Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 04:33 PM JST

PDB ID	:	5ZXG
Title	:	Cyclic alpha-maltosyl-(1-->6)-maltose hydrolase from Arthrobacter globiformis, ligand-free form
Authors	:	Kohno, M.; Arakawa, T.; Mori, T.; Nishimoto, T.; Fushinobu, S.
Deposited on	:	2018-05-20
Resolution	:	2.40 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:

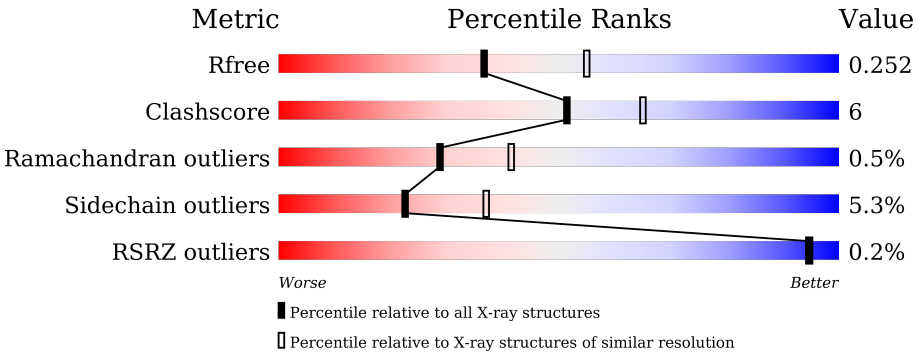
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	471	80% 11% • 7%
1	B	471	79% 12% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7103 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 Cyclic maltosyl-maltose hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3429	2173	598	647	11			
1	B	439	Total	C	N	O	S	0	0	0
			3417	2164	597	645	11			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP D2YYE1
A	-18	GLY	-	expression tag	UNP D2YYE1
A	-17	SER	-	expression tag	UNP D2YYE1
A	-16	SER	-	expression tag	UNP D2YYE1
A	-15	HIS	-	expression tag	UNP D2YYE1
A	-14	HIS	-	expression tag	UNP D2YYE1
A	-13	HIS	-	expression tag	UNP D2YYE1
A	-12	HIS	-	expression tag	UNP D2YYE1
A	-11	HIS	-	expression tag	UNP D2YYE1
A	-10	HIS	-	expression tag	UNP D2YYE1
A	-9	SER	-	expression tag	UNP D2YYE1
A	-8	SER	-	expression tag	UNP D2YYE1
A	-7	GLY	-	expression tag	UNP D2YYE1
A	-6	LEU	-	expression tag	UNP D2YYE1
A	-5	VAL	-	expression tag	UNP D2YYE1
A	-4	PRO	-	expression tag	UNP D2YYE1
A	-3	ARG	-	expression tag	UNP D2YYE1
A	-2	GLY	-	expression tag	UNP D2YYE1
A	-1	SER	-	expression tag	UNP D2YYE1
A	0	HIS	-	expression tag	UNP D2YYE1
A	1	MET	-	expression tag	UNP D2YYE1
A	2	VAL	-	expression tag	UNP D2YYE1
A	3	THR	-	expression tag	UNP D2YYE1
B	-19	MET	-	expression tag	UNP D2YYE1
B	-18	GLY	-	expression tag	UNP D2YYE1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP D2YYE1
B	-16	SER	-	expression tag	UNP D2YYE1
B	-15	HIS	-	expression tag	UNP D2YYE1
B	-14	HIS	-	expression tag	UNP D2YYE1
B	-13	HIS	-	expression tag	UNP D2YYE1
B	-12	HIS	-	expression tag	UNP D2YYE1
B	-11	HIS	-	expression tag	UNP D2YYE1
B	-10	HIS	-	expression tag	UNP D2YYE1
B	-9	SER	-	expression tag	UNP D2YYE1
B	-8	SER	-	expression tag	UNP D2YYE1
B	-7	GLY	-	expression tag	UNP D2YYE1
B	-6	LEU	-	expression tag	UNP D2YYE1
B	-5	VAL	-	expression tag	UNP D2YYE1
B	-4	PRO	-	expression tag	UNP D2YYE1
B	-3	ARG	-	expression tag	UNP D2YYE1
B	-2	GLY	-	expression tag	UNP D2YYE1
B	-1	SER	-	expression tag	UNP D2YYE1
B	0	HIS	-	expression tag	UNP D2YYE1
B	1	MET	-	expression tag	UNP D2YYE1
B	2	VAL	-	expression tag	UNP D2YYE1
B	3	THR	-	expression tag	UNP D2YYE1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is water.

