



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:15 AM UTC

PDB ID : 2PEE / pdb_00002pee
Title : Crystal Structure of a Thermophilic Serpin, Tengpin, in the Native State
Authors : Zhang, Q.W.; Buckle, A.M.; Whisstock, J.C.
Deposited on : 2007-04-02
Resolution : 2.70 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

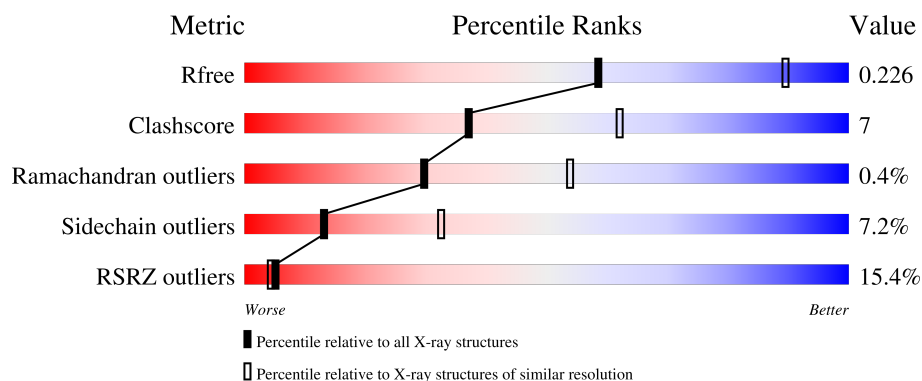
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	387	13% 83% 15% .
1	B	387	18% 80% 16% .

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
3	GOL	A	425	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5950 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.

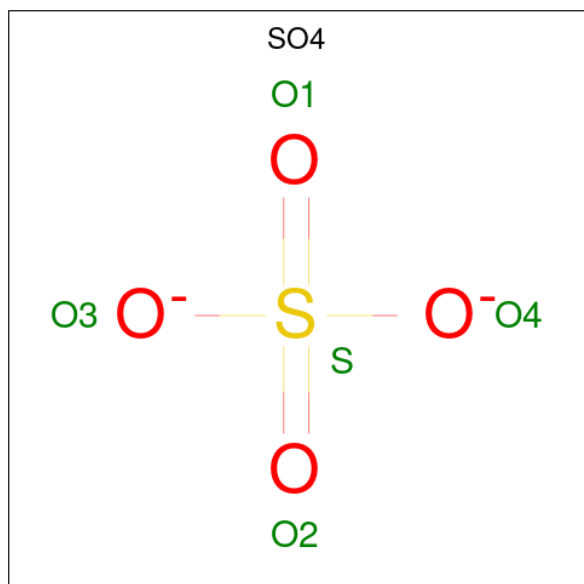
- Molecule 1 is a protein called Serine protease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3007	1938	469	589	11			
1	B	387	Total	C	N	O	S	0	0	0
			2888	1859	448	572	9			

There are 2 discrepancies between the modelled and reference sequences:

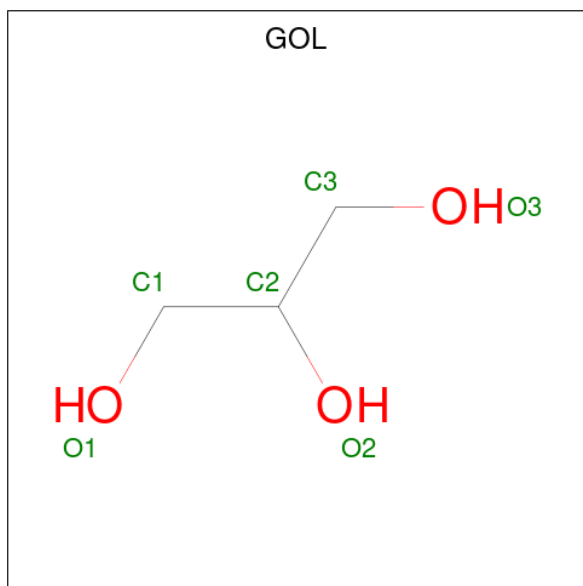
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ILE	VAL	engineered mutation	UNP Q8R9P5
B	261	ILE	VAL	engineered mutation	UNP Q8R9P5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

