Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2022 – 04:05 AM EST

PDB ID	:	2FGZ
Title	:	Crystal Structure Analysis of apo pullulanase from Klebsiella pneumoniae
Authors	:	Mikami, B.; Iwamoto, H.; Katsuya, Y.; Yoon, H.-J.; Demirkan-Sarikaya, E.; Malle, D.
Deposited on	:	2005-12-23
Resolution	:	1.75 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

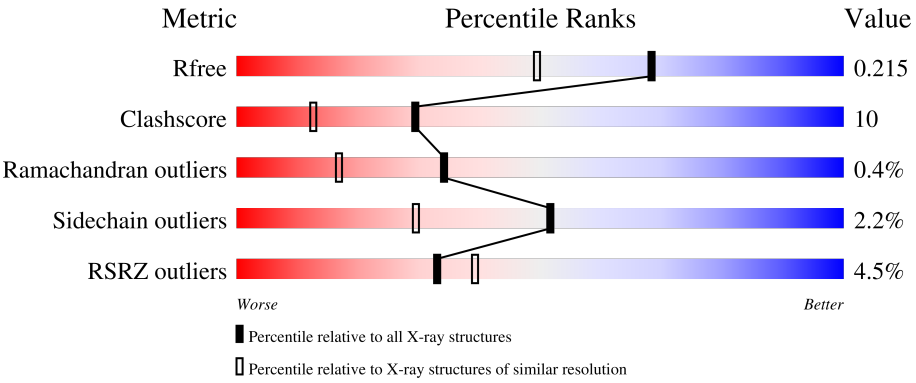
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	1083	4% 72% 13% · 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8383 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 Alpha-dextrin endo-1,6-alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	926	Total	C	N	O	S	0	13	0
			7168	4479	1226	1439	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	conflict	UNP W9BQ28

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is water.

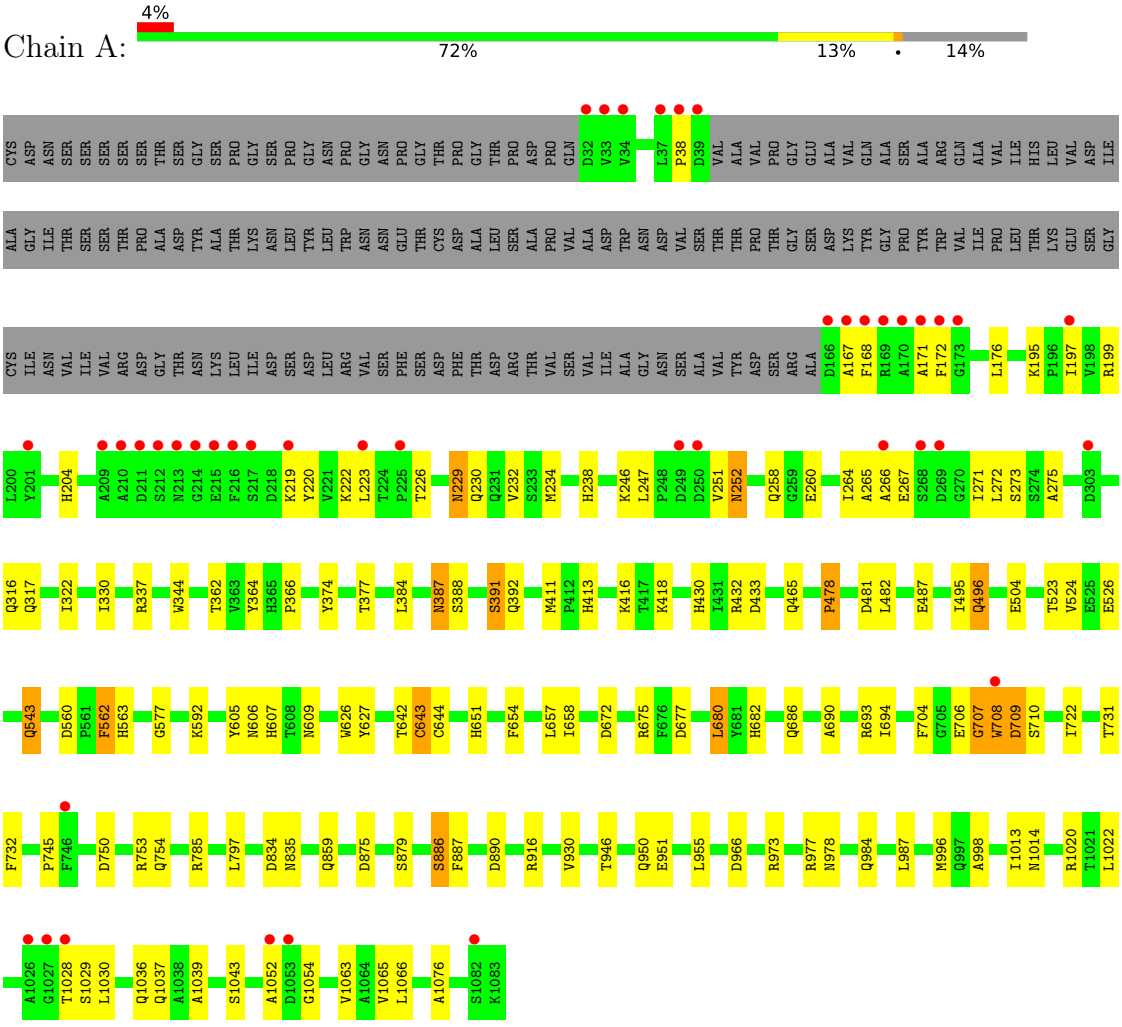
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1211	Total	O	0	0
			1211	1211		

