



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 6H44 / pdb_00006h44
Title : Flavín-dependent Tryptophan 6-halogenase Thal in complex with tryptophan
Authors : Moritzer, A.; Minges, H.; Sewald, N.; Niemann, H.H.
Deposited on : 2018-07-20
Resolution : 2.55 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

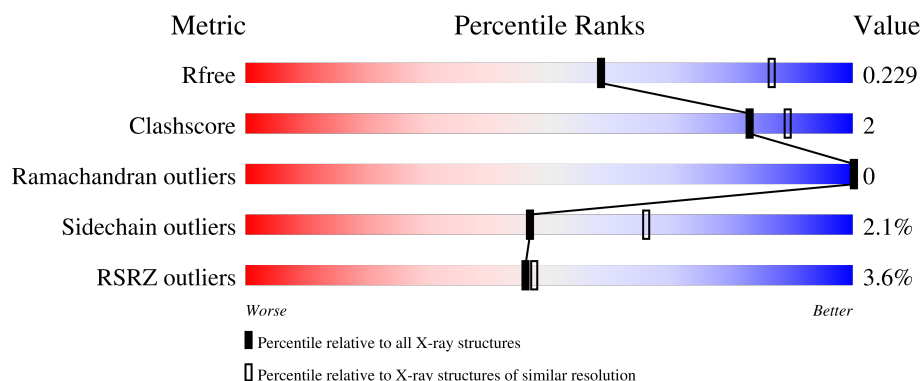
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	534	% 92% 7% .
1	B	534	6% 90% 8% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8820 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.

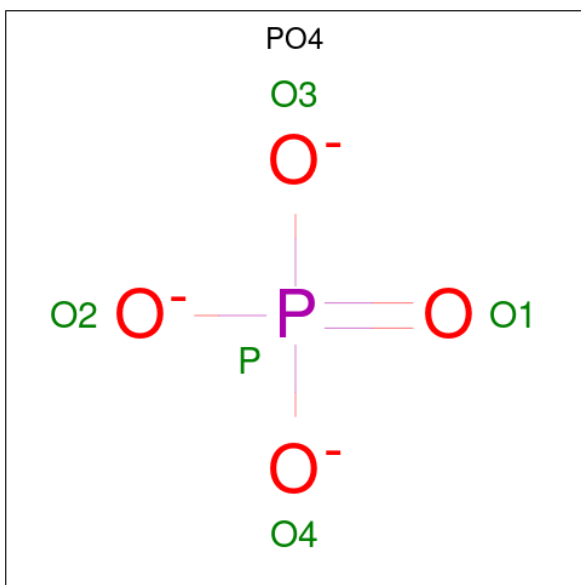
- Molecule 1 is a protein called Tryptophan 6-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	3	0
			4238	2704	728	785	21			
1	B	528	Total	C	N	O	S	0	2	0
			4235	2703	729	783	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A1E280
A	-1	ALA	-	expression tag	UNP A1E280
A	0	MET	-	expression tag	UNP A1E280
A	1	GLY	-	expression tag	UNP A1E280
B	-2	GLY	-	expression tag	UNP A1E280
B	-1	ALA	-	expression tag	UNP A1E280
B	0	MET	-	expression tag	UNP A1E280
B	1	GLY	-	expression tag	UNP A1E280

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



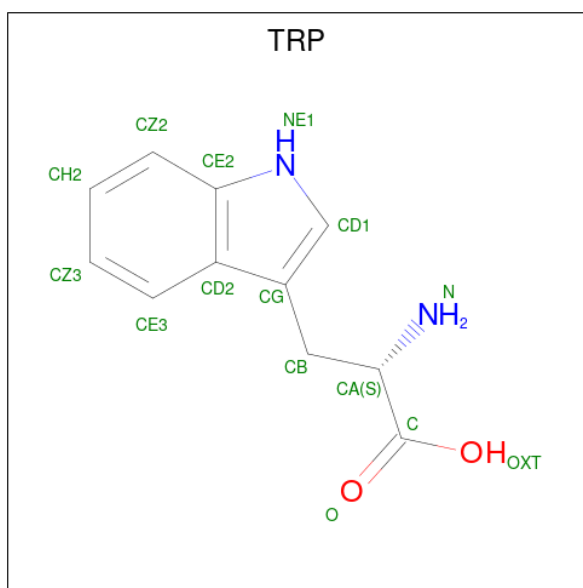
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- 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		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		

