



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 6FPZ / pdb_00006fpz
Title : Inter-alpha-inhibitor heavy chain 1, D298A
Authors : Briggs, D.C.; Day, A.J.
Deposited on : 2018-02-12
Resolution : 2.20 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

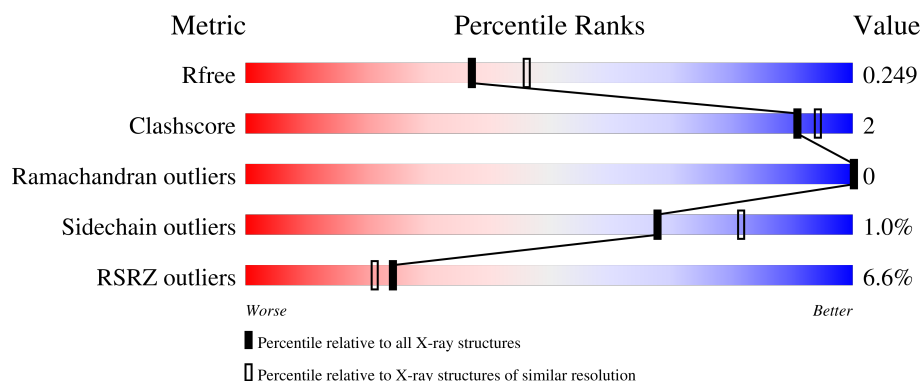
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	660	6% 86% • 9%
1	B	660	6% 86% 5% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19365 atoms, of which 9259 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 Inter-alpha-trypsin inhibitor heavy chain H1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	598	Total	C	H	N	O	S	0	2	0
			9255	2948	4591	818	879	19			
1	B	598	Total	C	H	N	O	S	0	3	0
			9269	2951	4598	820	881	19			

There are 46 discrepancies between the modelled and reference sequences:

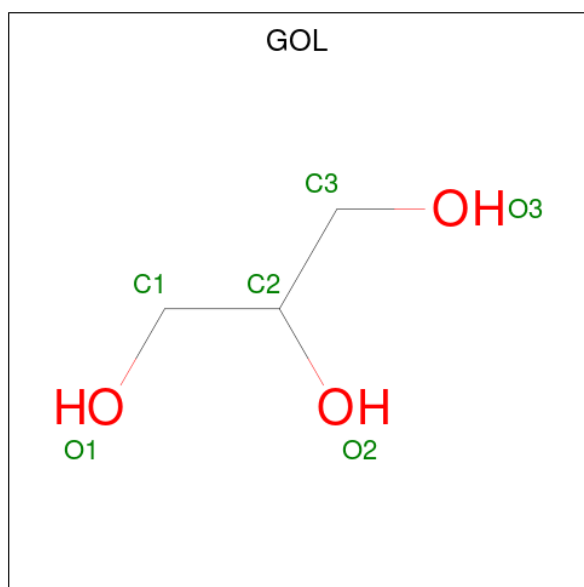
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP P19827
A	14	ALA	-	expression tag	UNP P19827
A	15	HIS	-	expression tag	UNP P19827
A	16	HIS	-	expression tag	UNP P19827
A	17	HIS	-	expression tag	UNP P19827
A	18	HIS	-	expression tag	UNP P19827
A	19	HIS	-	expression tag	UNP P19827
A	20	HIS	-	expression tag	UNP P19827
A	21	VAL	-	expression tag	UNP P19827
A	22	GLY	-	expression tag	UNP P19827
A	23	THR	-	expression tag	UNP P19827
A	24	GLY	-	expression tag	UNP P19827
A	25	SER	-	expression tag	UNP P19827
A	26	ASN	-	expression tag	UNP P19827
A	27	ASP	-	expression tag	UNP P19827
A	28	ASP	-	expression tag	UNP P19827
A	29	ASP	-	expression tag	UNP P19827
A	30	ASP	-	expression tag	UNP P19827
A	31	ASP	-	expression tag	UNP P19827
A	32	LYS	-	expression tag	UNP P19827
A	33	SER	-	expression tag	UNP P19827
A	34	PRO	-	expression tag	UNP P19827
A	298	ALA	ASP	engineered mutation	UNP P19827
B	13	MET	-	initiating methionine	UNP P19827
B	14	ALA	-	expression tag	UNP P19827

