Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2025 – 12:15 AM JST

PDB ID	:	8YUG
Title	:	X-ray Crystal structure of glycoside hydrolase family 18 chitinase from Serratia marcescens hexahistigine-tagged SmChiB apo enzyme
Authors	:	Ebi, S.; Sunagawa, N.; Yamaguchi, S.; Igarashi, K.
Deposited on	:	2024-03-27
Resolution	:	1.71 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:

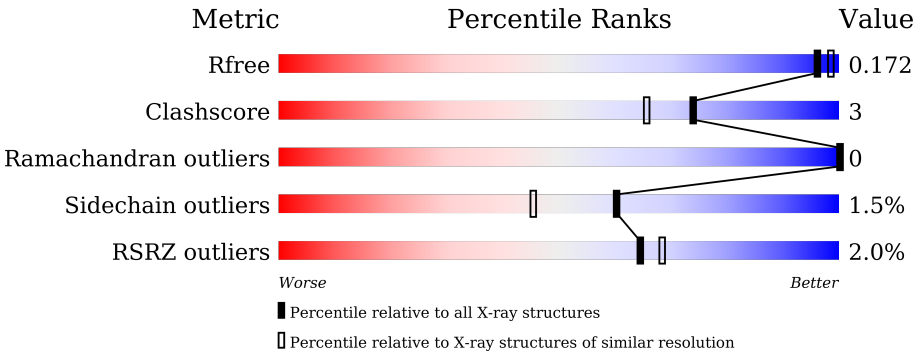
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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}	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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 <=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	511	2% 91% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5344 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.

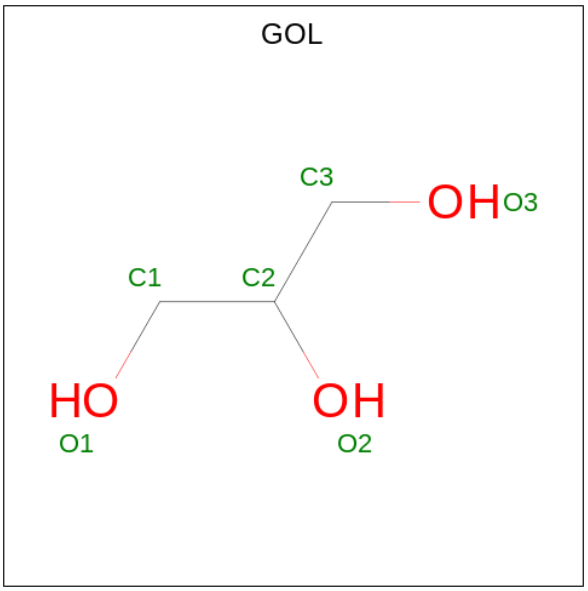
- Molecule 1 is a protein called Chitinase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	46	0
			4265	2718	724	801	22			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P11797
A	1	ASP	-	expression tag	UNP P11797
A	500	ALA	-	expression tag	UNP P11797
A	501	ALA	-	expression tag	UNP P11797
A	502	ALA	-	expression tag	UNP P11797
A	503	LEU	-	expression tag	UNP P11797
A	504	GLU	-	expression tag	UNP P11797
A	505	HIS	-	expression tag	UNP P11797
A	506	HIS	-	expression tag	UNP P11797
A	507	HIS	-	expression tag	UNP P11797
A	508	HIS	-	expression tag	UNP P11797
A	509	HIS	-	expression tag	UNP P11797
A	510	HIS	-	expression tag	UNP P11797