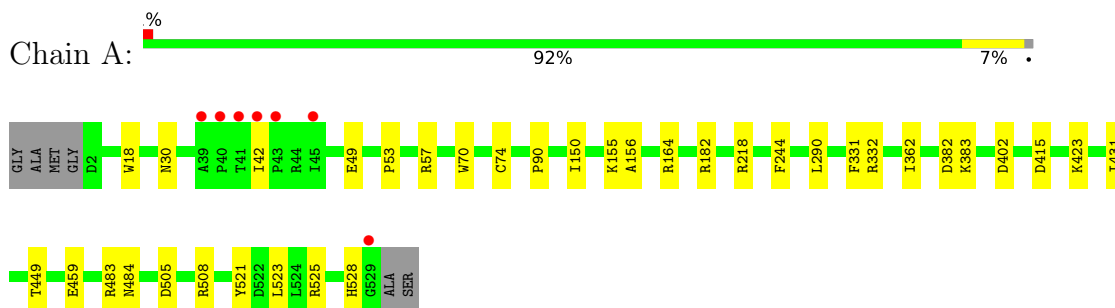
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	72	Total	O	0	0
			72	72		

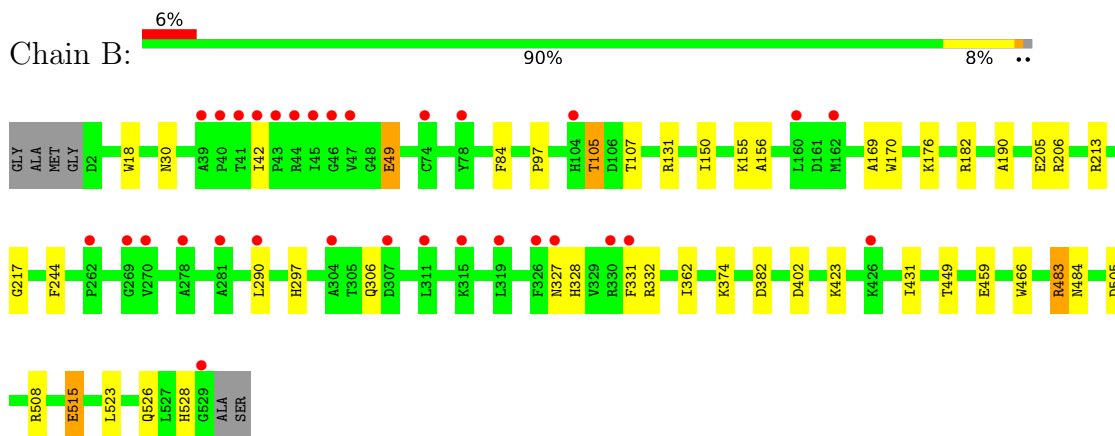
3 Residue-property plots

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: Tryptophan 6-halogenase



• Molecule 1: Tryptophan 6-halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	136.70Å 136.70Å 144.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 2.55 49.77 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.77-2.55) 99.9 (49.77-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.179 , 0.225 0.184 , 0.229	Depositor DCC
R_{free} test set	2462 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8820	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: K, PO4, 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	0.80	0/4353	0.97	1/5910 (0.0%)
1	B	0.75	0/4350	0.97	1/5905 (0.0%)
All	All	0.77	0/8703	0.97	2/11815 (0.0%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	PHE	CB-CA-C	-5.49	100.22	109.50
1	A	331	PHE	CB-CA-C	-5.44	100.31	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ARG	Sidechain
1	A	57	ARG	Sidechain
1	B	131	ARG	Sidechain

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	4238	0	4085	17	0
1	B	4235	0	4088	25	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
3	A	54	0	72	2	0
3	B	30	0	40	2	0
4	A	15	0	9	0	0
4	B	15	0	9	1	0
5	A	1	0	0	0	0
6	A	125	0	0	0	0
6	B	72	0	0	0	0
All	All	8820	0	8303	40	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 2.

