



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 AM UTC

PDB ID : 1VQU / pdb_00001vqu
Title : Crystal structure of Anthranilate phosphoribosyltransferase 2 (17130499)
from Nostoc sp. at 1.85 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-01-05
Resolution : 1.85 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

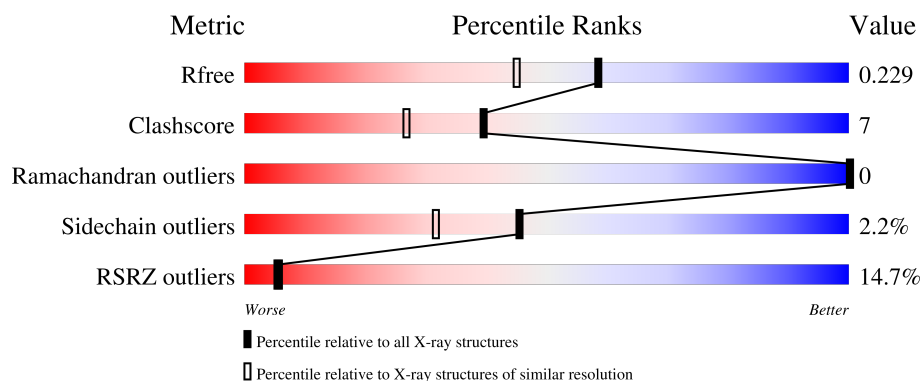
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	374	6% 79% 10% 11%
1	B	374	20% 73% 14% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5067 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 Anthranilate phosphoribosyltransferase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	Se	0	3	0
			2452	1554	421	473	1	3			
1	B	330	Total	C	N	O	S	Se	0	1	0
			2369	1504	410	451	1	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	cloning artifact	UNP Q8YXQ9
A	-10	GLY	-	cloning artifact	UNP Q8YXQ9
A	-9	SER	-	cloning artifact	UNP Q8YXQ9
A	-8	ASP	-	cloning artifact	UNP Q8YXQ9
A	-7	LYS	-	cloning artifact	UNP Q8YXQ9
A	-6	ILE	-	cloning artifact	UNP Q8YXQ9
A	-5	HIS	-	cloning artifact	UNP Q8YXQ9
A	-4	HIS	-	cloning artifact	UNP Q8YXQ9
A	-3	HIS	-	cloning artifact	UNP Q8YXQ9
A	-2	HIS	-	cloning artifact	UNP Q8YXQ9
A	-1	HIS	-	cloning artifact	UNP Q8YXQ9
A	0	HIS	-	cloning artifact	UNP Q8YXQ9
A	1	MSE	MET	modified residue	UNP Q8YXQ9
A	37	MSE	MET	modified residue	UNP Q8YXQ9
A	70	MSE	MET	modified residue	UNP Q8YXQ9
A	80	MSE	MET	modified residue	UNP Q8YXQ9
B	-11	MSE	-	cloning artifact	UNP Q8YXQ9
B	-10	GLY	-	cloning artifact	UNP Q8YXQ9
B	-9	SER	-	cloning artifact	UNP Q8YXQ9
B	-8	ASP	-	cloning artifact	UNP Q8YXQ9
B	-7	LYS	-	cloning artifact	UNP Q8YXQ9
B	-6	ILE	-	cloning artifact	UNP Q8YXQ9
B	-5	HIS	-	cloning artifact	UNP Q8YXQ9
B	-4	HIS	-	cloning artifact	UNP Q8YXQ9
B	-3	HIS	-	cloning artifact	UNP Q8YXQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	cloning artifact	UNP Q8YXQ9
B	-1	HIS	-	cloning artifact	UNP Q8YXQ9
B	0	HIS	-	cloning artifact	UNP Q8YXQ9
B	1	MSE	MET	modified residue	UNP Q8YXQ9
B	37	MSE	MET	modified residue	UNP Q8YXQ9
B	70	MSE	MET	modified residue	UNP Q8YXQ9
B	80	MSE	MET	modified residue	UNP Q8YXQ9

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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