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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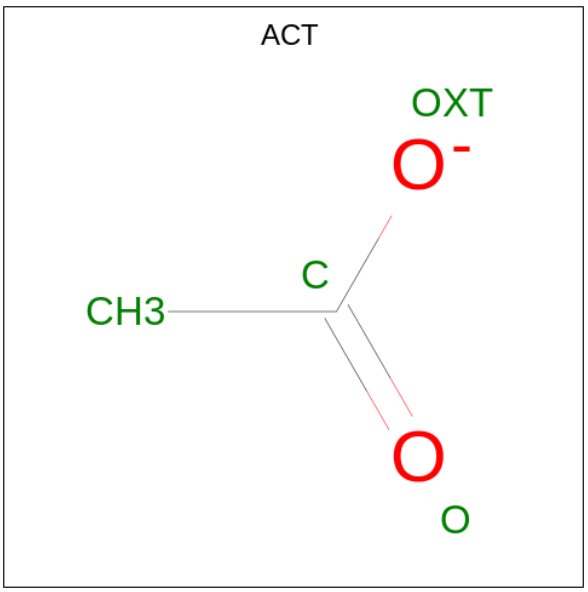
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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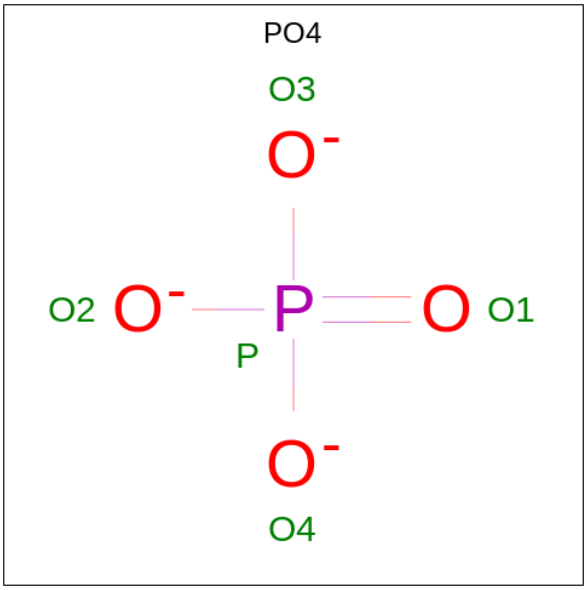
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

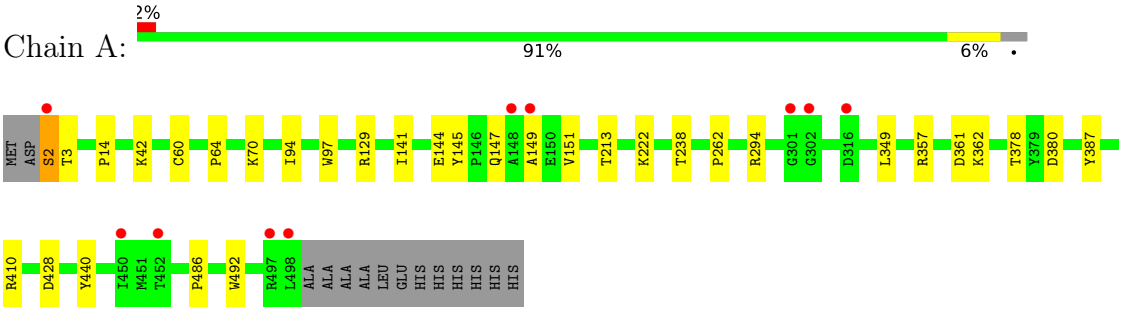
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	785	Total O 785 785	0	0

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: Chitinase B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.58Å 97.58Å 196.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 1.71 48.79 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.79-1.71) 99.9 (48.79-1.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.152 , 0.173 0.151 , 0.172	Depositor DCC
R_{free} test set	101183 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PO4

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	0.37	0/4393	0.58	0/5970

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

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	4265	0	4094	23	0
2	A	210	0	279	14	0
3	A	64	0	48	3	0
4	A	20	0	0	0	0
5	A	785	0	0	6	0
All	All	5344	0	4421	27	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 3.