All (40) 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:244:PHE:CE2	1:A:332:ARG:HG2	2.32	0.65
1:B:244:PHE:CE2	1:B:332:ARG:HG2	2.31	0.64
1:B:244:PHE:CZ	1:B:332:ARG:HG2	2.34	0.62
1:A:244:PHE:CZ	1:A:332:ARG:HG2	2.36	0.60
1:A:505:ASP:OD1	1:A:508:ARG:NH1	2.36	0.59
1:B:505:ASP:OD1	1:B:508:ARG:NH1	2.36	0.59
1:A:382:ASP:OD2	1:B:483:ARG:NH2	2.36	0.58
1:A:156:ALA:HB1	1:A:523:LEU:HD22	1.86	0.57
1:A:521:TYR:CZ	1:A:525:ARG:HD3	2.40	0.57
1:B:156:ALA:HB1	1:B:523:LEU:HD22	1.86	0.56
1:B:306:GLN:OE1	1:B:328:HIS:ND1	2.40	0.54
1:B:97:PRO:HB2	1:B:105:THR:HG22	1.90	0.53
1:B:213:ARG:HH21	1:B:217:GLY:HA2	1.74	0.53
1:B:205:GLU:HG2	1:B:206[A]:ARG:HG3	1.92	0.52
1:A:521:TYR:CE2	1:A:525:ARG:HD3	2.46	0.50
1:A:53:PRO:HB3	3:A:607:GOL:H2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:ND2	3:B:606:GOL:O3	2.47	0.47
1:B:190:ALA:HB3	3:B:606:GOL:H2	1.97	0.47
1:B:213:ARG:NH2	1:B:217:GLY:HA2	2.29	0.47
1:B:205:GLU:HG2	1:B:206[B]:ARG:HG3	1.96	0.47
1:A:402:ASP:HB3	1:A:431:ILE:HB	1.97	0.47
1:B:515:GLU:HA	1:B:515:GLU:OE1	2.15	0.46
1:B:402:ASP:HB3	1:B:431:ILE:HB	1.97	0.46
1:B:374:LYS:NZ	1:B:459:GLU:OE1	2.50	0.45
1:A:90:PRO:HB3	1:A:415:ASP:HB3	1.98	0.44
1:B:306:GLN:OE1	1:B:328:HIS:CG	2.70	0.44
1:A:70:TRP:HE3	1:A:74[A]:CYS:HG	1.61	0.44
1:A:150:ILE:HG23	1:A:155:LYS:HB2	2.00	0.43
1:A:290:LEU:HD22	1:A:528:HIS:CD2	2.54	0.43
1:B:290:LEU:HD22	1:B:528:HIS:CD2	2.54	0.43
1:A:49:GLU:HG2	1:A:362:ILE:HD12	2.01	0.43
1:B:18:TRP:CZ2	1:B:182:ARG:HG3	2.54	0.42
1:B:150:ILE:HG23	1:B:155:LYS:HB2	1.99	0.42
1:A:164:ARG:HH22	3:A:607:GOL:H32	1.85	0.42
1:A:18:TRP:CZ2	1:A:182:ARG:HG3	2.55	0.41
1:A:483:ARG:NH1	1:B:382:ASP:OD2	2.54	0.41
1:B:466:TRP:CZ3	4:B:610:TRP:CE3	3.08	0.41
1:B:84:PHE:O	1:B:107:THR:HA	2.21	0.40
1:B:49:GLU:HG2	1:B:362:ILE:HD12	2.02	0.40
1:B:169:ALA:HA	1:B:170:TRP:CE3	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	529/534 (99%)	516 (98%)	13 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	528/534 (99%)	515 (98%)	13 (2%)	0	100	100
All	All	1057/1068 (99%)	1031 (98%)	26 (2%)	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	446/445 (100%)	439 (98%)	7 (2%)	55	73
1	B	445/445 (100%)	433 (97%)	12 (3%)	39	58
All	All	891/890 (100%)	872 (98%)	19 (2%)	47	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	42	ILE
1	A	383	LYS
1	A	423	LYS
1	A	449	THR
1	A	459	GLU
1	A	484	ASN
1	B	42	ILE
1	B	49	GLU
1	B	105	THR
1	B	176	LYS
1	B	297	HIS
1	B	327	ASN
1	B	423	LYS
1	B	449	THR
1	B	483	ARG
1	B	484	ASN
1	B	515	GLU

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Mol	Chain	Res	Type
1	B	526	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	133	GLN
1	A	306	GLN
1	A	484	ASN
1	A	526	GLN
1	A	528	HIS
1	B	30	ASN
1	B	75	ASN
1	B	104	HIS
1	B	133	GLN
1	B	306	GLN
1	B	528	HIS

