Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:05 am BST

PDB ID	:	3A0O
Title	:	Crystal structure of alginate lyase from Agrobacterium tumefaciens C58
Authors	:	Ochiai, A.; Yamasaki, M.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on	:	2009-03-23
Resolution	:	2.11 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 ①) were used in the production of this report:

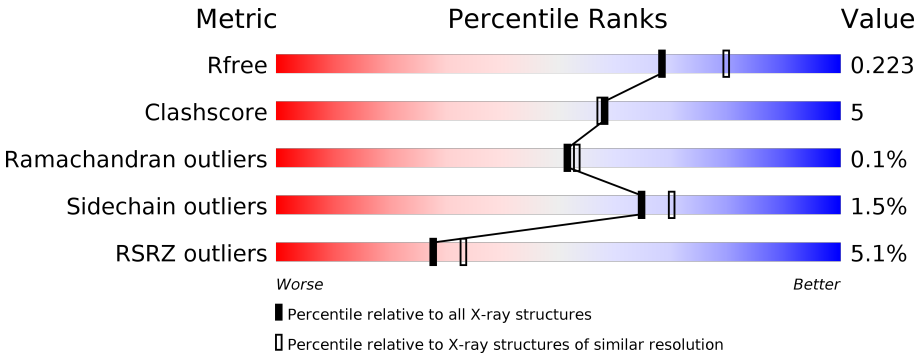
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 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	776	4% 89% 9%
1	B	776	6% 86% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13478 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 Oligo alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	764	Total	C	N	O	S	0	6	0
			6193	3948	1079	1152	14			
1	B	763	Total	C	N	O	S	0	9	0
			6216	3965	1083	1154	14			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

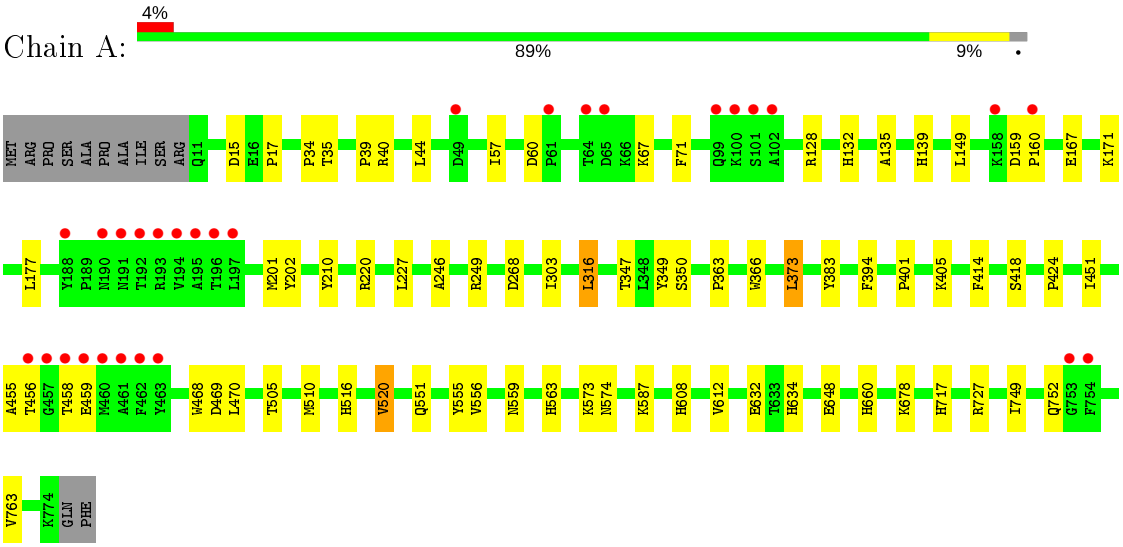
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	578	Total	O	0	0
			578	578		
3	B	489	Total	O	0	0
			489	489		

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.