All (27) 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:294:ARG:HH12	2:A:619:GOL:H12	1.52	0.75
1:A:440:TYR:HA	2:A:605:GOL:H31	1.78	0.64
1:A:147[B]:GLN:O	1:A:151:VAL:HG23	2.00	0.61
1:A:428[B]:ASP:HA	2:A:612:GOL:H12	1.85	0.59
1:A:64:PRO:HD2	2:A:626:GOL:H11	1.89	0.54
1:A:60[B]:CYS:SG	1:A:94:ILE:HD13	2.49	0.52
1:A:428[A]:ASP:HA	2:A:612:GOL:H12	1.93	0.49
1:A:70[A]:LYS:NZ	5:A:714:HOH:O	2.37	0.49
1:A:387:TYR:OH	3:A:635:ACT:H3	2.13	0.48
1:A:94:ILE:HD12	1:A:141[A]:ILE:HD13	1.97	0.47
1:A:129[A]:ARG:NH2	3:A:639:ACT:O	2.29	0.47
1:A:349[B]:LEU:HD11	1:A:357[B]:ARG:HB2	1.96	0.47
1:A:486:PRO:HA	1:A:492:TRP:CD1	2.52	0.45
1:A:144:GLU:HA	1:A:145:TYR:CG	2.52	0.44
1:A:97:TRP:CG	2:A:628:GOL:H2	2.52	0.44
1:A:294:ARG:HH12	2:A:619:GOL:C1	2.25	0.44
1:A:410[B]:ARG:NH2	2:A:610:GOL:H32	2.33	0.43
2:A:618:GOL:H11	5:A:740:HOH:O	2.19	0.43
2:A:632:GOL:H31	5:A:1210:HOH:O	2.18	0.43
2:A:623:GOL:H31	5:A:1135:HOH:O	2.18	0.42
1:A:42[B]:LYS:HE3	2:A:625:GOL:H12	2.02	0.42
3:A:643:ACT:H3	5:A:778:HOH:O	2.19	0.41
1:A:149[A]:ALA:O	5:A:702:HOH:O	2.21	0.41
1:A:14:PRO:HA	2:A:601:GOL:H31	2.03	0.41
1:A:2:SER:HB2	1:A:3:THR:H	1.60	0.40
1:A:362[B]:LYS:HG2	2:A:614:GOL:H2	2.04	0.40
1:A:238:THR:HB	1:A:262:PRO:HB2	2.04	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	541/511 (106%)	531 (98%)	10 (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	444/412 (108%)	436 (98%)	8 (2%)	54 37

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	213	THR
1	A	222[A]	LYS
1	A	222[B]	LYS
1	A	361[A]	ASP
1	A	361[B]	ASP
1	A	378	THR
1	A	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