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](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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	$\# Z > 2$
3	GOL	A	612	-	5,5,5	0.52	0	5,5,5	0.28	0
3	GOL	B	607	-	5,5,5	0.54	0	5,5,5	0.51	0
3	GOL	B	606	-	5,5,5	0.52	0	5,5,5	0.38	0
3	GOL	A	606	-	5,5,5	0.48	0	5,5,5	0.70	0
2	PO4	A	603	-	4,4,4	0.77	0	6,6,6	0.74	0
3	GOL	B	608	-	5,5,5	0.20	0	5,5,5	0.45	0
3	GOL	A	608	-	5,5,5	0.51	0	5,5,5	0.39	0
3	GOL	B	605	-	5,5,5	0.69	0	5,5,5	0.47	0
3	GOL	A	605	-	5,5,5	0.69	0	5,5,5	0.70	0
3	GOL	A	604	-	5,5,5	0.75	0	5,5,5	1.34	0
2	PO4	B	601	-	4,4,4	0.87	0	6,6,6	0.72	0
2	PO4	B	602	-	4,4,4	0.72	0	6,6,6	0.83	0
3	GOL	A	609	-	5,5,5	0.47	0	5,5,5	0.54	0
2	PO4	A	602	-	4,4,4	0.58	0	6,6,6	0.75	0
3	GOL	A	610	-	5,5,5	0.41	0	5,5,5	0.45	0
3	GOL	A	611	-	5,5,5	0.97	0	5,5,5	1.63	2 (40%)
2	PO4	B	604	-	4,4,4	0.87	0	6,6,6	0.44	0
4	TRP	A	613	-	15,16,16	0.58	0	18,22,22	0.79	0
4	TRP	B	610	-	15,16,16	0.86	1 (6%)	18,22,22	0.87	1 (5%)
2	PO4	B	603	-	4,4,4	0.93	0	6,6,6	0.72	0
2	PO4	A	601	-	4,4,4	1.12	0	6,6,6	1.93	2 (33%)
3	GOL	A	607	-	5,5,5	0.74	0	5,5,5	1.66	1 (20%)
3	GOL	B	609	-	5,5,5	0.60	0	5,5,5	0.74	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	A	612	-	-	2/4/4/4	-
3	GOL	A	609	-	-	2/4/4/4	-
3	GOL	B	608	-	-	0/4/4/4	-
3	GOL	A	608	-	-	2/4/4/4	-
4	TRP	A	613	-	-	2/8/8/8	0/2/2/2
4	TRP	B	610	-	-	3/8/8/8	0/2/2/2
3	GOL	B	607	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	A	610	-	-	2/4/4/4	-
3	GOL	A	611	-	-	0/4/4/4	-
3	GOL	A	605	-	-	4/4/4/4	-
3	GOL	B	606	-	-	2/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	A	607	-	-	2/4/4/4	-
3	GOL	A	606	-	-	0/4/4/4	-
3	GOL	B	609	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	610	TRP	OXT-C	-2.87	1.21	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	PO4	O4-P-O1	-3.96	96.96	110.95
4	B	610	TRP	OXT-C-O	-3.08	117.09	124.08
3	A	607	GOL	O2-C2-C3	2.77	120.66	109.18
3	A	611	GOL	O1-C1-C2	2.34	120.89	110.38
3	A	611	GOL	O2-C2-C1	2.29	118.66	109.18
2	A	601	PO4	O4-P-O2	2.26	114.94	107.91