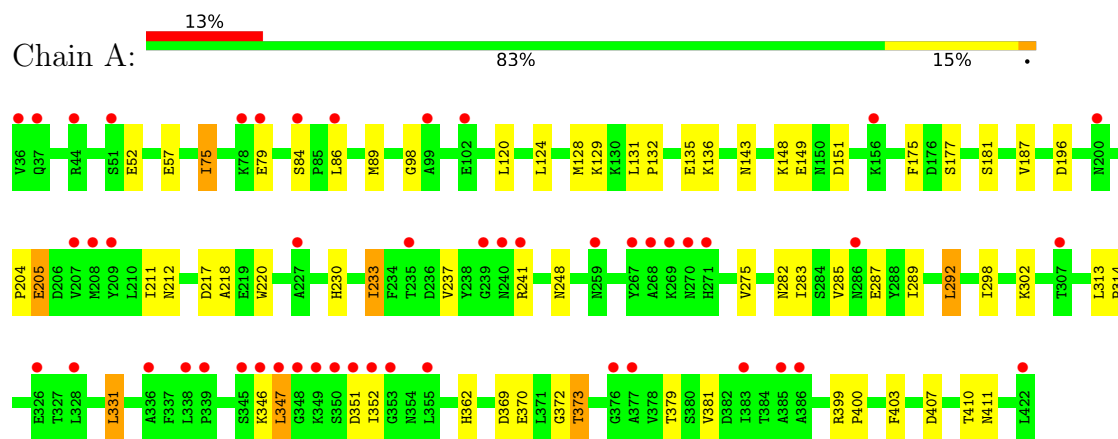
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	13	Total	O	0	0
			13	13		

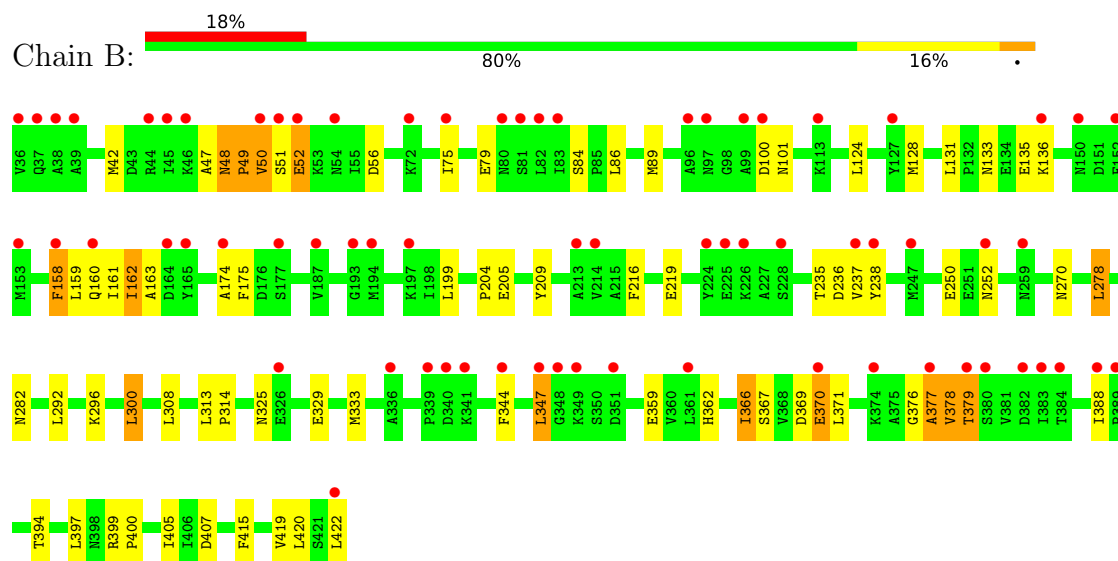
3 Residue-property plots [i](#)