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

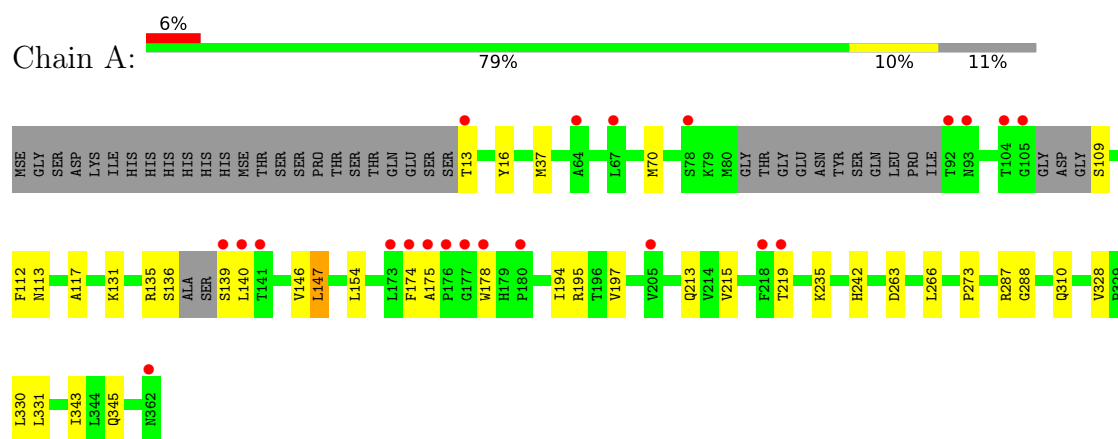
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	1
			153	153		
4	B	77	Total	O	0	2
			79	79		

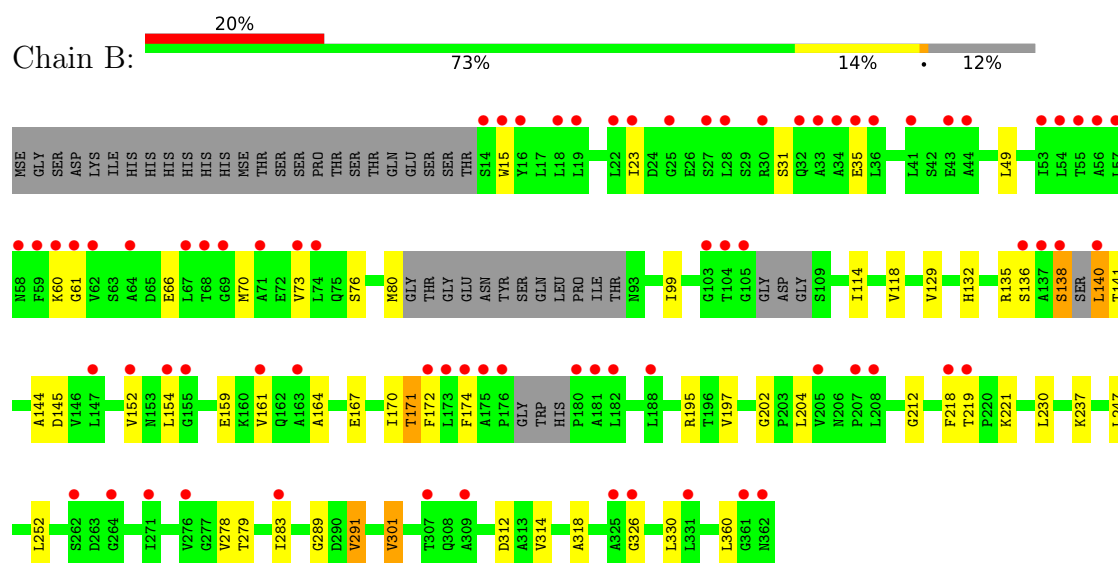
3 Residue-property plots [i](#)

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: Anthranilate phosphoribosyltransferase 2