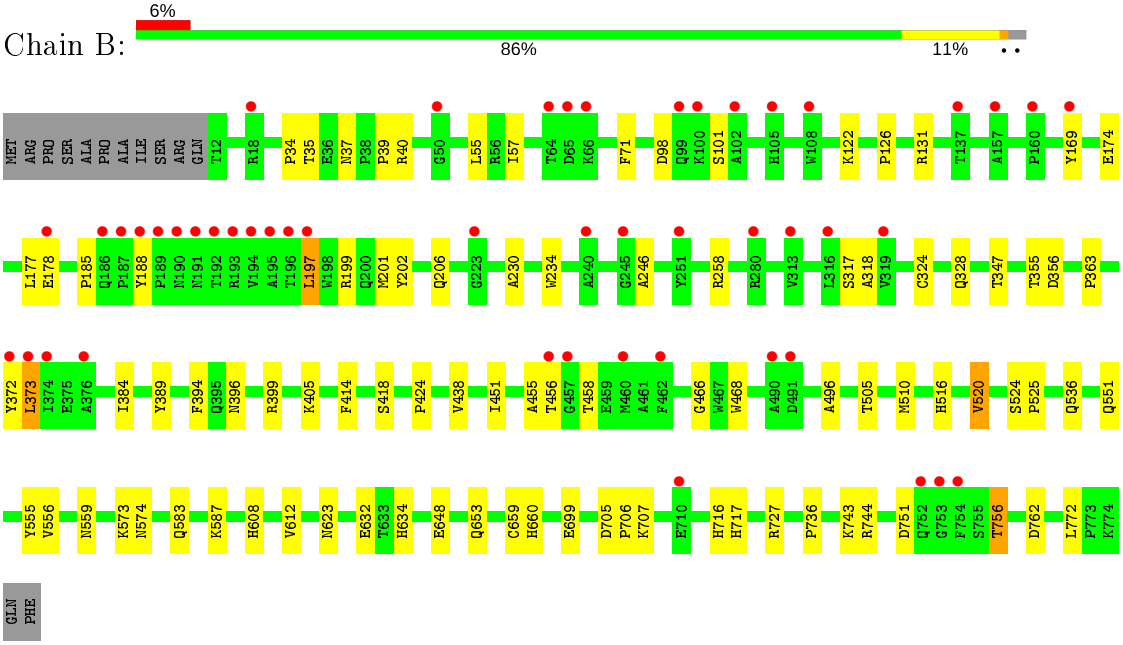
- Molecule 1: Oligo alginate lyase

Chain A:



- Molecule 1: Oligo alginate lyase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.15Å 68.24Å 108.89Å 78.32° 89.29° 88.56°	Depositor
Resolution (Å)	40.85 – 2.11 40.85 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.85-2.11) 96.4 (40.85-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.223 0.181 , 0.223	Depositor DCC
R_{free} test set	5044 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13478	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: CL

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	0.39	0/6386	0.53	0/8708
1	B	0.38	0/6410	0.52	0/8741
All	All	0.39	0/12796	0.52	0/17449

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	6193	0	5858	47	0
1	B	6216	0	5882	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	578	0	0	1	0
3	B	489	0	0	4	0
All	All	13478	0	11740	115	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 5.