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: Serine protease inhibitor



- Molecule 1: Serine protease inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	217.94Å 217.94Å 217.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.00 – 2.70 154.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (154.00-2.70) 97.8 (154.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	7.70	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.235 0.193 , 0.226	Depositor DCC
R_{free} test set	2321 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 82.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5950	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.68	0/3065	0.91	3/4159 (0.1%)
1	B	0.69	2/2945 (0.1%)	0.92	4/4021 (0.1%)
All	All	0.68	2/6010 (0.0%)	0.91	7/8180 (0.1%)

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	LEU	C-O	9.12	1.34	1.24
1	B	158	PHE	C-O	7.05	1.32	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ILE	N-CA-C	5.99	116.24	107.37
1	B	162	ILE	N-CA-C	5.75	117.17	110.62
1	B	388	ILE	CA-C-N	5.45	125.43	120.03
1	B	388	ILE	C-N-CA	5.45	125.43	120.03
1	A	79	GLU	N-CA-C	5.27	117.19	109.24
1	B	56	ASP	N-CA-C	5.16	114.96	108.45
1	A	149	GLU	N-CA-C	5.07	117.21	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	377	ALA	Peptide
1	B	50	VAL	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	3007	0	2922	33	0
1	B	2888	0	2634	49	0
2	A	5	0	0	0	0
3	A	12	0	16	1	0
4	A	25	0	0	0	0
4	B	13	0	0	0	0
All	All	5950	0	5572	81	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 (81) 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:A:86:LEU:HD21	1:A:128:MET:HE1	1.53	0.89
1:A:204:PRO:O	1:A:205:GLU:HB2	1.72	0.89
1:B:86:LEU:HD21	1:B:128:MET:HE1	1.57	0.85
1:B:51:SER:O	1:B:52:GLU:C	2.29	0.75
1:B:47:ALA:C	1:B:48:ASN:OD1	2.30	0.75
1:B:250:GLU:HG2	1:B:308:LEU:HD11	1.73	0.70
1:B:371:LEU:CD1	1:B:376:GLY:HA3	2.24	0.68
1:A:84:SER:H	1:A:362:HIS:HE1	1.41	0.67
1:A:52:GLU:OE2	1:A:129:LYS:HE2	1.94	0.67
1:B:399:ARG:HB2	1:B:400:PRO:HD2	1.77	0.66
1:A:220:TRP:NE1	1:A:372:GLY:HA2	2.12	0.64
1:B:369:ASP:OD1	1:B:370:GLU:HG2	2.00	0.62
1:B:371:LEU:HG	1:B:376:GLY:HA3	1.81	0.62
1:B:84:SER:H	1:B:362:HIS:CE1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:HD11	1:B:376:GLY:HA3	1.83	0.60
1:B:399:ARG:HB2	1:B:400:PRO:CD	2.32	0.59
1:B:378:VAL:CG2	1:B:379:THR:N	2.64	0.59
1:B:329:GLU:HA	1:B:333:MET:O	2.03	0.59
1:B:42:MET:CE	1:B:163:ALA:HB2	2.32	0.58
1:B:377:ALA:O	1:B:378:VAL:HG12	2.03	0.57
1:B:136:LYS:HE3	1:B:219:GLU:CD	2.29	0.57
1:A:220:TRP:CD1	1:A:372:GLY:HA2	2.39	0.57
1:B:366:ILE:HD11	1:B:405:ILE:HD11	1.87	0.56
1:B:344:PHE:HB3	1:B:347:LEU:HD22	1.87	0.56
1:A:98:GLY:HA3	1:A:347:LEU:HB2	1.87	0.56
