



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:18 pm GMT

PDB ID : 4QWP
Title : co-crystal structure of chitosanase OU01 with substrate
Authors : Lyu, Q.; Liu, W.; Han, B.
Deposited on : 2014-07-17
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

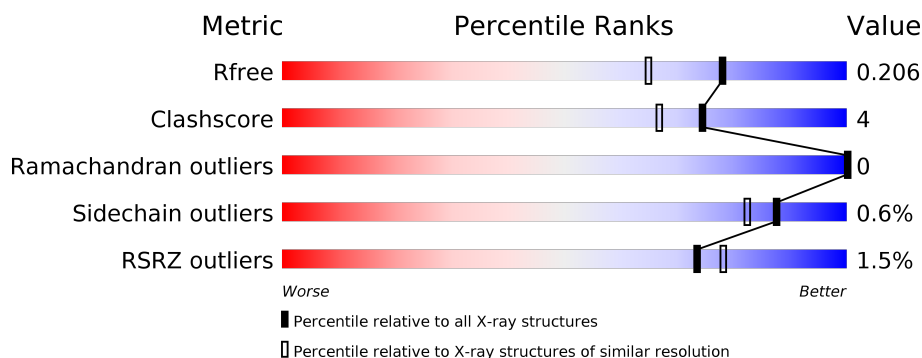
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	248	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 93%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 93% • • </div> </div>
1	B	248	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 88%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 2% 88% 7% • • </div> </div>

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
2	GCS	B	307	X	-	-	-
3	ACT	A	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4182 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.

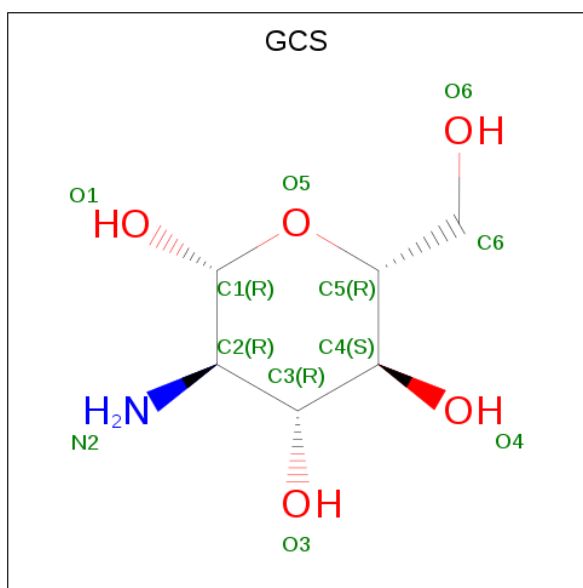
- Molecule 1 is a protein called Chitosanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	0
			1813	1126	307	376	4			
1	B	237	Total	C	N	O	S	0	9	0
			1874	1159	324	388	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q8KZM5
A	-6	PRO	-	EXPRESSION TAG	UNP Q8KZM5
A	-5	LEU	-	EXPRESSION TAG	UNP Q8KZM5
A	-4	GLY	-	EXPRESSION TAG	UNP Q8KZM5
A	-3	SER	-	EXPRESSION TAG	UNP Q8KZM5
A	-2	PRO	-	EXPRESSION TAG	UNP Q8KZM5
A	-1	GLU	-	EXPRESSION TAG	UNP Q8KZM5
A	0	PHE	-	EXPRESSION TAG	UNP Q8KZM5
A	2	THR	ALA	SEE REMARK 999	UNP Q8KZM5
A	43	ALA	ASP	SEE REMARK 999	UNP Q8KZM5
A	145	ALA	VAL	SEE REMARK 999	UNP Q8KZM5
A	237	TYR	PHE	SEE REMARK 999	UNP Q8KZM5
B	-7	GLY	-	EXPRESSION TAG	UNP Q8KZM5
B	-6	PRO	-	EXPRESSION TAG	UNP Q8KZM5
B	-5	LEU	-	EXPRESSION TAG	UNP Q8KZM5
B	-4	GLY	-	EXPRESSION TAG	UNP Q8KZM5
B	-3	SER	-	EXPRESSION TAG	UNP Q8KZM5
B	-2	PRO	-	EXPRESSION TAG	UNP Q8KZM5
B	-1	GLU	-	EXPRESSION TAG	UNP Q8KZM5
B	0	PHE	-	EXPRESSION TAG	UNP Q8KZM5
B	2	THR	ALA	SEE REMARK 999	UNP Q8KZM5
B	43	ALA	ASP	SEE REMARK 999	UNP Q8KZM5
B	145	ALA	VAL	SEE REMARK 999	UNP Q8KZM5
B	237	TYR	PHE	SEE REMARK 999	UNP Q8KZM5