- Molecule 1: Anthranilate phosphoribosyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.56Å 47.23Å 99.38Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	99.05 – 1.85 99.05 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (99.05-1.85) 97.8 (99.05-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.179 , 0.221 0.187 , 0.229	Depositor DCC
R_{free} test set	2636 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5067	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: ACT, 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	1.13	5/2491 (0.2%)	1.08	2/3384 (0.1%)
1	B	0.93	4/2397 (0.2%)	0.99	2/3257 (0.1%)
All	All	1.03	9/4888 (0.2%)	1.04	4/6641 (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	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	MSE	SE-CE	-9.93	1.65	1.95
1	B	31	SER	C-O	9.42	1.36	1.24
1	A	117	ALA	CA-CB	6.97	1.64	1.53
1	B	35	GLU	C-O	6.43	1.31	1.24
1	A	343	ILE	CA-C	-5.77	1.45	1.52
1	B	114	ILE	CA-CB	5.65	1.61	1.54
1	B	301	VAL	CA-CB	5.54	1.60	1.54
1	A	310	GLN	C-O	5.49	1.30	1.24
1	A	215	VAL	C-O	-5.06	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	VAL	N-CA-C	-5.88	104.37	109.19
1	A	147	LEU	N-CA-C	-5.57	105.21	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	GLY	CA-C-N	5.40	125.22	119.28
1	B	202	GLY	C-N-CA	5.40	125.22	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	THR	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	2452	0	2498	21	1
1	B	2369	0	2404	46	1
2	A	8	0	6	0	0
3	B	6	0	8	0	0
4	A	153	0	0	6	0
4	B	79	0	0	4	0
All	All	5067	0	4916	65	1