55 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	625	-	5,5,5	0.83	0	5,5,5	0.87	0
2	GOL	A	620	-	5,5,5	0.86	0	5,5,5	1.05	0
3	ACT	A	635	-	3,3,3	1.16	0	3,3,3	1.43	0
2	GOL	A	610	-	5,5,5	1.17	0	5,5,5	1.07	0
3	ACT	A	643	-	3,3,3	1.13	0	3,3,3	1.39	0
2	GOL	A	626	-	5,5,5	1.14	0	5,5,5	0.96	0
2	GOL	A	649	-	5,5,5	0.90	0	5,5,5	1.03	0
2	GOL	A	654	-	5,5,5	0.82	0	5,5,5	1.09	0
3	ACT	A	638	-	3,3,3	1.34	0	3,3,3	1.39	0
4	PO4	A	617	-	4,4,4	1.02	0	6,6,6	0.53	0
4	PO4	A	609	-	4,4,4	0.85	0	6,6,6	0.53	0
3	ACT	A	641	-	3,3,3	1.38	1 (33%)	3,3,3	1.36	0
2	GOL	A	616	-	5,5,5	1.01	0	5,5,5	0.97	0
3	ACT	A	608	-	3,3,3	1.32	0	3,3,3	1.40	0
2	GOL	A	632	-	5,5,5	0.89	0	5,5,5	0.98	0
2	GOL	A	627	-	5,5,5	1.08	1 (20%)	5,5,5	0.95	0
2	GOL	A	652	-	5,5,5	0.80	0	5,5,5	1.07	0
3	ACT	A	646	-	3,3,3	1.47	1 (33%)	3,3,3	1.39	0
2	GOL	A	606	-	5,5,5	0.77	0	5,5,5	1.22	1 (20%)
2	GOL	A	619	-	5,5,5	0.91	0	5,5,5	0.96	0
3	ACT	A	642	-	3,3,3	1.26	0	3,3,3	1.40	0
4	PO4	A	613	-	4,4,4	0.81	0	6,6,6	0.54	0
2	GOL	A	624	-	5,5,5	0.89	0	5,5,5	0.89	0
2	GOL	A	648	-	5,5,5	0.72	0	5,5,5	1.10	0
2	GOL	A	615	-	5,5,5	0.92	0	5,5,5	0.98	0
2	GOL	A	621	-	5,5,5	0.88	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	647	-	5,5,5	0.96	0	5,5,5	1.09	0
2	GOL	A	618	-	5,5,5	0.83	0	5,5,5	1.03	0
3	ACT	A	639	-	3,3,3	1.31	0	3,3,3	1.38	0
2	GOL	A	611	-	5,5,5	1.28	1 (20%)	5,5,5	1.03	0
3	ACT	A	640	-	3,3,3	1.32	0	3,3,3	1.40	0
3	ACT	A	634	-	3,3,3	1.02	0	3,3,3	1.53	1 (33%)
2	GOL	A	650	-	5,5,5	0.88	0	5,5,5	0.82	0
3	ACT	A	645	-	3,3,3	1.42	1 (33%)	3,3,3	1.31	0
2	GOL	A	612	-	5,5,5	0.82	0	5,5,5	1.11	0
3	ACT	A	655	-	3,3,3	1.36	0	3,3,3	1.37	0
2	GOL	A	653	-	5,5,5	0.96	0	5,5,5	0.96	0
2	GOL	A	628	-	5,5,5	0.76	0	5,5,5	1.04	0
3	ACT	A	604	-	3,3,3	1.07	0	3,3,3	1.44	0
3	ACT	A	644	-	3,3,3	1.35	1 (33%)	3,3,3	1.37	0
2	GOL	A	603	-	5,5,5	0.80	0	5,5,5	1.03	0
2	GOL	A	631	-	5,5,5	0.94	0	5,5,5	1.09	0
2	GOL	A	630	-	5,5,5	0.89	0	5,5,5	1.06	0
4	PO4	A	622	-	4,4,4	0.88	0	6,6,6	0.51	0
2	GOL	A	614	-	5,5,5	0.75	0	5,5,5	0.94	0
3	ACT	A	637	-	3,3,3	1.36	1 (33%)	3,3,3	1.32	0
2	GOL	A	601	-	5,5,5	1.20	1 (20%)	5,5,5	0.87	0
2	GOL	A	607	-	5,5,5	0.90	0	5,5,5	1.18	0
2	GOL	A	629	-	5,5,5	0.87	0	5,5,5	0.94	0
2	GOL	A	651	-	5,5,5	0.88	0	5,5,5	1.12	1 (20%)
2	GOL	A	605	-	5,5,5	1.08	0	5,5,5	0.87	0
3	ACT	A	636	-	3,3,3	1.36	0	3,3,3	1.41	0
2	GOL	A	633	-	5,5,5	0.89	0	5,5,5	0.73	0
2	GOL	A	602	-	5,5,5	1.06	0	5,5,5	0.89	0
2	GOL	A	623	-	5,5,5	0.95	0	5,5,5	0.89	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	625	-	-	2/4/4/4	-
2	GOL	A	620	-	-	2/4/4/4	-
2	GOL	A	610	-	-	0/4/4/4	-
2	GOL	A	626	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	649	-	-	0/4/4/4	-
2	GOL	A	654	-	-	0/4/4/4	-
2	GOL	A	616	-	-	1/4/4/4	-
2	GOL	A	632	-	-	0/4/4/4	-
2	GOL	A	627	-	-	3/4/4/4	-
2	GOL	A	652	-	-	0/4/4/4	-
2	GOL	A	606	-	-	0/4/4/4	-
2	GOL	A	619	-	-	2/4/4/4	-
2	GOL	A	624	-	-	4/4/4/4	-
2	GOL	A	648	-	-	2/4/4/4	-
2	GOL	A	615	-	-	1/4/4/4	-
2	GOL	A	621	-	-	2/4/4/4	-
2	GOL	A	647	-	-	2/4/4/4	-
2	GOL	A	618	-	-	2/4/4/4	-
2	GOL	A	611	-	-	3/4/4/4	-
2	GOL	A	650	-	-	0/4/4/4	-
2	GOL	A	612	-	-	2/4/4/4	-
2	GOL	A	653	-	-	4/4/4/4	-
2	GOL	A	628	-	-	2/4/4/4	-
2	GOL	A	603	-	-	0/4/4/4	-
2	GOL	A	631	-	-	4/4/4/4	-
2	GOL	A	630	-	-	4/4/4/4	-
2	GOL	A	614	-	-	1/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	A	607	-	-	2/4/4/4	-
2	GOL	A	629	-	-	2/4/4/4	-
2	GOL	A	651	-	-	0/4/4/4	-
2	GOL	A	605	-	-	3/4/4/4	-
2	GOL	A	633	-	-	4/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	A	623	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	646	ACT	CH3-C	2.20	1.58	1.49
2	A	601	GOL	O2-C2	-2.19	1.36	1.43
2	A	627	GOL	O2-C2	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	611	GOL	C1-C2	2.03	1.60	1.51
3	A	644	ACT	CH3-C	2.03	1.57	1.49
3	A	637	ACT	CH3-C	2.02	1.57	1.49
3	A	641	ACT	CH3-C	2.02	1.57	1.49
3	A	645	ACT	CH3-C	2.01	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	606	GOL	C3-C2-C1	-2.33	102.65	111.70
2	A	651	GOL	C3-C2-C1	-2.10	103.53	111.70
3	A	634	ACT	OXT-C-O	2.08	129.72	122.05