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	HIS	-	expression tag	UNP P19827
B	16	HIS	-	expression tag	UNP P19827
B	17	HIS	-	expression tag	UNP P19827
B	18	HIS	-	expression tag	UNP P19827
B	19	HIS	-	expression tag	UNP P19827
B	20	HIS	-	expression tag	UNP P19827
B	21	VAL	-	expression tag	UNP P19827
B	22	GLY	-	expression tag	UNP P19827
B	23	THR	-	expression tag	UNP P19827
B	24	GLY	-	expression tag	UNP P19827
B	25	SER	-	expression tag	UNP P19827
B	26	ASN	-	expression tag	UNP P19827
B	27	ASP	-	expression tag	UNP P19827
B	28	ASP	-	expression tag	UNP P19827
B	29	ASP	-	expression tag	UNP P19827
B	30	ASP	-	expression tag	UNP P19827
B	31	ASP	-	expression tag	UNP P19827
B	32	LYS	-	expression tag	UNP P19827
B	33	SER	-	expression tag	UNP P19827
B	34	PRO	-	expression tag	UNP P19827
B	298	ALA	ASP	engineered mutation	UNP P19827

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



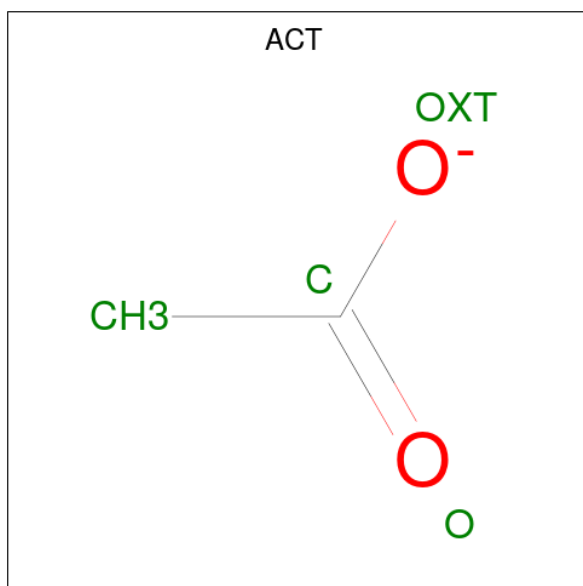
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			13	3	7	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			13	3	7	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			7	2	3	2		

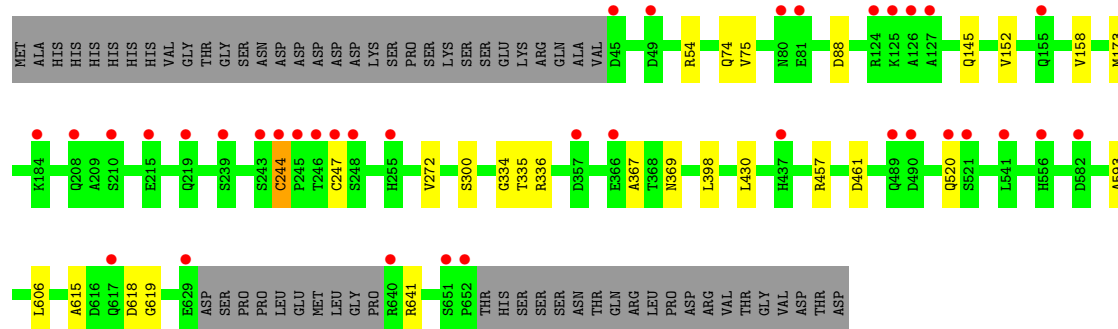
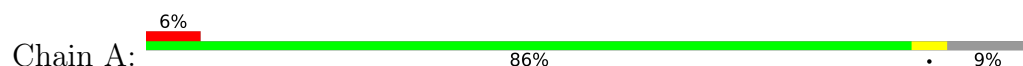
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	357	Total 357	O 357	0	0
4	B	356	Total 356	O 356	0	0