1:B:371:LEU:CG	1:B:376:GLY:HA3	2.35	0.56
1:A:84:SER:H	1:A:362:HIS:CE1	2.24	0.55
1:B:216:PHE:HB2	1:B:415:PHE:HE1	1.72	0.55
1:B:160:GLN:O	1:B:161:ILE:C	2.48	0.55
1:B:84:SER:H	1:B:362:HIS:HE1	1.54	0.55
1:B:136:LYS:HE3	1:B:219:GLU:OE2	2.07	0.54
1:B:282:ASN:H	1:B:282:ASN:HD22	1.56	0.54
1:B:209:TYR:CE2	1:B:359:GLU:HB2	2.44	0.53
1:A:135:GLU:O	1:A:136:LYS:HB2	2.08	0.53
1:A:217:ASP:HA	1:A:373:THR:HG21	1.89	0.53
1:A:399:ARG:HB2	1:A:400:PRO:CD	2.39	0.52
1:A:233:ILE:HG21	1:A:241:ARG:HB3	1.93	0.51
1:B:209:TYR:HE2	1:B:359:GLU:HB2	1.75	0.50
1:B:48:ASN:O	1:B:49:PRO:O	2.30	0.50
1:B:400:PRO:HA	1:B:419:VAL:O	2.12	0.49
1:B:158:PHE:O	1:B:162:ILE:HG12	2.12	0.49
1:B:89:MET:HE3	1:B:124:LEU:HD21	1.95	0.48
1:A:89:MET:CE	1:A:124:LEU:HD21	2.43	0.48
1:B:377:ALA:C	1:B:378:VAL:HG12	2.37	0.48
1:B:174:ALA:O	1:B:175:PHE:HB2	2.14	0.48
1:A:151:ASP:OD1	1:A:351:ASP:N	2.44	0.47
1:A:230:HIS:HD2	1:A:248:ASN:HD22	1.62	0.47
1:B:366:ILE:HG12	1:B:367:SER:N	2.30	0.46
1:A:212:ASN:OD1	1:A:362:HIS:HD2	1.98	0.46
1:B:296:LYS:O	1:B:300:LEU:HB2	2.15	0.46
1:B:236:ASP:HB2	1:B:420:LEU:O	2.16	0.46
1:A:75:ILE:H	1:A:75:ILE:HG13	1.64	0.46
1:A:220:TRP:CE2	1:A:372:GLY:HA2	2.51	0.45
1:B:366:ILE:HG12	1:B:367:SER:H	1.81	0.45
1:A:148:LYS:HG3	1:A:175:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:OD1	1:B:48:ASN:N	2.45	0.45
1:A:205:GLU:HG3	1:B:238:TYR:CG	2.52	0.45
1:A:313:LEU:HD12	1:A:314:PRO:HD2	1.99	0.44
1:A:283:ILE:HG13	1:A:287:GLU:CD	2.42	0.44
1:B:370:GLU:HG2	1:B:370:GLU:H	1.61	0.44
1:B:42:MET:HE1	1:B:163:ALA:HB2	1.99	0.44
1:A:218:ALA:O	1:A:373:THR:HB	2.17	0.44
1:B:325:ASN:HD21	1:B:359:GLU:HA	1.82	0.44
1:A:143:ASN:H	3:A:424:GOL:HO2	1.61	0.43
1:B:100:ASP:OD1	1:B:101:ASN:N	2.49	0.43
1:A:298:ILE:HG22	1:A:302:LYS:HE2	2.00	0.43
1:B:278:LEU:HG	1:B:397:LEU:HD23	2.00	0.43
1:B:378:VAL:HG23	1:B:379:THR:N	2.33	0.43
1:A:151:ASP:OD2	1:A:352:ILE:N	2.51	0.43
1:A:275:VAL:O	1:A:403:PHE:HA	2.19	0.43
1:B:128:MET:HE2	1:B:128:MET:HA	2.01	0.42
1:B:51:SER:O	1:B:52:GLU:O	2.38	0.42
1:A:289:ILE:O	1:A:292:LEU:HB2	2.19	0.42
1:A:233:ILE:CG2	1:A:241:ARG:HB3	2.50	0.41
1:B:325:ASN:OD1	1:B:325:ASN:N	2.53	0.41
1:B:313:LEU:HD12	1:B:314:PRO:HD2	2.03	0.41
1:B:204:PRO:O	1:B:205:GLU:CB	2.68	0.41
1:A:211:ILE:C	1:A:212:ASN:HD22	2.29	0.41
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.93	0.40
1:A:331:LEU:HD12	1:A:331:LEU:HA	1.92	0.40
1:A:410:THR:O	1:A:411:ASN:HB2	2.21	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	385/387 (100%)	362 (94%)	23 (6%)	0	100	100
1	B	385/387 (100%)	358 (93%)	24 (6%)	3 (1%)	16	37
All	All	770/774 (100%)	720 (94%)	47 (6%)	3 (0%)	30	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	VAL
1	B	52	GLU
1	B	49	PRO