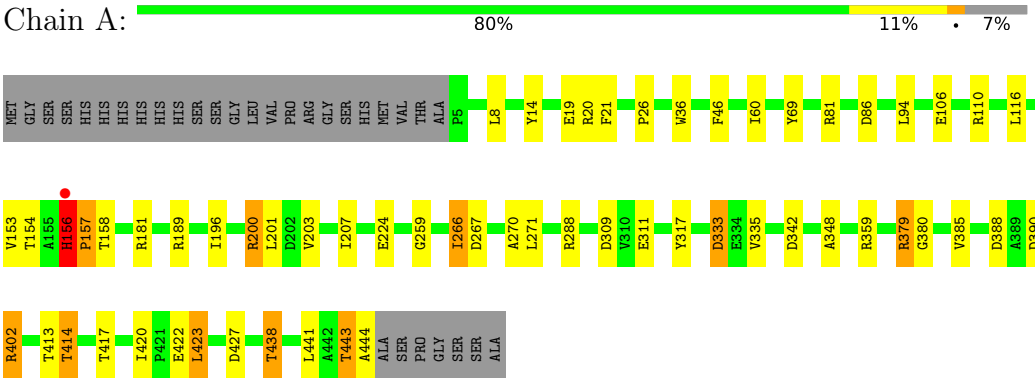
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	173	Total O 173 173	0	0
3	B	83	Total O 83 83	0	0

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.

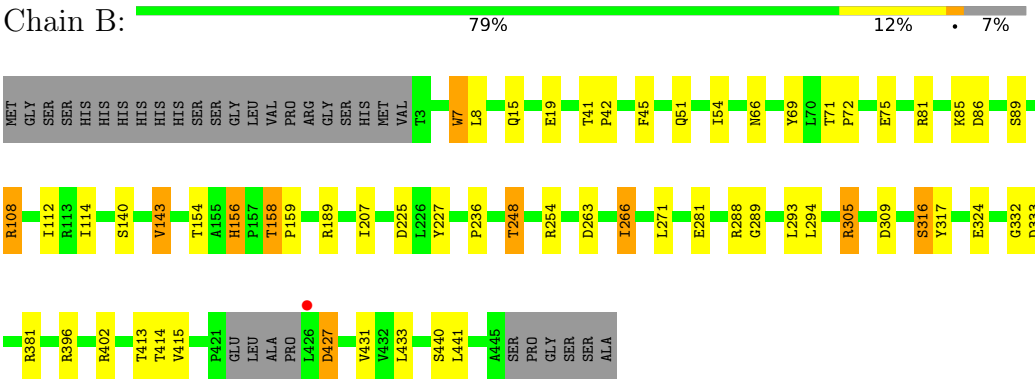
• Molecule 1: Cyclic maltosyl-maltose hydrolase

Chain A:



• Molecule 1: Cyclic maltosyl-maltose hydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.25Å 179.80Å 63.41Å 90.00° 113.61° 90.00°	Depositor
Resolution (Å)	89.90 – 2.40 19.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.5 (89.90-2.40) 91.7 (19.92-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.54 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.188 , 0.248 0.194 , 0.252	Depositor DCC
R_{free} test set	1836 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 10.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7103	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: CA

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	0.83	0/3528	0.94	12/4824 (0.2%)
1	B	0.89	0/3514	0.95	10/4804 (0.2%)
All	All	0.86	0/7042	0.95	22/9628 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	181	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	254	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	402	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	309	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	189	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	86	ASP	CB-CG-OD1	6.52	124.16	118.30
1	A	181	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	189	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	359	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	288	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	86	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	267	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	8	LEU	CA-CB-CG	-5.70	102.20	115.30
1	B	288	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	110	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	309	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	254	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	333	ASP	CB-CG-OD1	5.12	122.90	118.30
1	B	81	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	108	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	143	VAL	CB-CA-C	-5.00	101.89	111.40

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	3429	0	3230	41	0
1	B	3417	0	3216	35	0
2	A	1	0	0	0	0
3	A	173	0	0	3	0
3	B	83	0	0	1	0
All	All	7103	0	6446	74	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 6.