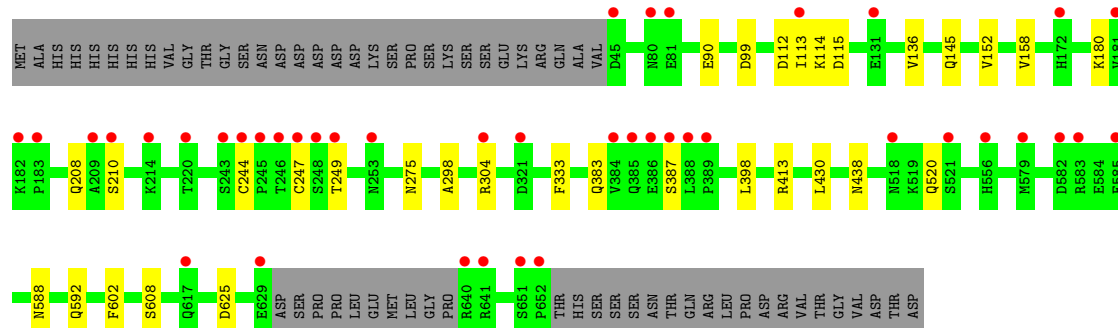
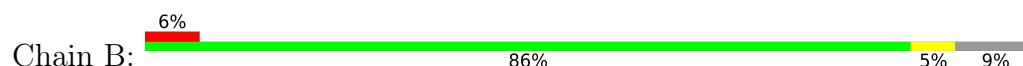
3 Residue-property plots [i](#)

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: Inter-alpha-trypsin inhibitor heavy chain H1



- Molecule 1: Inter-alpha-trypsin inhibitor heavy chain H1



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	159.70Å 159.70Å 65.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.41 – 2.20 71.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (71.41-2.20) 94.2 (71.41-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.248 0.220 , 0.249	Depositor DCC
R_{free} test set	4175 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19365	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, ACT

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	0.10	0/4765	0.28	0/6448
1	B	0.10	0/4765	0.28	0/6448
All	All	0.10	0/9530	0.28	0/12896

There are no bond length outliers.

There are no bond angle outliers.