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	605	GOL	C1-C2-C3-O3
2	A	607	GOL	O1-C1-C2-C3
2	A	612	GOL	O1-C1-C2-C3
2	A	619	GOL	C1-C2-C3-O3
2	A	621	GOL	O2-C2-C3-O3
2	A	623	GOL	O1-C1-C2-C3
2	A	623	GOL	C1-C2-C3-O3
2	A	625	GOL	C1-C2-C3-O3
2	A	626	GOL	C1-C2-C3-O3
2	A	626	GOL	O2-C2-C3-O3
2	A	630	GOL	C1-C2-C3-O3
2	A	633	GOL	O1-C1-C2-C3
2	A	633	GOL	C1-C2-C3-O3
2	A	633	GOL	O2-C2-C3-O3
2	A	647	GOL	C1-C2-C3-O3
2	A	648	GOL	C1-C2-C3-O3
2	A	653	GOL	C1-C2-C3-O3
2	A	605	GOL	O2-C2-C3-O3
2	A	607	GOL	O1-C1-C2-O2
2	A	624	GOL	O2-C2-C3-O3
2	A	630	GOL	O2-C2-C3-O3
2	A	631	GOL	O2-C2-C3-O3
2	A	653	GOL	O2-C2-C3-O3
2	A	611	GOL	O1-C1-C2-C3
2	A	616	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	618	GOL	O1-C1-C2-C3
2	A	620	GOL	C1-C2-C3-O3
2	A	621	GOL	C1-C2-C3-O3
2	A	624	GOL	O1-C1-C2-C3
2	A	624	GOL	C1-C2-C3-O3
2	A	627	GOL	O1-C1-C2-C3
2	A	628	GOL	C1-C2-C3-O3
2	A	629	GOL	C1-C2-C3-O3
2	A	630	GOL	O1-C1-C2-C3
2	A	631	GOL	O1-C1-C2-C3
2	A	631	GOL	C1-C2-C3-O3
2	A	612	GOL	O1-C1-C2-O2
2	A	618	GOL	O1-C1-C2-O2
2	A	619	GOL	O2-C2-C3-O3
2	A	623	GOL	O2-C2-C3-O3
2	A	624	GOL	O1-C1-C2-O2
2	A	625	GOL	O2-C2-C3-O3
2	A	633	GOL	O1-C1-C2-O2
2	A	647	GOL	O2-C2-C3-O3
2	A	648	GOL	O2-C2-C3-O3
2	A	623	GOL	O1-C1-C2-O2
2	A	630	GOL	O1-C1-C2-O2
2	A	627	GOL	O1-C1-C2-O2
2	A	631	GOL	O1-C1-C2-O2
2	A	653	GOL	O1-C1-C2-O2
2	A	653	GOL	O1-C1-C2-C3
2	A	611	GOL	O1-C1-C2-O2
2	A	615	GOL	O2-C2-C3-O3
2	A	629	GOL	O2-C2-C3-O3
2	A	614	GOL	O1-C1-C2-O2
2	A	628	GOL	O1-C1-C2-C3
2	A	620	GOL	O2-C2-C3-O3
2	A	605	GOL	O1-C1-C2-C3
2	A	627	GOL	C1-C2-C3-O3
2	A	611	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	625	GOL	1	0
3	A	635	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	610	GOL	1	0
3	A	643	ACT	1	0
2	A	626	GOL	1	0
2	A	632	GOL	1	0
2	A	619	GOL	2	0
2	A	618	GOL	1	0
3	A	639	ACT	1	0
2	A	612	GOL	2	0
2	A	628	GOL	1	0
2	A	614	GOL	1	0
2	A	601	GOL	1	0
2	A	605	GOL	1	0
2	A	623	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	497/511 (97%)	-0.51	10 (2%) 64 68	7, 19, 30, 43	47 (9%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301[A]	GLY	3.3
1	A	2	SER	3.2
1	A	148[A]	ALA	3.1
1	A	450[A]	ILE	2.7
1	A	302[A]	GLY	2.7
1	A	149[A]	ALA	2.5
1	A	498	LEU	2.4
1	A	452	THR	2.4
1	A	497	ARG	2.0
1	A	316[A]	ASP	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 monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	ACT	A	655	4/4	0.58	0.26	52,54,56,57	4