All (74) 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:156:HIS:HB2	1:A:157:PRO:CD	1.62	1.29
1:A:156:HIS:HB2	1:A:157:PRO:HD2	1.24	1.13
1:A:156:HIS:HB2	1:A:157:PRO:HD3	1.44	0.99
1:A:156:HIS:CB	1:A:157:PRO:CD	2.37	0.99
1:B:8:LEU:HD21	1:B:227:TYR:CE1	2.08	0.89
1:B:7:TRP:HZ3	1:B:225:ASP:O	1.57	0.86
1:A:156:HIS:CB	1:A:157:PRO:HD2	1.99	0.85
1:A:156:HIS:CB	1:A:157:PRO:HD3	2.17	0.67
1:A:385:VAL:HG21	1:A:422:GLU:HG3	1.77	0.66
1:A:81:ARG:HH21	1:A:94:LEU:HG	1.61	0.66
1:A:380:GLY:O	1:A:396:ARG:NH1	2.32	0.62
1:B:8:LEU:HD21	1:B:227:TYR:CD1	2.35	0.61
1:B:294:LEU:HD13	1:B:316:SER:HB3	1.82	0.60
1:A:427:ASP:HB2	1:B:427:ASP:HB2	1.82	0.60
1:B:381:ARG:O	1:B:396:ARG:HA	2.02	0.59
1:B:236:PRO:HB3	1:B:248:THR:HG21	1.85	0.58
1:A:154:THR:OG1	1:A:156:HIS:ND1	2.35	0.57
1:A:397:SER:HB3	1:A:402:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HH11	1:A:379:ARG:HG3	1.69	0.56
1:B:317:TYR:OH	1:B:333:ASP:HB3	2.07	0.55
1:B:54:ILE:HD13	1:B:103:LEU:HA	1.88	0.54
1:A:266:ILE:HG13	1:A:270:ALA:HB3	1.90	0.54
1:B:263:ASP:OD2	1:B:305:ARG:NH1	2.41	0.53
1:B:266:ILE:HD11	1:B:271:LEU:HB2	1.90	0.53
1:B:19:GLU:OE2	1:B:45:PHE:HA	2.09	0.52
1:B:305:ARG:NH2	3:B:502:HOH:O	2.41	0.52
1:A:116:LEU:HG	1:A:196:ILE:HD12	1.92	0.52
1:A:438:THR:CG2	3:A:644:HOH:O	2.58	0.52
1:B:140:SER:O	1:B:143:VAL:HG23	2.10	0.52
1:A:427:ASP:CB	1:B:427:ASP:HB2	2.41	0.51
1:B:7:TRP:CZ3	1:B:225:ASP:O	2.49	0.51
1:B:431:VAL:HG21	1:B:441:LEU:HD21	1.93	0.49
1:B:158:THR:HG23	1:B:159:PRO:HD2	1.95	0.49
1:A:438:THR:HG23	3:A:644:HOH:O	2.11	0.49
1:A:36:TRP:CE2	1:A:348:ALA:HB1	2.48	0.48
1:A:156:HIS:ND1	1:A:156:HIS:N	2.55	0.48
1:A:317:TYR:OH	1:A:333:ASP:HB3	2.13	0.48
1:A:420:ILE:HG21	1:A:423:LEU:HD22	1.94	0.48
1:A:266:ILE:HD11	1:A:271:LEU:CA	2.44	0.48
1:A:14:TYR:CE2	1:A:60:ILE:HD12	2.49	0.47
1:A:203:VAL:O	1:A:203:VAL:HG23	2.13	0.47
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.27	0.47
1:A:69:TYR:CZ	1:A:200:ARG:HD3	2.50	0.46
1:B:54:ILE:CD1	1:B:103:LEU:HA	2.45	0.46
1:A:266:ILE:HD11	1:A:271:LEU:HA	1.96	0.46
1:B:263:ASP:OD1	1:B:305:ARG:NH1	2.46	0.46
1:B:66:ASN:O	1:B:112:ILE:HA	2.16	0.46
1:B:15:GLN:HG3	1:B:69:TYR:CD2	2.51	0.45
1:B:41:THR:HB	1:B:42:PRO:CD	2.48	0.44
1:B:440:SER:C	1:B:441:LEU:HD12	2.38	0.44
1:A:21:PHE:CZ	1:A:60:ILE:HD11	2.53	0.44
1:A:413:THR:OG1	1:A:414:THR:N	2.50	0.44
1:B:154:THR:HB	1:B:156:HIS:O	2.17	0.44
1:A:402:ARG:HD3	1:A:422:GLU:O	2.18	0.43
1:B:8:LEU:HD23	1:B:289:GLY:HA2	1.99	0.43
1:B:7:TRP:CH2	1:B:227:TYR:HB2	2.53	0.43
1:A:137:GLU:HA	1:A:151:PHE:CE1	2.54	0.43
1:A:259:GLY:C	1:A:266:ILE:HG23	2.38	0.43
1:B:71:THR:HB	1:B:72:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:THR:OG1	1:B:414:THR:N	2.51	0.43
1:A:154:THR:HG1	1:A:156:HIS:CE1	2.30	0.43
1:B:332:GLY:HA3	1:B:337:LEU:HD12	2.00	0.43
1:A:20:ARG:NE	1:A:46:PHE:CD1	2.87	0.42
1:A:154:THR:OG1	1:A:156:HIS:CG	2.73	0.42
1:A:36:TRP:O	1:A:348:ALA:HB3	2.19	0.42
1:B:7:TRP:CD1	1:B:7:TRP:C	2.93	0.42
1:B:51:GLN:HA	1:B:54:ILE:HG13	2.02	0.41
1:A:14:TYR:CD2	1:A:60:ILE:HD12	2.56	0.41
1:A:26:PRO:HB3	3:A:728:HOH:O	2.21	0.41
1:B:8:LEU:CD2	1:B:227:TYR:CE1	2.94	0.41
1:A:388:ASP:HB3	1:A:390:ASP:H	1.86	0.41
1:B:75:GLU:HG3	1:B:85:LYS:HD3	2.02	0.40
1:A:443:THR:HG23	1:A:444:ALA:CB	2.51	0.40
1:B:107:CYS:SG	1:B:114:ILE:HD11	2.61	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	438/471 (93%)	419 (96%)	16 (4%)	3 (1%)	22	32
1	B	435/471 (92%)	420 (97%)	14 (3%)	1 (0%)	47	62
All	All	873/942 (93%)	839 (96%)	30 (3%)	4 (0%)	29	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	157	PRO
1	B	207	ILE