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	4664	4591	4582	13	0
1	B	4671	4598	4605	18	0
2	A	30	37	40	0	0
2	B	24	30	32	0	0
3	B	4	3	3	0	0
4	A	357	0	0	1	0
4	B	356	0	0	6	0
All	All	10106	9259	9262	31	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 (31) 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:210:SER:OG	4:B:801:HOH:O	1.99	0.81
1:B:413:ARG:NH1	4:B:805:HOH:O	2.20	0.74
1:B:90:GLU:OE1	4:B:803:HOH:O	2.09	0.71
1:B:180:LYS:O	4:B:802:HOH:O	2.09	0.70
1:B:304:ARG:NH1	4:B:806:HOH:O	2.26	0.69
1:B:438[B]:ASN:OD1	4:B:804:HOH:O	2.12	0.68
1:B:113:ILE:HD11	1:B:602:PHE:O	1.94	0.68
1:A:54:ARG:NH1	1:A:74:GLN:OE1	2.31	0.59
1:B:398:LEU:HD23	1:B:430:LEU:HD13	1.85	0.58
1:B:152:VAL:HG11	1:B:158:VAL:HG21	1.88	0.56
1:A:398:LEU:HD23	1:A:430:LEU:HD13	1.88	0.56
1:B:152:VAL:CG1	1:B:158:VAL:HG21	2.39	0.53
1:A:244:CYS:N	1:A:247:CYS:SG	2.84	0.50
1:B:275:ASN:OD1	1:B:520:GLN:NE2	2.44	0.50
1:A:615:ALA:HB1	1:A:619:GLY:HA2	1.94	0.49
1:A:618:ASP:OD2	1:A:641:ARG:NH2	2.43	0.48
1:B:608:SER:OG	1:B:625:ASP:OD1	2.19	0.46
1:A:152:VAL:HG11	1:A:158:VAL:HG21	1.96	0.46
1:A:88:ASP:OD1	1:A:145:GLN:NE2	2.48	0.46
1:A:593:ALA:HB3	1:A:606:LEU:CD1	2.48	0.44
1:B:244:CYS:SG	1:B:247:CYS:N	2.92	0.42
1:B:136:VAL:HA	1:B:145:GLN:O	2.19	0.42
1:A:334:GLY:O	1:A:369:ASN:N	2.47	0.42
1:B:112:ASP:OD1	1:B:114:LYS:NZ	2.36	0.42
1:B:298:ALA:HB2	1:B:333:PHE:CZ	2.54	0.42
1:A:272:VAL:HG11	1:A:520:GLN:HG3	2.01	0.41
1:A:152:VAL:CG1	1:A:158:VAL:HG21	2.51	0.41
1:A:335:THR:HB	1:A:367:ALA:HB3	2.01	0.41
1:B:383:GLN:O	1:B:387:SER:O	2.38	0.41
1:A:173:MET:HE1	4:A:1118:HOH:O	2.20	0.41
1:B:588:ASN:OD1	1:B:592:GLN:NE2	2.50	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	596/660 (90%)	585 (98%)	11 (2%)	0	100	100
1	B	597/660 (90%)	586 (98%)	11 (2%)	0	100	100
All	All	1193/1320 (90%)	1171 (98%)	22 (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	502/574 (88%)	496 (99%)	6 (1%)	63	78
1	B	503/574 (88%)	499 (99%)	4 (1%)	73	85
All	All	1005/1148 (88%)	995 (99%)	10 (1%)	68	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	244	CYS
1	A	300	SER
1	A	336	ARG
1	A	457	ARG
1	A	461	ASP
1	B	99	ASP
1	B	115	ASP

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Mol	Chain	Res	Type
1	B	208	GLN
1	B	249	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	185	GLN
1	A	208	GLN
1	A	255	HIS
1	A	371	ASN
1	A	415	GLN
1	A	419	ASN
1	B	59	ASN
1	B	132	ASN
1	B	155	GLN
1	B	161	GLN
1	B	288	ASN
1	B	323	GLN
1	B	415	GLN
1	B	442	ASN
1	B	456	GLN
1	B	500	HIS
1	B	520	GLN
1	B	561	HIS

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

10 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	702	-	5,5,5	0.98	0	5,5,5	1.04	0
2	GOL	A	703	-	5,5,5	0.96	0	5,5,5	1.04	0
2	GOL	A	701	-	5,5,5	0.96	0	5,5,5	1.06	0
2	GOL	B	701	-	5,5,5	1.00	0	5,5,5	0.99	0
2	GOL	A	704	-	5,5,5	1.04	0	5,5,5	0.93	0
2	GOL	B	703	-	5,5,5	0.95	0	5,5,5	1.05	0
3	ACT	B	705	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
2	GOL	A	705	-	5,5,5	0.94	0	5,5,5	1.06	0
2	GOL	B	702	-	5,5,5	0.91	0	5,5,5	1.10	0
2	GOL	B	704	-	5,5,5	0.95	0	5,5,5	1.03	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	702	-	-	2/4/4/4	-
2	GOL	A	703	-	-	1/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	B	703	-	-	0/4/4/4	-
2	GOL	A	705	-	-	0/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	B	704	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	ACT	CH3-C	2.02	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	C1-C2-C3-O3
2	A	702	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-C3
2	B	704	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	A	704	GOL	C1-C2-C3-O3
2	A	701	GOL	O2-C2-C3-O3
2	A	704	GOL	O2-C2-C3-O3
2	B	704	GOL	O2-C2-C3-O3
2	A	702	GOL	O2-C2-C3-O3
2	A	703	GOL	O1-C1-C2-O2