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: Alpha-dextrin endo-1,6-alpha-glucosidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.98Å 60.21Å 132.79Å 90.00° 112.61° 90.00°	Depositor
Resolution (Å)	14.94 – 1.75 43.16 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (14.94-1.75) 98.3 (43.16-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.214 0.186 , 0.215	Depositor DCC
R_{free} test set	10814 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8383	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.30	0/7364	0.61	0/10010

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	7168	0	6904	134	0
2	A	4	0	0	0	0
3	A	1211	0	0	16	1
All	All	8383	0	6904	134	1

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 10.

All (134) 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:680:LEU:HD22	1:A:707:GLY:HA3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HG	1:A:710:SER:CB	2.01	0.90
1:A:680:LEU:HD13	1:A:708:TRP:H	1.39	0.88
1:A:978:ASN:HD21	1:A:984:GLN:H	1.19	0.86
1:A:680:LEU:HG	1:A:710:SER:HB3	1.61	0.83
1:A:606:ASN:HD21	1:A:607:HIS:HD2	1.25	0.82
1:A:680:LEU:HD11	1:A:710:SER:H	1.44	0.81
1:A:680:LEU:HD13	1:A:708:TRP:N	1.99	0.78
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.65	0.78
1:A:722[B]:ILE:HD11	3:A:1809:HOH:O	1.83	0.77
1:A:680:LEU:HG	1:A:710:SER:HB2	1.67	0.77
1:A:654:PHE:O	1:A:658[B]:ILE:HG12	1.85	0.76
1:A:680:LEU:CD1	1:A:710:SER:H	2.00	0.73
1:A:680:LEU:HD11	1:A:709:ASP:H	1.52	0.72
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.71	0.72
1:A:680:LEU:HD11	1:A:709:ASP:N	2.05	0.72
1:A:1013[B]:ILE:HD13	1:A:1063:VAL:HG13	1.69	0.72
1:A:229:ASN:ND2	1:A:232:VAL:H	1.86	0.72
1:A:229:ASN:HD21	1:A:232:VAL:HG23	1.56	0.71
1:A:627:TYR:O	1:A:651:HIS:HD2	1.74	0.70
1:A:680:LEU:HD21	3:A:1411:HOH:O	1.91	0.70
1:A:606:ASN:ND2	1:A:607:HIS:HD2	1.89	0.70
1:A:722[B]:ILE:HG12	3:A:1584:HOH:O	1.92	0.69
1:A:680:LEU:CD2	1:A:707:GLY:HA3	2.24	0.67
1:A:229:ASN:HD21	1:A:232:VAL:H	1.41	0.66
1:A:605:TYR:CD1	1:A:658[B]:ILE:HD12	2.31	0.66
1:A:682:HIS:HD2	1:A:686:GLN:HE22	1.44	0.65
1:A:1030:LEU:HG	1:A:1066:LEU:HB3	1.78	0.65
1:A:1013[B]:ILE:CD1	1:A:1063:VAL:HG13	2.28	0.64
1:A:680:LEU:CG	1:A:710:SER:HB3	2.28	0.63
1:A:682:HIS:HD2	1:A:686:GLN:NE2	1.98	0.62
1:A:708:TRP:N	1:A:708:TRP:CE3	2.69	0.61