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	320/342 (94%)	299 (93%)	21 (7%)	15	36
1	B	280/342 (82%)	258 (92%)	22 (8%)	11	28
All	All	600/684 (88%)	557 (93%)	43 (7%)	13	32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	75	ILE
1	A	120	LEU
1	A	177	SER
1	A	181	SER
1	A	187	VAL
1	A	196	ASP
1	A	205	GLU
1	A	237	VAL
1	A	282	ASN
1	A	285	VAL
1	A	292	LEU
1	A	331	LEU

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Mol	Chain	Res	Type
1	A	346	LYS
1	A	347	LEU
1	A	369	ASP
1	A	370	GLU
1	A	373	THR
1	A	379	THR
1	A	381	VAL
1	A	407	ASP
1	B	48	ASN
1	B	75	ILE
1	B	79	GLU
1	B	131	LEU
1	B	133	ASN
1	B	135	GLU
1	B	199	LEU
1	B	235	THR
1	B	237	VAL
1	B	252	ASN
1	B	270	ASN
1	B	278	LEU
1	B	292	LEU
1	B	300	LEU
1	B	347	LEU
1	B	366	ILE
1	B	370	GLU
1	B	378	VAL
1	B	379	THR
1	B	394	THR
1	B	407	ASP
1	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	230	HIS
1	A	282	ASN
1	A	286	ASN
1	A	303	ASN
1	A	362	HIS
1	B	133	ASN
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	212	ASN
1	B	240	ASN
1	B	252	ASN
1	B	282	ASN
1	B	286	ASN
1	B	303	ASN
1	B	362	HIS
1	B	391	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	A	423	-	4,4,4	0.30	0	6,6,6	0.32	0
3	GOL	A	424	-	5,5,5	0.48	0	5,5,5	0.61	0
3	GOL	A	425	-	5,5,5	0.49	0	5,5,5	5.14	3 (60%)