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Mol	Chain	Res	Type
1	A	207	ILE

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	348/372 (94%)	328 (94%)	20 (6%)	20	33
1	B	346/372 (93%)	329 (95%)	17 (5%)	25	40
All	All	694/744 (93%)	657 (95%)	37 (5%)	22	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	106	GLU
1	A	153	VAL
1	A	156	HIS
1	A	158	THR
1	A	201	LEU
1	A	224	GLU
1	A	266	ILE
1	A	311	GLU
1	A	335	VAL
1	A	342	ASP
1	A	379	ARG
1	A	397	SER
1	A	402	ARG
1	A	414	THR
1	A	417	THR
1	A	423	LEU
1	A	438	THR
1	A	441	LEU
1	A	443	THR
1	B	7	TRP
1	B	89	SER

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Mol	Chain	Res	Type
1	B	106	GLU
1	B	108	ARG
1	B	156	HIS
1	B	158	THR
1	B	248	THR
1	B	266	ILE
1	B	281	GLU
1	B	293	LEU
1	B	305	ARG
1	B	316	SER
1	B	324	GLU
1	B	359	ARG
1	B	415	VAL
1	B	427	ASP
1	B	433	LEU

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	440/471 (93%)	-0.57	1 (0%)	95	94	15, 25, 47, 89	0
1	B	439/471 (93%)	-0.56	1 (0%)	95	94	15, 25, 44, 91	0
All	All	879/942 (93%)	-0.57	2 (0%)	95	94	15, 25, 45, 91	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	HIS	5.1
1	B	426	LEU	2.2

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
2	CA	A	501	1/1	0.97	0.15	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.