All (115) 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:608:HIS:HE1	1:A:634:HIS:HD2	1.21	0.88
1:B:206:GLN:HG2	1:B:258:ARG:HE	1.41	0.84
1:A:559:ASN:H	1:A:563:HIS:HD2	1.25	0.82
1:B:608:HIS:HE1	1:B:634:HIS:HD2	1.28	0.81
1:B:536:GLN:H	1:B:583:GLN:HE22	1.34	0.76
1:A:608:HIS:CE1	1:A:634:HIS:HD2	2.05	0.75
1:B:608:HIS:CE1	1:B:634:HIS:HD2	2.05	0.74
1:A:559:ASN:H	1:A:563:HIS:CD2	2.06	0.73
1:B:455:ALA:O	1:B:458:THR:HG22	1.86	0.73
1:B:551:GLN:HE22	1:B:573:LYS:NZ	1.87	0.72
1:B:574:ASN:ND2	1:B:660:HIS:H	1.88	0.71
1:B:608:HIS:HE1	1:B:634:HIS:CD2	2.10	0.70
1:A:201:MET:HE1	1:A:246:ALA:O	1.91	0.70
1:A:608:HIS:HE1	1:A:634:HIS:CD2	2.07	0.70
1:B:206:GLN:HG2	1:B:258:ARG:NE	2.08	0.69
1:A:414:PHE:HE2	1:A:520:VAL:HG22	1.59	0.68
1:A:551:GLN:HE22	1:A:573:LYS:NZ	1.91	0.67
1:A:551:GLN:HE22	1:A:573:LYS:HZ1	1.40	0.67
1:A:574:ASN:ND2	1:A:660:HIS:H	1.94	0.66
1:B:414:PHE:HE2	1:B:520:VAL:HG22	1.60	0.65
1:B:612:VAL:HG22	1:B:632:GLU:HG2	1.78	0.65
1:A:17:PRO:HB3	1:B:744[B]:ARG:HG3	1.80	0.64
1:B:174:GLU:HA	1:B:177:LEU:HD12	1.79	0.64
1:B:717:HIS:HD2	3:B:2155:HOH:O	1.80	0.63
1:A:17:PRO:HG2	1:A:44:LEU:HB3	1.79	0.63
1:B:206:GLN:HG3	1:B:466:GLY:O	2.00	0.62
1:B:206:GLN:CG	1:B:258:ARG:HE	2.13	0.61
1:B:574:ASN:HD21	1:B:660:HIS:H	1.48	0.60
1:B:188:TYR:CD1	1:B:197:LEU:HD13	2.37	0.59
1:B:230:ALA:O	1:B:234:TRP:HD1	1.86	0.59
1:A:414:PHE:CE2	1:A:520:VAL:HG22	2.38	0.58
1:A:505:THR:HG22	1:A:520:VAL:HB	1.86	0.58
1:B:623:ASN:HD21	1:B:653:GLN:HE21	1.51	0.57
1:B:751:ASP:OD1	1:B:756:THR:HB	2.05	0.56
1:B:756:THR:HG23	1:B:772:LEU:HB2	1.88	0.56
1:A:40:ARG:HG3	1:A:347:THR:HA	1.87	0.56
1:B:98:ASP:OD2	1:B:101:SER:HB3	2.06	0.56
1:B:40:ARG:HG3	1:B:347:THR:HA	1.88	0.55
1:B:414:PHE:CE2	1:B:520:VAL:HG22	2.40	0.55
1:A:15:ASP:OD2	1:B:744[B]:ARG:NH1	2.40	0.55
1:B:648:GLU:HG2	1:B:727:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:CE	1:A:246:ALA:O	2.54	0.54
1:B:551:GLN:NE2	1:B:573:LYS:NZ	2.56	0.54
1:B:744[B]:ARG:HG2	3:B:2150:HOH:O	2.08	0.54
1:A:60:ASP:HB2	1:A:67:LYS:HD2	1.90	0.53
1:A:717:HIS:HD2	3:A:2086:HOH:O	1.90	0.53
1:A:648:GLU:HG2	1:A:727:ARG:HD3	1.91	0.53
1:A:373:LEU:HD22	1:A:394:PHE:CE1	2.44	0.53
1:A:574:ASN:HD21	1:A:660:HIS:H	1.56	0.52
1:B:131:ARG:HG2	1:B:384:ILE:HD12	1.90	0.52
1:B:35:THR:HG21	1:B:355:THR:HG21	1.91	0.52
1:A:612:VAL:HG22	1:A:632:GLU:HG2	1.92	0.52
1:B:551:GLN:HE22	1:B:573:LYS:HZ1	1.57	0.51
1:B:324:CYS:O	1:B:328:GLN:HG2	2.11	0.50
1:B:551:GLN:HE22	1:B:573:LYS:HZ2	1.57	0.50
1:A:167:GLU:HG2	1:A:171:LYS:HD2	1.94	0.49
1:A:455:ALA:O	1:A:458:THR:HG22	2.12	0.49
1:A:373:LEU:O	1:A:373:LEU:HG	2.13	0.49
1:A:135:ALA:HB1	1:A:383:TYR:CZ	2.47	0.49
1:B:505:THR:HG22	1:B:520:VAL:HB	1.94	0.49