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
3	GOL	A	424	-	-	2/4/4/4	-
3	GOL	A	425	-	-	3/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	425	GOL	O2-C2-C1	-7.17	79.50	109.18
3	A	425	GOL	O2-C2-C3	-6.83	80.89	109.18
3	A	425	GOL	C3-C2-C1	5.78	132.99	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	425	GOL	C1-C2-C3-O3
3	A	425	GOL	O1-C1-C2-O2
3	A	425	GOL	O2-C2-C3-O3
3	A	424	GOL	O1-C1-C2-C3
3	A	424	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
3	A	424	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	387/387 (100%)	0.88	49 (12%) 8 7	40, 60, 74, 85	0
1	B	387/387 (100%)	1.21	70 (18%) 3 3	40, 60, 77, 90	0
All	All	774/774 (100%)	1.04	119 (15%) 5 4	40, 60, 76, 90	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	ASN	6.3
1	B	36	VAL	6.1
1	B	351	ASP	6.0
1	B	382	ASP	5.4
1	B	340	ASP	4.2
1	A	259	ASN	4.2
1	A	351	ASP	4.1
1	A	383	ILE	4.1
1	B	380	SER	4.1
1	A	346	LYS	4.0
1	B	388	ILE	4.0
1	B	225	GLU	3.9
1	B	164	ASP	3.9
1	B	384	THR	3.8
1	B	150	ASN	3.8
1	B	158	PHE	3.8
1	B	136	LYS	3.7
1	B	81	SER	3.6
1	B	349	LYS	3.6
1	B	224	TYR	3.6
1	B	37	GLN	3.5
1	B	377	ALA	3.4
1	A	269	LYS	3.4
1	B	113	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	3.4
1	B	347	LEU	3.3
1	B	348	GLY	3.3
1	A	36	VAL	3.3
1	A	352	ILE	3.2
1	B	44	ARG	3.2
1	B	160	GLN	3.2
1	B	97	ASN	3.1
1	B	174	ALA	3.1
1	B	165	TYR	3.1
1	B	214	VAL	3.1
1	A	386	ALA	3.1
1	B	226	LYS	3.1
1	B	361	LEU	3.0
1	A	326	GLU	3.0
1	B	326	GLU	3.0
1	B	194	MET	3.0
1	B	177	SER	3.0
1	B	389	PRO	3.0
1	B	100	ASP	2.9
1	B	339	PRO	2.9
1	A	339	PRO	2.8
1	B	72	LYS	2.8
1	A	336	ALA	2.8
1	B	379	THR	2.8
1	B	228	SER	2.8
1	B	51	SER	2.8
1	B	238	TYR	2.8
1	B	45	ILE	2.8
1	A	239	GLY	2.8
1	B	82	LEU	2.8
1	A	376	GLY	2.7
1	A	99	ALA	2.7
1	A	353	GLY	2.7
1	B	259	ASN	2.7
1	A	37	GLN	2.7
1	B	193	GLY	2.7
1	A	328	LEU	2.6
1	A	385	ALA	2.6
1	B	54	ASN	2.6
1	B	344	PHE	2.6
1	A	377	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	52	GLU	2.5
1	B	237	VAL	2.5
1	B	383	ILE	2.5
1	A	209	TYR	2.5
1	A	207	VAL	2.5
1	B	39	ALA	2.5
1	B	213	ALA	2.5
1	B	247	MET	2.5
1	B	197	LYS	2.5
1	B	96	ALA	2.5
1	A	156	LYS	2.4
1	B	152	PHE	2.4
1	B	46	LYS	2.4
1	B	50	VAL	2.4
1	A	348	GLY	2.4
1	B	422	LEU	2.3
1	B	341	LYS	2.3
1	A	347	LEU	2.3
1	A	307	THR	2.3
1	B	374	LYS	2.3
1	A	267	TYR	2.3
1	A	268	ALA	2.3
1	B	153	MET	2.3
1	A	200	ASN	2.3
1	A	240	ASN	2.3
1	B	187	VAL	2.3
1	A	355	LEU	2.2
1	A	349	LYS	2.2
1	B	83	ILE	2.2
1	A	345	SER	2.2
1	A	227	ALA	2.2
1	B	99	ALA	2.2
1	A	235	THR	2.2
1	A	102	GLU	2.2
1	B	127	TYR	2.2
1	A	271	HIS	2.2
1	A	286	ASN	2.1
1	A	79	GLU	2.1
1	B	75	ILE	2.1
1	A	338	LEU	2.1
1	B	252	ASN	2.1
1	A	51	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	SER	2.1
1	A	241	ARG	2.1
1	A	86	LEU	2.1
1	B	336	ALA	2.0
1	B	370	GLU	2.0
1	A	350	SER	2.0
1	A	78	LYS	2.0
1	B	38	ALA	2.0
1	A	208	MET	2.0
1	A	422	LEU	2.0
1	A	270	ASN	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	GOL	A	425	6/6	0.83	0.25	97,105,106,108	0
3	GOL	A	424	6/6	0.85	0.24	97,105,108,109	0
2	SO4	A	423	5/5	0.91	0.18	96,97,98,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.