2	GOL	A	630	6/6	0.65	0.28	27,32,39,48	6
3	ACT	A	638	4/4	0.73	0.17	56,65,66,66	0
3	ACT	A	643	4/4	0.75	0.22	41,46,49,55	4
3	ACT	A	639	4/4	0.75	0.33	30,32,37,44	4
3	ACT	A	646	4/4	0.76	0.29	29,37,41,44	4
3	ACT	A	635	4/4	0.77	0.20	41,46,48,55	4
2	GOL	A	652	6/6	0.77	0.22	32,33,40,47	6
2	GOL	A	647	6/6	0.78	0.26	32,44,55,55	6
2	GOL	A	619	6/6	0.78	0.24	35,44,47,50	6
2	GOL	A	648	6/6	0.79	0.21	33,48,56,58	0
2	GOL	A	624	6/6	0.79	0.21	38,41,49,54	6
4	PO4	A	622	5/5	0.79	0.17	42,47,54,61	5
3	ACT	A	637	4/4	0.80	0.25	39,40,44,45	4
2	GOL	A	625	6/6	0.81	0.15	43,50,61,63	0
2	GOL	A	632	6/6	0.81	0.21	30,34,43,43	6
2	GOL	A	626	6/6	0.81	0.20	27,41,45,45	6
3	ACT	A	641	4/4	0.81	0.21	49,50,50,52	4
2	GOL	A	650	6/6	0.82	0.18	41,47,51,55	0
4	PO4	A	613	5/5	0.83	0.13	35,48,62,66	5
2	GOL	A	653	6/6	0.83	0.18	30,35,39,46	6
2	GOL	A	628	6/6	0.84	0.19	39,43,47,48	6
2	GOL	A	627	6/6	0.84	0.18	36,38,41,46	6
2	GOL	A	629	6/6	0.85	0.19	32,37,43,45	6
3	ACT	A	642	4/4	0.85	0.18	48,49,50,54	4
3	ACT	A	640	4/4	0.85	0.18	28,36,39,41	4
3	ACT	A	644	4/4	0.85	0.22	31,41,46,48	4
2	GOL	A	623	6/6	0.86	0.20	31,49,51,54	6
4	PO4	A	609	5/5	0.86	0.14	25,31,46,50	5
2	GOL	A	606	6/6	0.86	0.14	32,33,37,51	6
2	GOL	A	651	6/6	0.86	0.18	19,37,40,45	6
2	GOL	A	615	6/6	0.87	0.19	24,40,47,51	6
2	GOL	A	620	6/6	0.87	0.16	31,35,37,42	6
2	GOL	A	621	6/6	0.87	0.20	20,36,43,43	6
2	GOL	A	631	6/6	0.87	0.17	31,39,44,47	6
2	GOL	A	618	6/6	0.87	0.14	24,33,38,47	6
2	GOL	A	610	6/6	0.88	0.15	23,33,36,44	6
2	GOL	A	654	6/6	0.88	0.14	29,36,48,54	6
2	GOL	A	616	6/6	0.88	0.18	26,41,47,49	6
2	GOL	A	649	6/6	0.88	0.15	27,29,33,34	6
2	GOL	A	633	6/6	0.89	0.15	27,37,42,61	6
3	ACT	A	636	4/4	0.89	0.17	43,44,44,46	4
2	GOL	A	611	6/6	0.89	0.15	19,22,35,47	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	614	6/6	0.89	0.14	26,36,40,41	6
3	ACT	A	634	4/4	0.89	0.17	35,36,46,46	4
3	ACT	A	645	4/4	0.90	0.15	24,35,39,48	4
4	PO4	A	617	5/5	0.90	0.14	22,35,42,54	5
2	GOL	A	612	6/6	0.90	0.13	32,34,37,42	6
2	GOL	A	607	6/6	0.91	0.15	23,35,40,59	0
2	GOL	A	605	6/6	0.91	0.15	17,30,34,41	6
2	GOL	A	601	6/6	0.92	0.15	19,30,34,41	6
2	GOL	A	602	6/6	0.92	0.12	19,29,32,36	0
3	ACT	A	608	4/4	0.92	0.14	35,43,49,50	0
2	GOL	A	603	6/6	0.93	0.10	29,34,36,43	0
3	ACT	A	604	4/4	0.97	0.06	20,25,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.