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	598/660 (90%)	0.34	37 (6%)	26 23	19, 46, 86, 134	1 (0%)
1	B	598/660 (90%)	0.42	42 (7%)	22 19	21, 46, 84, 139	3 (0%)
All	All	1196/1320 (90%)	0.38	79 (6%)	24 21	19, 46, 85, 139	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	GLU	7.4
1	B	45	ASP	7.1
1	B	629	GLU	6.4
1	A	45	ASP	6.2
1	A	640	ARG	6.0
1	A	246	THR	5.8
1	B	246	THR	5.7
1	B	652	PRO	5.6
1	B	582	ASP	5.4
1	B	640	ARG	5.3
1	B	245	PRO	4.4
1	B	386	GLU	4.4
1	B	243	SER	4.4
1	A	248	SER	4.2
1	A	245	PRO	3.9
1	A	247	CYS	3.8
1	B	579	MET	3.7
1	A	244	CYS	3.6
1	A	125	LYS	3.5
1	A	489	GLN	3.4
1	A	210	SER	3.4
1	B	80	ASN	3.4
1	B	183	PRO	3.3
1	A	124	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	SER	3.3
1	A	652	PRO	3.2
1	A	208	GLN	3.2
1	B	210	SER	3.2
1	A	490	ASP	3.2
1	B	385	GLN	3.2
1	B	387	SER	3.0
1	A	49	ASP	3.0
1	B	389	PRO	3.0
1	B	641	ARG	2.9
1	B	249	THR	2.9
1	B	388	LEU	2.9
1	B	244	CYS	2.9
1	A	617	GLN	2.9
1	A	556	HIS	2.9
1	A	255	HIS	2.8
1	B	247	CYS	2.7
1	B	651	SER	2.6
1	B	248	SER	2.5
1	B	214	LYS	2.5
1	A	521	SER	2.4
1	B	131	GLU	2.4
1	A	184	LYS	2.4
1	B	384	VAL	2.4
1	B	321	ASP	2.4
1	A	127	ALA	2.3
1	B	521	SER	2.3
1	B	304	ARG	2.3
1	A	155	GLN	2.3
1	A	126	ALA	2.3
1	B	253	ASN	2.3
1	B	556	HIS	2.3
1	B	585	GLU	2.3
1	A	541	LEU	2.3
1	B	182	LYS	2.3
1	B	113	ILE	2.2
1	A	520	GLN	2.2
1	B	220	THR	2.2
1	B	181	VAL	2.2
1	A	81	GLU	2.2
1	B	209	ALA	2.2
1	B	518	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	617	GLN	2.2
1	A	239	SER	2.2
1	A	582	ASP	2.1
1	A	437	HIS	2.1
1	A	651	SER	2.1
1	A	215	GLU	2.1
1	A	366	GLU	2.1
1	B	172	HIS	2.1
1	B	81	GLU	2.1
1	A	80	ASN	2.1
1	A	219	GLN	2.1
1	A	357	ASP	2.1
1	B	583	ARG	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	GOL	A	703	6/6	0.79	0.25	87,105,108,109	0
2	GOL	B	703	6/6	0.79	0.20	68,82,85,89	0
2	GOL	A	704	6/6	0.81	0.24	96,97,116,116	0
2	GOL	A	701	6/6	0.81	0.21	54,58,69,70	0
3	ACT	B	705	4/4	0.83	0.27	58,62,75,75	0
2	GOL	A	702	6/6	0.84	0.23	89,91,108,109	0
2	GOL	B	701	6/6	0.86	0.21	63,69,80,82	0
2	GOL	B	702	6/6	0.89	0.16	57,69,72,72	0
2	GOL	B	704	6/6	0.91	0.16	64,68,80,81	0
2	GOL	A	705	6/6	0.92	0.12	49,59,67,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.