1:A:722[B]:ILE:HD12	3:A:2353:HOH:O	2.01	0.60
1:A:560:ASP:HB3	1:A:609:ASN:ND2	2.17	0.59
1:A:675[A]:ARG:HD3	1:A:732:PHE:HE2	1.67	0.59
1:A:251:VAL:HG12	3:A:2279:HOH:O	2.03	0.59
1:A:642:THR:O	1:A:643:CYS:HB3	2.03	0.58
1:A:322:ILE:HG22	1:A:330:ILE:HD11	1.83	0.58
1:A:680:LEU:CD2	1:A:680:LEU:H	2.15	0.58
1:A:223:LEU:CD2	1:A:247:LEU:HG	2.34	0.58
1:A:675[B]:ARG:NH1	1:A:677:ASP:HA	2.19	0.58
1:A:219:LYS:NZ	1:A:219:LYS:HB3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:PHE:CZ	1:A:658[B]:ILE:HD11	2.39	0.57
1:A:750:ASP:O	1:A:754:GLN:HG3	2.05	0.57
1:A:495:ILE:HA	1:A:524:VAL:HB	1.87	0.56
1:A:706:GLU:HG2	1:A:707:GLY:N	2.21	0.55
1:A:465:GLN:HG3	1:A:950:GLN:HE22	1.73	0.54
1:A:675[A]:ARG:HD3	1:A:732:PHE:CE2	2.43	0.54
1:A:680:LEU:H	1:A:680:LEU:HD23	1.72	0.53
1:A:680:LEU:HD23	1:A:680:LEU:N	2.23	0.53
1:A:430:HIS:CD2	1:A:432:ARG:H	2.26	0.53
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.23	0.53
1:A:682:HIS:CD2	1:A:686:GLN:HE22	2.24	0.53
1:A:430:HIS:HD2	1:A:433:ASP:H	1.55	0.53
1:A:642:THR:O	1:A:643:CYS:CB	2.57	0.52
1:A:258:GLN:HE22	1:A:316:GLN:HA	1.75	0.52
1:A:238:HIS:HE1	3:A:1438:HOH:O	1.92	0.51
1:A:387:ASN:ND2	1:A:487:GLU:H	2.07	0.51
1:A:197:ILE:HB	1:A:266:ALA:HB3	1.92	0.51
1:A:523:THR:OG1	1:A:526:GLU:HG3	2.11	0.51
1:A:246[B]:LYS:HD3	1:A:247:LEU:O	2.09	0.51
1:A:680:LEU:CD1	1:A:708:TRP:N	2.70	0.51
1:A:834:ASP:O	1:A:835:ASN:HB2	2.10	0.51
1:A:229:ASN:HD21	1:A:232:VAL:CG2	2.23	0.51
1:A:260:GLU:HB2	1:A:364:TYR:CE1	2.46	0.51
1:A:951[B]:GLU:OE1	1:A:1036:GLN:HG2	2.10	0.51
1:A:272:LEU:C	1:A:272:LEU:HD23	2.32	0.50
1:A:496:GLN:NE2	1:A:496:GLN:H	2.09	0.50
1:A:745:PRO:HA	3:A:2486:HOH:O	2.12	0.50
1:A:693[B]:ARG:NH2	3:A:1576:HOH:O	2.44	0.50
1:A:886:SER:O	1:A:887:PHE:HB2	2.12	0.50
1:A:592:LYS:HE2	1:A:672:ASP:OD2	2.12	0.50
1:A:706:GLU:CG	1:A:707:GLY:N	2.74	0.49
1:A:606:ASN:ND2	1:A:607:HIS:CD2	2.75	0.49
1:A:411:MET:HG2	1:A:672:ASP:OD1	2.13	0.49
1:A:675[A]:ARG:HG2	1:A:704:PHE:CE2	2.48	0.49
1:A:643:CYS:SG	1:A:644:CYS:N	2.86	0.49
1:A:978:ASN:ND2	1:A:984:GLN:H	2.00	0.49
1:A:317:GLN:HB2	1:A:362:THR:HB	1.95	0.48
1:A:377:THR:OG1	1:A:563:HIS:HE1	1.95	0.48
1:A:204:HIS:HE1	3:A:1651:HOH:O	1.96	0.48
1:A:418:LYS:HD2	1:A:966[B]:ASP:OD1	2.15	0.47
1:A:465:GLN:HG3	1:A:950:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:ALA:C	1:A:1054:GLY:H	2.18	0.47
