	537	LYS	2.2
1	B	400	SER	2.2
1	A	362	THR	2.2
1	B	547	ASN	2.1
1	B	572	GLN	2.1
1	B	447	THR	2.1
1	B	576	ALA	2.1
1	A	535	PHE	2.1
2	b	128	SER	2.0
1	B	376	LYS	2.0
1	B	416	ARG	2.0
1	B	535	PHE	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	601	5/5	0.75	0.16	72,77,82,86	0
4	GOL	b	202	6/6	0.75	0.16	47,51,59,59	0
4	GOL	a	201	6/6	0.81	0.16	35,39,40,49	0
4	GOL	b	201	6/6	0.83	0.15	35,48,56,65	0
4	GOL	a	202	6/6	0.84	0.15	49,59,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.