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	607	GOL	C1-C2-C3-O3
3	A	609	GOL	O1-C1-C2-O2
3	A	609	GOL	O1-C1-C2-C3
3	A	610	GOL	O1-C1-C2-C3
3	A	612	GOL	O1-C1-C2-C3
3	B	605	GOL	O1-C1-C2-C3
3	B	606	GOL	C1-C2-C3-O3
3	B	609	GOL	O1-C1-C2-C3
3	B	609	GOL	C1-C2-C3-O3
4	B	610	TRP	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	A	608	GOL	O2-C2-C3-O3
3	A	612	GOL	O1-C1-C2-O2
3	B	609	GOL	O1-C1-C2-O2
4	A	613	TRP	OXT-C-CA-N
3	A	605	GOL	O1-C1-C2-C3
3	A	608	GOL	C1-C2-C3-O3
3	B	607	GOL	C1-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	B	605	GOL	O1-C1-C2-O2
3	B	609	GOL	O2-C2-C3-O3
3	A	605	GOL	O1-C1-C2-O2
3	A	605	GOL	O2-C2-C3-O3
3	A	607	GOL	O2-C2-C3-O3
3	B	606	GOL	O2-C2-C3-O3
3	B	607	GOL	O2-C2-C3-O3
3	A	610	GOL	O1-C1-C2-O2
4	B	610	TRP	O-C-CA-N
3	A	605	GOL	C1-C2-C3-O3
4	B	610	TRP	OXT-C-CA-CB
4	A	613	TRP	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	GOL	2	0
4	B	610	TRP	1	0
3	A	607	GOL	2	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	528/534 (98%)	-0.21	7 (1%) 75 75	25, 46, 72, 124	3 (0%)
1	B	528/534 (98%)	0.43	31 (5%) 28 27	31, 61, 103, 154	2 (0%)
All	All	1056/1068 (98%)	0.11	38 (3%) 46 47	25, 52, 96, 154	5 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	4.8
1	B	45	ILE	4.4
1	B	42	ILE	4.4
1	B	39	ALA	4.1
1	B	311	LEU	4.0
1	A	43	PRO	3.8
1	B	40	PRO	3.7
1	A	39	ALA	3.3
1	B	160	LEU	3.3
1	B	529	GLY	3.0
1	A	45	ILE	2.9
1	B	43	PRO	2.9
1	A	529	GLY	2.9
1	B	47	VAL	2.9
1	B	319	LEU	2.9
1	A	41	THR	2.8
1	B	326	PHE	2.8
1	A	40	PRO	2.6
1	B	331	PHE	2.5
1	B	41	THR	2.5
1	B	426	LYS	2.5
1	B	44	ARG	2.5
1	B	315	LYS	2.4
1	B	281	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	2.3
1	B	162	MET	2.2
1	B	278	ALA	2.2
1	B	307	ASP	2.2
1	B	262	PRO	2.2
1	B	270	VAL	2.1
1	B	269	GLY	2.1
1	B	104	HIS	2.1
1	B	330	ARG	2.1
1	B	78	TYR	2.1
1	B	304	ALA	2.0
1	B	74	CYS	2.0
1	B	290	LEU	2.0
1	B	327	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(Å ²)	Q<0.9
2	PO4	B	604	5/5	0.63	0.10	92,93,103,107	5
3	GOL	B	609	6/6	0.75	0.24	73,83,90,90	0
2	PO4	B	601	5/5	0.78	0.12	75,75,83,90	5
3	GOL	A	606	6/6	0.78	0.20	68,76,79,79	0
2	PO4	B	602	5/5	0.78	0.14	76,79,90,97	5
3	GOL	A	612	6/6	0.82	0.21	71,82,87,88	0
3	GOL	A	609	6/6	0.84	0.17	64,69,79,86	0
3	GOL	A	604	6/6	0.86	0.18	53,62,71,72	0
3	GOL	A	605	6/6	0.87	0.15	48,65,72,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	607	6/6	0.88	0.17	73,84,89,97	0
3	GOL	A	608	6/6	0.89	0.13	83,100,101,104	0
2	PO4	B	603	5/5	0.89	0.12	69,71,75,82	5
3	GOL	B	608	6/6	0.89	0.12	87,94,94,97	0
3	GOL	A	611	6/6	0.89	0.19	51,65,74,74	0
3	GOL	B	605	6/6	0.90	0.15	67,79,85,85	0
2	PO4	A	603	5/5	0.91	0.15	65,68,70,78	5
3	GOL	A	610	6/6	0.94	0.14	50,55,58,59	0
2	PO4	A	602	5/5	0.95	0.08	49,61,62,64	5
3	GOL	A	607	6/6	0.95	0.09	41,42,47,47	0
3	GOL	B	606	6/6	0.95	0.10	52,58,62,69	0
2	PO4	A	601	5/5	0.97	0.06	40,46,50,52	0
4	TRP	A	613	15/15	0.97	0.07	41,43,47,50	0
4	TRP	B	610	15/15	0.97	0.06	47,52,61,62	0
5	K	A	614	1/1	0.98	0.06	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.