1:A:680:LEU:CD2	1:A:680:LEU:N	2.78	0.47
1:A:543:GLN:HE21	1:A:916:ARG:HA	1.81	0.46
1:A:416:LYS:HE2	3:A:1649:HOH:O	2.15	0.46
1:A:38:PRO:HG2	1:A:172:PHE:CE2	2.51	0.46
1:A:785:ARG:NH2	3:A:1603:HOH:O	2.49	0.45
1:A:875:ASP:OD1	1:A:879:SER:HB2	2.16	0.45
1:A:413:HIS:HD2	3:A:1488:HOH:O	1.99	0.45
1:A:708:TRP:N	1:A:708:TRP:CD2	2.84	0.45
1:A:230:GLN:O	1:A:234:MET:HG2	2.17	0.45
1:A:1014:ASN:HD21	1:A:1020:ARG:HH11	1.64	0.45
1:A:219:LYS:HB3	1:A:219:LYS:HZ3	1.82	0.45
1:A:272:LEU:HD23	1:A:273:SER:N	2.32	0.44
1:A:955:LEU:HD13	1:A:1065:VAL:HG21	1.99	0.44
1:A:238:HIS:H	1:A:238:HIS:CD2	2.36	0.44
1:A:226:THR:HG21	1:A:246[A]:LYS:HD3	1.99	0.44
1:A:708:TRP:HB2	3:A:1786:HOH:O	2.18	0.44
1:A:657:LEU:C	1:A:657:LEU:HD23	2.37	0.44
1:A:797:LEU:HD12	1:A:797:LEU:C	2.38	0.44
1:A:264:ILE:HG12	1:A:275:ALA:CB	2.48	0.43
1:A:195:LYS:HG2	1:A:265:ALA:HB1	2.01	0.43
1:A:229:ASN:C	1:A:229:ASN:HD22	2.21	0.43
1:A:977:ARG:NH2	3:A:1636:HOH:O	2.52	0.43
1:A:337:ARG:HD2	1:A:344:TRP:CZ2	2.54	0.43
1:A:708:TRP:CH2	1:A:731:THR:HB	2.54	0.43
1:A:366:PRO:HB2	1:A:626:TRP:CE2	2.55	0.42
1:A:481:ASP:OD2	1:A:563:HIS:HD2	2.02	0.42
1:A:1028:THR:O	1:A:1029:SER:HB2	2.19	0.42
1:A:1066:LEU:HD22	1:A:1066:LEU:N	2.35	0.42
1:A:199:ARG:HD3	1:A:220:TYR:CD2	2.54	0.42
1:A:384:LEU:HD23	1:A:391:SER:HA	2.00	0.42
1:A:392:GLN:HE22	1:A:577:GLY:HA2	1.85	0.42
1:A:168:PHE:O	1:A:171:ALA:HB3	2.19	0.42
1:A:388:SER:HB2	1:A:562:PHE:CE1	2.54	0.42
1:A:753:ARG:HD2	1:A:930:VAL:HG11	2.01	0.42
1:A:946:THR:O	1:A:950:GLN:HG3	2.20	0.41
1:A:973:ARG:HG2	1:A:998:ALA:HB1	2.01	0.41
1:A:267:GLU:HA	1:A:267:GLU:OE1	2.20	0.41
1:A:654:PHE:CE1	1:A:658[B]:ILE:HD11	2.55	0.41
1:A:252:ASN:C	1:A:252:ASN:HD22	2.22	0.41
1:A:465:GLN:NE2	3:A:2099:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:ND2	1:A:229:ASN:C	2.74	0.41
1:A:176:LEU:HA	3:A:1854:HOH:O	2.20	0.41
1:A:223:LEU:HD22	1:A:247:LEU:HG	2.03	0.41
1:A:682:HIS:CD2	1:A:686:GLN:NE2	2.83	0.41
1:A:890:ASP:HB3	1:A:916:ARG:HH21	1.86	0.41
1:A:690:ALA:O	1:A:694:ILE:HG12	2.21	0.41
1:A:996:MET:HE3	1:A:1076:ALA:HA	2.03	0.41
1:A:222:LYS:NZ	1:A:222:LYS:CB	2.84	0.40
1:A:38:PRO:HG3	1:A:271:ILE:CG2	2.52	0.40
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2098:HOH:O	3:A:2098:HOH:O[2_756]	1.96	0.24