1:A:424:PRO:HB2	1:A:451:ILE:HD12	1.94	0.48
1:B:201:MET:HE1	1:B:246:ALA:O	2.13	0.48
1:B:373:LEU:CD2	1:B:394:PHE:CE1	2.97	0.47
1:A:373:LEU:CD2	1:A:394:PHE:CE1	2.98	0.47
1:B:510:MET:HA	1:B:516:HIS:CD2	2.49	0.47
1:B:131:ARG:HG2	1:B:384:ILE:CD1	2.45	0.47
1:B:373:LEU:HD21	1:B:394:PHE:CE1	2.49	0.47
1:B:699:GLU:HG2	1:B:716:HIS:CD2	2.50	0.47
1:A:139:HIS:HD2	1:A:268:ASP:OD1	1.98	0.47
1:B:418:SER:HA	1:B:555:TYR:CG	2.50	0.46
1:A:418:SER:HA	1:A:555:TYR:CG	2.50	0.46
1:B:716:HIS:HD2	3:B:2101:HOH:O	1.98	0.46
1:B:126:PRO:O	1:B:131:ARG:HD3	2.15	0.46
1:A:128[B]:ARG:HE	1:A:132:HIS:HE1	1.63	0.46
1:B:389:TYR:HB3	1:B:438:VAL:HG11	1.97	0.45
1:A:303:ILE:HD11	1:A:316:LEU:HD13	1.99	0.45
1:B:399:ARG:NH2	1:B:496:ALA:HB1	2.32	0.45
1:B:424:PRO:HB2	1:B:451:ILE:HD12	1.99	0.45
1:A:177:LEU:HD21	1:A:227:LEU:CD2	2.47	0.45
1:A:366:TRP:CH2	1:A:401:PRO:HG3	2.53	0.44
1:B:57:ILE:HD12	1:B:71:PHE:HE1	1.83	0.44
1:B:736:PRO:O	1:B:743:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PRO:HB3	1:A:39:PRO:HB3	1.99	0.44
1:A:459:GLU:HG3	1:A:470:LEU:HD12	2.00	0.44
1:B:705:ASP:OD1	1:B:707:LYS:HE3	2.17	0.44
1:A:57:ILE:HD12	1:A:71:PHE:HE1	1.84	0.43
1:B:317:SER:HB3	1:B:372[B]:TYR:O	2.18	0.43
1:A:559:ASN:HD21	1:A:587:LYS:NZ	2.17	0.43
1:A:149:LEU:HD21	1:A:220:ARG:HB3	2.00	0.43
1:A:510:MET:HA	1:A:516:HIS:CD2	2.54	0.43
1:B:551:GLN:NE2	1:B:573:LYS:HZ2	2.16	0.43
1:B:37:ASN:O	1:B:122:LYS:HA	2.18	0.42
1:B:623:ASN:HD21	1:B:653:GLN:NE2	2.17	0.42
1:A:349:TYR:HA	1:A:350:SER:HA	1.82	0.42
1:B:373:LEU:O	1:B:373:LEU:HG	2.14	0.42
1:A:210:TYR:CE1	1:A:469:ASP:HB2	2.54	0.42
1:B:396:ASN:O	1:B:399:ARG:HG2	2.19	0.42
1:A:159:ASP:HA	1:A:160:PRO:HD2	1.92	0.42
1:B:169:TYR:CE1	1:B:174:GLU:HG3	2.55	0.42
1:B:363:PRO:HB2	1:B:405:LYS:HG3	2.01	0.42
1:A:363:PRO:HB2	1:A:405:LYS:HG3	2.02	0.41
1:B:185:PRO:HB3	1:B:201:MET:HG3	2.01	0.41
1:B:34:PRO:HB3	1:B:39:PRO:HB3	2.01	0.41
1:B:559:ASN:HD21	1:B:587:LYS:NZ	2.17	0.41
1:B:206:GLN:HG2	1:B:258:ARG:CD	2.51	0.41
1:B:705:ASP:HA	1:B:706:PRO:HD2	1.94	0.41
1:B:318:ALA:HB2	1:B:372[B]:TYR:HB3	2.02	0.41
1:B:199:ARG:HA	1:B:202:TYR:CE2	2.56	0.41
1:A:648:GLU:HG2	1:A:727:ARG:CD	2.51	0.41
1:B:559:ASN:HD22	1:B:559:ASN:HA	1.68	0.41
1:B:762:ASP:HB2	3:B:2105:HOH:O	2.21	0.41
1:B:524:SER:HA	1:B:525:PRO:HD3	1.93	0.40
1:B:356:ASP:HB3	1:B:399:ARG:HH11	1.86	0.40
1:A:749:ILE:N	1:A:749:ILE:HD12	2.37	0.40
1:B:574:ASN:HD22	1:B:659:CYS:HA	1.86	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	768/776 (99%)	742 (97%)	25 (3%)	1 (0%)	51 53
1	B	770/776 (99%)	746 (97%)	23 (3%)	1 (0%)	51 53
All	All	1538/1552 (99%)	1488 (97%)	48 (3%)	2 (0%)	51 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	VAL
1	B	556	VAL