- Molecule 2 is D-GLUCOSAMINE (three-letter code: GCS) (formula: $C_6H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	1	5		
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	A	1	Total	C	N	O	0	0
			12	6	1	5		
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			12	6	1	5		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			12	6	1	5		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

- 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	0	0
			3	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

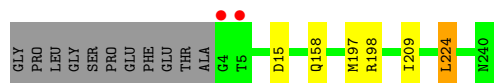
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total 176	O 176	0	0
5	B	187	Total 187	O 187	0	0

3 Residue-property plots [i](#)

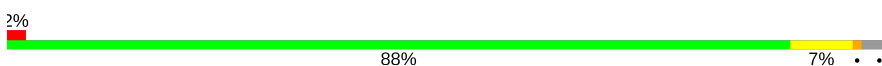
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Chitosanase

Chain A:  93%



● Molecule 1: Chitosanase

Chain B:  88%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.23Å 40.88Å 105.31Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 33.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-1.70) 96.9 (33.60-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.18 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.166 , 0.204 0.167 , 0.206	Depositor DCC
R_{free} test set	2765 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4182	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: GOL, GCS, 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	0.98	0/1853	0.98	3/2518 (0.1%)
1	B	1.02	1/1914 (0.1%)	1.02	5/2597 (0.2%)
All	All	1.00	1/3767 (0.0%)	1.00	8/5115 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	TYR	CE1-CZ	5.68	1.46	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	191	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	198	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	224	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	123[A]	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	B	123[B]	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	15	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	223	ASP	CB-CG-OD1	5.13	122.92	118.30

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	1813	0	1668	2	0
1	B	1874	0	1725	19	0
2	A	57	0	56	0	0
2	B	66	0	61	3	0
3	A	3	0	0	3	0
4	B	6	0	8	0	0
5	A	176	0	0	1	0
5	B	187	0	0	3	0
All	All	4182	0	3518	26	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 4.

All (26) 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:7:ASP:OD2	1:B:134[B]:LYS:HE2	1.68	0.94
1:B:7:ASP:CG	1:B:134[B]:LYS:HE2	1.90	0.92
3:A:306:ACT:O	3:A:306:ACT:CH3	2.33	0.77
3:A:306:ACT:OXT	3:A:306:ACT:CH3	2.40	0.69
1:B:64:LEU:HB2	1:B:120[A]:GLU:OE1	1.94	0.68
1:B:123[A]:ARG:HG2	1:B:123[A]:ARG:NH1	2.09	0.66
1:B:120[B]:GLU:HG2	5:B:424:HOH:O	1.96	0.65
1:B:7:ASP:OD2	1:B:134[A]:LYS:NZ	2.32	0.61
1:B:130:VAL:CG1	1:B:134[B]:LYS:HE3	2.32	0.59
1:B:7:ASP:OD2	1:B:134[B]:LYS:CE	2.48	0.57
1:B:66:ARG:NH2	1:B:85:GLU:OE2	2.33	0.57
1:B:123[A]:ARG:HH11	1:B:123[A]:ARG:HG2	1.70	0.57
3:A:306:ACT:OXT	3:A:306:ACT:O	2.23	0.56
1:A:197[B]:MET:SD	1:A:209:ILE:CD1	2.94	0.56
2:B:302:GCS:O4	2:B:307:GCS:C1	2.56	0.54
1:B:45:ARG:CZ	2:B:307:GCS:C6	2.85	0.54
1:B:123[A]:ARG:CG	1:B:123[A]:ARG:HH11	2.20	0.54
1:B:201:PRO:HD3	5:B:544:HOH:O	2.08	0.53
2:B:303:GCS:HN21	2:B:304:GCS:H62	1.75	0.51
1:A:158:GLN:HG3	5:A:521:HOH:O	2.14	0.48
1:B:123[A]:ARG:CG	1:B:123[A]:ARG:NH1	2.74	0.47
1:B:152:VAL:HG21	1:B:193:ARG:NH2	2.30	0.46
1:B:130:VAL:HG12	1:B:134[B]:LYS:HE3	1.99	0.45
1:B:194:ASN:O	1:B:198:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:NE	5:B:493:HOH:O	2.43	0.41
1:B:63:GLU:CD	1:B:123[B]:ARG:HH22	2.25	0.41