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 (65) 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:161:VAL:O	1:B:171[A]:THR:HG21	1.58	1.03
1:A:70:MSE:HE1	1:A:197:VAL:HG21	1.45	0.96
1:B:360:LEU:HB2	4:B:395[B]:HOH:O	1.67	0.94
1:B:247:LEU:HD21	1:B:283:ILE:HD11	1.50	0.90
1:A:136:SER:HG	1:A:139:SER:N	1.71	0.88
1:B:164:ALA:HB3	1:B:171[A]:THR:HG23	1.62	0.79
1:B:164:ALA:HB3	1:B:171[A]:THR:CG2	2.18	0.73
1:B:138:SER:OG	1:B:140:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:SER:HB2	1:B:140:LEU:HD11	1.75	0.68
1:B:167:GLU:HG3	4:B:387:HOH:O	1.95	0.64
1:B:140:LEU:CD1	1:B:140:LEU:N	2.61	0.64
1:B:247:LEU:HD21	1:B:283:ILE:CD1	2.26	0.63
1:B:219:THR:HG22	1:B:221:LYS:H	1.66	0.60
1:B:144:ALA:HB2	1:B:174:PHE:CE1	2.38	0.59
1:A:136:SER:OG	1:A:139:SER:N	2.35	0.57
1:B:278:VAL:HG13	1:B:312:ASP:HB3	1.88	0.56
1:A:195:ARG:HD3	4:A:428:HOH:O	2.05	0.55
1:B:60:LYS:NZ	1:B:66:GLU:OE1	2.38	0.55
1:B:60:LYS:HE2	1:B:61:GLY:O	2.06	0.55
1:B:140:LEU:O	1:B:291:VAL:HG22	2.07	0.55
1:A:263:ASP:HB2	4:A:486:HOH:O	2.07	0.53
1:B:159:GLU:N	4:B:419:HOH:O	2.41	0.52
1:B:161:VAL:HG13	1:B:171[B]:THR:CG2	2.38	0.52
1:B:15:TRP:HB2	1:B:49:LEU:HD13	1.91	0.52
1:A:194:ILE:HD13	1:B:23:ILE:CD1	2.40	0.52
1:B:70:MSE:HE1	1:B:197:VAL:HG21	1.91	0.52
1:A:113:ASN:HD21	1:A:146:VAL:HG21	1.74	0.51
1:B:252:LEU:HD22	1:B:278:VAL:HG11	1.92	0.51
1:B:140:LEU:N	1:B:140:LEU:HD13	2.26	0.50
1:B:60:LYS:NZ	1:B:66:GLU:OE2	2.45	0.49
1:B:118:VAL:HG13	1:B:318:ALA:HA	1.94	0.49
1:B:161:VAL:O	1:B:171[B]:THR:HG21	2.11	0.49
1:A:135:ARG:HB2	1:A:174:PHE:HB3	1.93	0.49
1:B:326:GLY:HA2	4:B:428:HOH:O	2.13	0.48
1:A:112:PHE:O	4:A:370:HOH:O	2.20	0.48
1:B:172:PHE:HB3	1:B:174:PHE:CE2	2.48	0.48
1:A:109:SER:HB3	4:A:490:HOH:O	2.15	0.47
1:A:242:HIS:HD2	4:A:397:HOH:O	1.96	0.47
1:B:152:VAL:HG12	1:B:154:LEU:HD23	1.96	0.47
1:A:213:GLN:OE1	1:A:235:LYS:HE3	2.15	0.46
1:B:161:VAL:HG13	1:B:171[B]:THR:HG21	1.97	0.46
1:B:60:LYS:NZ	1:B:66:GLU:CD	2.74	0.46
1:B:99:ILE:HA	1:B:212:GLY:O	2.16	0.46
1:B:301:VAL:HG11	1:B:314:VAL:HG21	1.99	0.45
1:A:154:LEU:HD13	1:A:174:PHE:CD2	2.52	0.45
1:B:73:VAL:O	1:B:76:SER:OG	2.29	0.45
1:B:141:THR:HG21	1:B:289:GLY:O	2.17	0.44
1:B:212:GLY:HA2	1:B:237:LYS:O	2.18	0.44
1:A:135:ARG:O	1:A:135:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:N	1:B:140:LEU:HD12	2.33	0.44
1:B:161:VAL:O	1:B:171[A]:THR:CG2	2.48	0.44
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.80	0.43
1:A:194:ILE:HD13	1:B:23:ILE:HD11	2.01	0.43
1:B:140:LEU:HD22	1:B:141:THR:H	1.84	0.43
1:B:161:VAL:HG13	1:B:171[B]:THR:HG22	2.01	0.43
1:A:330:LEU:O	1:A:331:LEU:HB2	2.18	0.42
1:B:129:VAL:O	1:B:170:ILE:HA	2.20	0.42
1:A:175:ALA:HB3	1:A:178:TRP:O	2.20	0.42
1:A:287:ARG:HG2	1:A:288:GLY:O	2.20	0.41
1:A:345:GLN:HG2	4:A:482:HOH:O	2.20	0.41
1:B:135:ARG:HG3	1:B:145:ASP:OD2	2.21	0.41
1:B:195:ARG:HH22	1:B:218:PHE:HB2	1.86	0.41
1:A:139:SER:OG	1:A:140:LEU:HG	2.21	0.40
1:B:252:LEU:HD22	1:B:278:VAL:CG1	2.51	0.40
1:B:204:LEU:HD23	1:B:230:LEU:CD2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:OH	1:B:279:THR:OG1[2_556]	1.97	0.23

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	328/374 (88%)	318 (97%)	10 (3%)	0	100	100
1	B	321/374 (86%)	308 (96%)	13 (4%)	0	100	100
All	All	649/748 (87%)	626 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	257/287 (90%)	253 (98%)	4 (2%)	55	44
1	B	240/287 (84%)	232 (97%)	8 (3%)	33	18
All	All	497/574 (87%)	485 (98%)	12 (2%)	45	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	219	THR
1	A	266	LEU
1	A	273	PRO
1	B	80	MSE
1	B	132	HIS
1	B	138	SER
1	B	140	LEU
1	B	171[A]	THR
1	B	171[B]	THR
1	B	291	VAL
1	B	330	LEU

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	38	GLN
1	A	153	ASN
1	B	166	GLN
1	B	199	ASN
1	B	213	GLN
1	B	232	ASN
1	B	308	GLN