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	935/1083 (86%)	912 (98%)	19 (2%)	4 (0%)	34 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	CYS
1	A	478	PRO
1	A	167	ALA
1	A	707	GLY

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	774/891 (87%)	757 (98%)	17 (2%)	52 29

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	252	ASN
1	A	374	TYR
1	A	387	ASN
1	A	391	SER
1	A	478	PRO
1	A	482	LEU
1	A	496	GLN
1	A	504	GLU
1	A	543	GLN
1	A	562	PHE
1	A	680	LEU
1	A	708	TRP
1	A	709	ASP
1	A	859	GLN
1	A	886	SER
1	A	1037	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	229	ASN
1	A	230	GLN
1	A	238	HIS
1	A	252	ASN
1	A	258	GLN
1	A	279	GLN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	387	ASN
1	A	392	GLN
1	A	413	HIS
1	A	430	HIS
1	A	455	GLN
1	A	458	ASN
1	A	461	GLN
1	A	465	GLN
1	A	496	GLN
1	A	533	GLN
1	A	541	GLN
1	A	543	GLN
1	A	551	GLN
1	A	563	HIS
1	A	593	GLN
1	A	606	ASN
1	A	607	HIS
1	A	609	ASN
1	A	629	GLN
1	A	651	HIS
1	A	682	HIS
1	A	686	GLN
1	A	712	GLN
1	A	859	GLN
1	A	899	ASN
1	A	911	ASN
1	A	944	GLN
1	A	950	GLN
1	A	978	ASN
1	A	983	GLN
1	A	1014	ASN
1	A	1023	GLN
1	A	1037	GLN
1	A	1074	GLN

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 4 ligands modelled in this entry, 4 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 (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	926/1083 (85%)	-0.13	42 (4%) 33 39	10, 17, 43, 70	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	PHE	15.6
1	A	167	ALA	13.0
1	A	172	PHE	8.5
1	A	169	ARG	6.9
1	A	170	ALA	5.6
1	A	212	SER	5.3
1	A	213	ASN	4.8
1	A	217	SER	4.7
1	A	166	ASP	4.5
1	A	214	GLY	4.3
1	A	171	ALA	4.1
1	A	173	GLY	4.1
1	A	249	ASP	3.5
1	A	268	SER	3.5
1	A	1027	GLY	3.3
1	A	37	LEU	3.2
1	A	708	TRP	3.2
1	A	746	PHE	3.2
1	A	1052	ALA	3.0
1	A	38	PRO	2.9
1	A	269	ASP	2.9
1	A	34	VAL	2.8
1	A	266	ALA	2.6
1	A	250	ASP	2.6
1	A	1053	ASP	2.6
1	A	1028	THR	2.6
1	A	223	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	216	PHE	2.4
1	A	1026	ALA	2.3
1	A	32	ASP	2.2
1	A	1082	SER	2.2
1	A	210	ALA	2.2
1	A	201	TYR	2.1
1	A	215	GLU	2.1
1	A	39	ASP	2.1
1	A	219	LYS	2.1
1	A	303	ASP	2.1
1	A	225	PRO	2.1
1	A	197	ILE	2.1
1	A	209	ALA	2.1
1	A	33	VAL	2.0
1	A	211	ASP	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 monosaccharides 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	CA	A	1193	1/1	0.94	0.04	38,38,38,38	0
2	CA	A	1192	1/1	0.98	0.14	32,32,32,32	0
2	CA	A	1194	1/1	0.99	0.02	16,16,16,16	0
2	CA	A	1191	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.