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	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
1	B	244/248 (98%)	240 (98%)	4 (2%)	0	100	100
All	All	481/496 (97%)	473 (98%)	8 (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	182/188 (97%)	181 (100%)	1 (0%)	90	85
1	B	189/188 (100%)	188 (100%)	1 (0%)	90	85
All	All	371/376 (99%)	369 (100%)	2 (0%)	87	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	B	198	ARG

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	GCS	A	301	2	12,12,12	0.93	0	16,17,17	1.05	1 (6%)
2	GCS	A	302	2	11,11,12	1.03	1 (9%)	13,15,17	1.48	2 (15%)
2	GCS	A	303	2	12,12,12	1.01	1 (8%)	16,17,17	1.29	3 (18%)
2	GCS	A	304	2	11,11,12	1.51	3 (27%)	13,15,17	1.21	2 (15%)
2	GCS	A	305	2	11,11,12	1.01	1 (9%)	13,15,17	2.14	3 (23%)
3	ACT	A	306	-	0,0,3	0.00	-	0,0,3	0.00	-
4	GOL	B	301	-	5,5,5	0.58	0	5,5,5	1.17	0
2	GCS	B	302	2	12,12,12	1.13	1 (8%)	16,17,17	1.38	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GCS	B	303	2	11,11,12	1.41	2 (18%)	13,15,17	1.39	2 (15%)
2	GCS	B	304	2	11,11,12	0.94	1 (9%)	13,15,17	1.41	3 (23%)
2	GCS	B	305	2	12,12,12	0.95	1 (8%)	16,17,17	1.94	2 (12%)
2	GCS	B	306	2	11,11,12	1.04	1 (9%)	13,15,17	1.18	1 (7%)
2	GCS	B	307	2	9,9,12	1.54	2 (22%)	10,12,17	2.28	2 (20%)