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	ACT	A	363	-	3,3,3	0.59	0	3,3,3	1.42	0
2	ACT	A	364	-	3,3,3	1.14	0	3,3,3	1.43	1 (33%)
3	GOL	B	363	-	5,5,5	0.46	0	5,5,5	0.69	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
3	GOL	B	363	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	364	ACT	OXT-C-O	-2.06	114.40	122.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	363	GOL	C1-C2-C3-O3
3	B	363	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	331/374 (88%)	0.68	22 (6%) 24 26	25, 38, 64, 87	3 (0%)
1	B	327/374 (87%)	1.25	75 (22%) 2 2	17, 38, 65, 85	1 (0%)
All	All	658/748 (87%)	0.96	97 (14%) 6 5	17, 38, 66, 87	4 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	5.2
1	B	176	PRO	4.8
1	B	61	GLY	4.7
1	B	62	VAL	4.4
1	B	22	LEU	4.4
1	B	180	PRO	4.3
1	A	178	TRP	4.0
1	B	140	LEU	3.9
1	A	140	LEU	3.8
1	B	54	LEU	3.8
1	B	41	LEU	3.7
1	B	208	LEU	3.7
1	A	105[A]	GLY	3.5
1	B	74	LEU	3.4
1	A	176	PRO	3.3
1	B	33	ALA	3.3
1	A	141	THR	3.3
1	B	68	THR	3.3
1	B	34	ALA	3.2
1	B	64	ALA	3.2
1	B	71	ALA	3.2
1	B	57	LEU	3.1
1	B	25	GLY	3.0
1	B	218	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	56	ALA	3.0
1	B	27	SER	2.9
1	A	177	GLY	2.9
1	B	104	THR	2.9
1	B	105	GLY	2.9
1	B	174	PHE	2.9
1	B	271	ILE	2.8
1	A	67	LEU	2.8
1	B	59	PHE	2.7
1	B	19	LEU	2.7
1	B	67	LEU	2.7
1	B	32	GLN	2.7
1	B	276	VAL	2.7
1	B	44	ALA	2.6
1	B	30	ARG	2.6
1	B	182	LEU	2.6
1	B	137	ALA	2.6
1	B	325	ALA	2.6
1	A	173	LEU	2.5
1	B	60	LYS	2.5
1	B	361	GLY	2.5
1	B	163	ALA	2.5
1	B	18	LEU	2.5
1	B	28	LEU	2.5
1	B	283	ILE	2.4
1	A	175	ALA	2.4
1	B	73	VAL	2.4
1	A	78	SER	2.4
1	B	138	SER	2.4
1	B	36	LEU	2.4
1	A	174	PHE	2.4
1	B	172	PHE	2.4
1	B	55	THR	2.4
1	B	331	LEU	2.3
1	B	219	THR	2.3
1	B	69	GLY	2.3
1	B	14	SER	2.3
1	A	92	THR	2.3
1	A	104	THR	2.3
1	B	53	ILE	2.3
1	A	139	SER	2.3
1	A	219	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	307	THR	2.3
1	A	13	THR	2.3
1	B	23	ILE	2.2
1	A	205	VAL	2.2
1	A	93	ASN	2.2
1	B	154	LEU	2.2
1	B	136	SER	2.2
1	B	35	GLU	2.2
1	B	173	LEU	2.2
1	B	262	SER	2.2
1	B	147	LEU	2.2
1	B	188	LEU	2.2
1	B	326	GLY	2.2
1	A	180	PRO	2.2
1	B	205	VAL	2.1
1	B	264	GLY	2.1
1	A	64	ALA	2.1
1	A	362	ASN	2.1
1	B	181	ALA	2.1
1	B	103	GLY	2.1
1	B	152	VAL	2.1
1	B	43	GLU	2.1
1	B	58	ASN	2.1
1	B	155	GLY	2.1
1	B	15	TRP	2.1
1	B	362	ASN	2.1
1	B	207	PRO	2.1
1	B	16	TYR	2.0
1	B	309	ALA	2.0
1	A	218	PHE	2.0
1	B	161	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
3	GOL	B	363	6/6	0.65	0.16	71,77,78,79	0
2	ACT	A	364	4/4	0.67	0.20	67,68,68,69	0
2	ACT	A	363	4/4	0.80	0.20	36,42,45,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.