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	643/647 (99%)	632 (98%)	11 (2%)	60 66
1	B	645/647 (100%)	637 (99%)	8 (1%)	71 77
All	All	1288/1294 (100%)	1269 (98%)	19 (2%)	65 70

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

Mol	Chain	Res	Type
1	A	35	THR
1	A	202	TYR
1	A	249	ARG
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	456	THR
1	A	468	TRP
1	A	520	VAL
1	A	678	LYS
1	A	752	GLN
1	A	763	VAL
1	B	55	LEU
1	B	178	GLU
1	B	197	LEU
1	B	373	LEU
1	B	456	THR
1	B	468	TRP
1	B	520	VAL
1	B	756	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	161	ASN
1	A	296	HIS
1	A	396	ASN
1	A	551	GLN
1	A	559	ASN
1	A	563	HIS
1	A	574	ASN
1	A	608	HIS
1	A	634	HIS
1	A	716	HIS
1	A	717	HIS
1	B	99	GLN
1	B	139	HIS
1	B	364	HIS
1	B	483	GLN
1	B	551	GLN
1	B	559	ASN
1	B	574	ASN
1	B	583	GLN
1	B	608	HIS
1	B	634	HIS
1	B	653	GLN

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Mol	Chain	Res	Type
1	B	716	HIS
1	B	717	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

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	764/776 (98%)	0.04	29 (3%)	40	46	12, 22, 40, 53	0
1	B	763/776 (98%)	0.30	49 (6%)	19	23	12, 26, 49, 72	0
All	All	1527/1552 (98%)	0.17	78 (5%)	28	33	12, 24, 46, 72	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	TYR	8.8
1	B	754	PHE	8.8
1	B	192	THR	8.4
1	B	190	ASN	6.7
1	A	457	GLY	6.6
1	A	754	PHE	6.4
1	A	191	ASN	6.3
1	B	191	ASN	5.5
1	B	462	PHE	5.4
1	A	190	ASN	5.3
1	A	192	THR	5.1
1	B	197	LEU	5.1
1	B	194	VAL	5.0
1	B	189	PRO	5.0
1	A	456	THR	5.0
1	B	196	THR	4.8
1	A	462	PHE	4.7
1	B	193	ARG	4.7
1	B	100	LYS	4.7
1	B	160	PRO	4.2
1	B	195	ALA	4.0
1	B	372[A]	TYR	4.0
1	B	187	PRO	3.9
1	B	186	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	102	ALA	3.8
1	B	753	GLY	3.7
1	B	457	GLY	3.4
1	B	178	GLU	3.4
1	A	460	MET	3.3
1	A	100	LYS	3.3
1	A	193	ARG	3.2
1	A	65	ASP	3.2
1	B	752	GLN	3.2
1	B	313	VAL	3.1
1	A	194	VAL	3.1
1	B	105	HIS	3.0
1	A	99	GLN	3.0
1	B	65	ASP	2.9
1	B	50	GLY	2.9
1	B	99	GLN	2.9
1	B	280	ARG	2.9
1	A	463	TYR	2.9
1	A	188	TYR	2.8
1	B	456	THR	2.8
1	A	461	ALA	2.8
1	B	376	ALA	2.8
1	B	102	ALA	2.8
1	B	251	TYR	2.8
1	B	245	GLY	2.7
1	A	195	ALA	2.5
1	A	101	SER	2.5
1	A	459	GLU	2.5
1	B	240	ALA	2.5
1	B	223	GLY	2.5
1	A	64	THR	2.4
1	B	373	LEU	2.4
1	B	491	ASP	2.4
1	A	196	THR	2.4
1	B	66	LYS	2.4
1	B	710	GLU	2.3
1	A	197	LEU	2.2
1	B	137	THR	2.2
1	B	316	LEU	2.2
1	B	490	ALA	2.2
1	B	18	ARG	2.2
1	B	374	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	169	TYR	2.2
1	A	753	GLY	2.2
1	B	460	MET	2.2
1	A	160	PRO	2.2
1	B	319	VAL	2.1
1	B	157	ALA	2.1
1	B	108	TRP	2.1
1	B	64	THR	2.0
1	A	61	PRO	2.0
1	A	458	THR	2.0
1	A	49	ASP	2.0
1	A	158	LYS	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, 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	CL	B	1001	1/1	0.99	0.09	20,20,20,20	0
2	CL	A	1001	1/1	0.99	0.07	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.