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	GCS	A	301	2	-	0/2/22/22	0/1/1/1
2	GCS	A	302	2	-	0/2/18/22	0/1/1/1
2	GCS	A	303	2	-	0/2/22/22	0/1/1/1
2	GCS	A	304	2	-	0/2/18/22	0/1/1/1
2	GCS	A	305	2	-	0/2/18/22	0/1/1/1
3	ACT	A	306	-	-	0/0/0/0	0/0/0/0
4	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GCS	B	302	2	-	0/2/22/22	0/1/1/1
2	GCS	B	303	2	-	0/2/18/22	0/1/1/1
2	GCS	B	304	2	-	0/2/18/22	0/1/1/1
2	GCS	B	305	2	-	0/2/22/22	0/1/1/1
2	GCS	B	306	2	-	0/2/18/22	0/1/1/1
2	GCS	B	307	2	1/1/3/5	0/0/13/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	306	GCS	O5-C5	-2.65	1.39	1.44
2	A	303	GCS	O5-C5	-2.41	1.38	1.44
2	A	305	GCS	C2-N2	-2.40	1.43	1.47
2	B	307	GCS	O5-C1	-2.16	1.40	1.43
2	A	304	GCS	C1-C2	-2.15	1.50	1.52
2	B	307	GCS	C2-N2	-2.12	1.39	1.47
2	A	304	GCS	C2-N2	2.07	1.50	1.47
2	B	304	GCS	C1-C2	2.11	1.55	1.52
2	A	304	GCS	C6-C5	2.14	1.56	1.50
2	B	303	GCS	C6-C5	2.15	1.56	1.50
2	B	305	GCS	C2-N2	2.23	1.50	1.47
2	A	302	GCS	C1-C2	2.36	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	GCS	C2-N2	2.51	1.51	1.47
2	B	302	GCS	C3-C2	2.52	1.56	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	GCS	C1-C2-C3	-6.06	102.62	110.60
2	A	302	GCS	C1-O5-C5	-3.47	107.08	113.69
2	B	305	GCS	C4-C3-C2	-3.39	105.08	111.03
2	B	307	GCS	C1-O5-C5	-3.34	106.83	111.63
2	B	304	GCS	O5-C1-C2	-2.93	106.09	109.51
2	B	302	GCS	C1-C2-C3	-2.52	107.29	110.60
2	A	302	GCS	O1-C1-O5	-2.46	103.03	110.44
2	B	304	GCS	C1-C2-C3	-2.46	107.37	110.60
2	B	302	GCS	O1-C1-O5	-2.43	103.12	110.44
2	A	304	GCS	O6-C6-C5	-2.35	105.32	111.74
2	A	303	GCS	C1-C2-C3	-2.20	107.70	110.60
2	B	304	GCS	O6-C6-C5	-2.17	105.81	111.74
2	A	305	GCS	C3-C2-N2	-2.14	106.70	111.11
2	B	302	GCS	O3-C3-C2	-2.11	106.42	110.22
2	B	303	GCS	O6-C6-C5	-2.11	105.98	111.74
2	A	301	GCS	C4-C3-C2	-2.02	107.49	111.03
2	A	303	GCS	C4-C3-C2	-2.01	107.50	111.03
2	B	306	GCS	O5-C5-C6	2.07	110.30	106.88
2	A	304	GCS	O5-C1-C2	2.35	112.25	109.51
2	A	303	GCS	C6-C5-C4	2.44	118.76	112.99
2	B	303	GCS	O5-C1-C2	2.73	112.69	109.51
2	A	305	GCS	O5-C5-C4	3.85	116.25	109.97
2	A	305	GCS	C1-O5-C5	5.01	123.23	113.69
2	B	307	GCS	C4-C3-C2	5.28	119.10	111.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	307	GCS	C4

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	ACT	3	0
2	B	302	GCS	1	0
2	B	303	GCS	1	0
2	B	304	GCS	1	0
2	B	307	GCS	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	237/248 (95%)	-0.30	2 (0%) 86 88	9, 18, 33, 45	0
1	B	237/248 (95%)	-0.16	5 (2%) 63 68	7, 16, 32, 54	0
All	All	474/496 (95%)	-0.23	7 (1%) 73 78	7, 17, 33, 54	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	4.0
1	B	5	THR	2.4
1	B	201	PRO	2.2
1	A	5	THR	2.2
1	B	202	ALA	2.1
1	A	4	GLY	2.1
1	B	198	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 carbohydrates 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(\AA^2)	Q<0.9
2	GCS	B	307	9/12	0.67	0.31	32,42,51,52	0
2	GCS	B	305	12/12	0.78	0.23	30,41,52,54	0
3	ACT	A	306	3/4	0.79	0.14	43,43,44,48	0
4	GOL	B	301	6/6	0.85	0.13	28,34,35,36	0
2	GCS	B	306	11/12	0.86	0.14	21,25,31,33	0
2	GCS	A	305	11/12	0.88	0.13	30,36,43,50	0
2	GCS	B	304	11/12	0.92	0.10	16,21,29,41	0
2	GCS	A	304	11/12	0.94	0.07	19,21,23,24	0
2	GCS	A	301	12/12	0.95	0.08	20,25,35,46	0
2	GCS	B	302	12/12	0.96	0.10	13,16,19,22	0
2	GCS	A	302	11/12	0.96	0.06	16,17,20,20	0
2	GCS	B	303	11/12	0.96	0.07	14,16,17,18	0
2	GCS	A	303	12/12	0.97	0.10	16,18,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.