Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:21 PM EDT

PDB ID	:	4YPJ
Title	:	X-ray Structure of The Mutant of Glycoside Hydrolase
Authors	:	Ishikawa, K.; Kataoka, M.; Yanamoto, T.; Nakabayashi, M.; Watanabe, M.
Deposited on	:	2015-03-13
Resolution	:	2.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

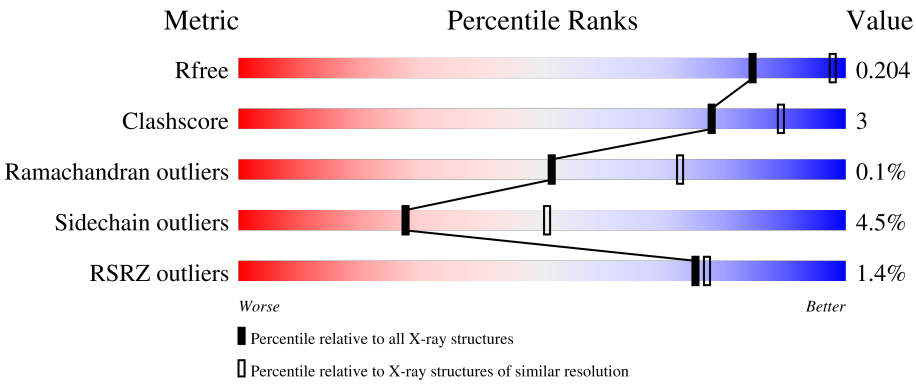
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

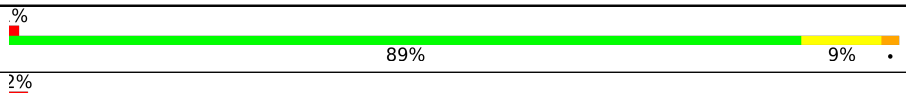
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	810	
1	B	810	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13764 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 Beta galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	810	6422	4065	1092	1255	10	0	0	0
1	B	810	6422	4065	1092	1255	10	0	0	0

- Molecule 2 is water.

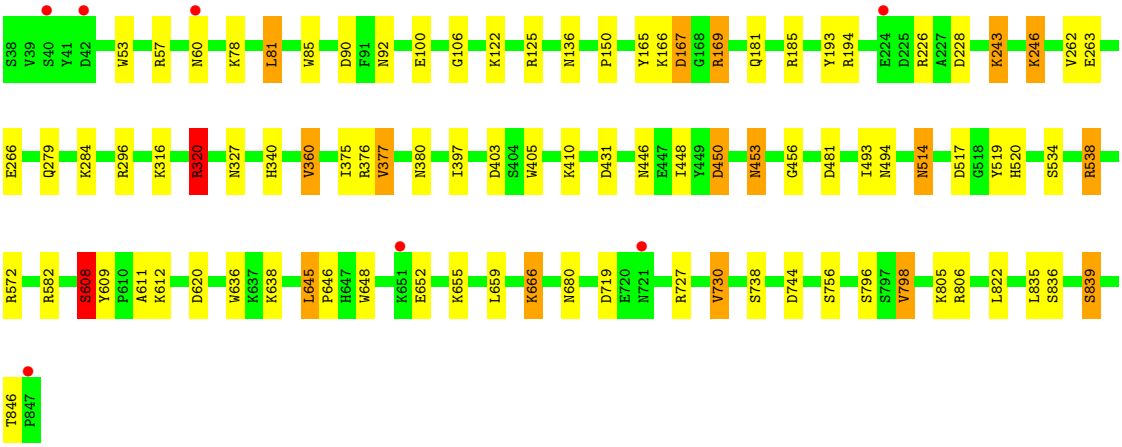
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	455	455	455	0	0
2	B	465	465	465	0	0

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.

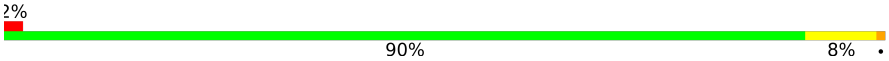
• Molecule 1: Beta galactosidase

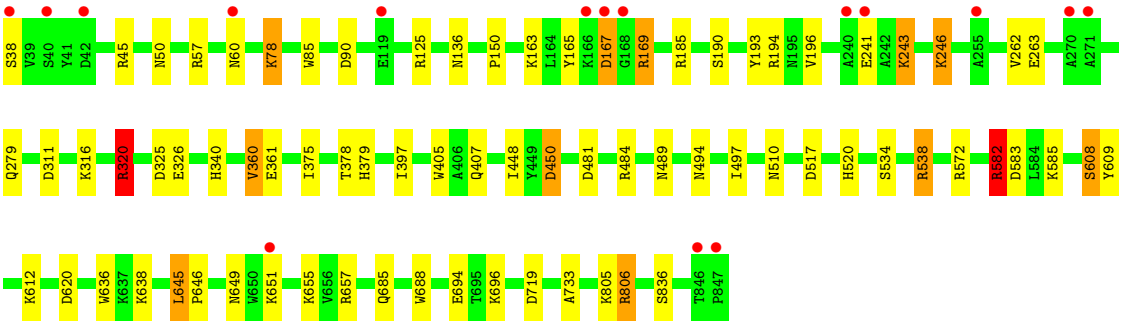
Chain A:



• Molecule 1: Beta galactosidase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	161.41Å 161.41Å 275.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.50 29.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.97-2.50) 98.9 (29.97-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.163 , 0.198 0.172 , 0.204	Depositor DCC
R_{free} test set	6246 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 (i)

5.1 Standard geometry (i)

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	0.90	3/6580 (0.0%)	0.98	24/8930 (0.3%)
1	B	0.87	1/6580 (0.0%)	1.00	30/8930 (0.3%)
All	All	0.89	4/13160 (0.0%)	0.99	54/17860 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	SER	CB-OG	9.27	1.54	1.42
1	B	361	GLU	CD-OE1	5.88	1.32	1.25
1	A	839	SER	CB-OG	-5.81	1.34	1.42
1	A	608	SER	CB-OG	-5.60	1.34	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	538	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	538	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	A	538	ARG	NE-CZ-NH2	11.30	125.95	120.30
1	A	538	ARG	NE-CZ-NH1	-9.83	115.39	120.30
1	B	484	ARG	NE-CZ-NH2	9.79	125.19	120.30
1	B	806	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	806	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	657	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	582	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	57	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	57	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	B	582	ARG	CG-CD-NE	7.30	127.13	111.80
1	B	484	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	B	325	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	481	ASP	CB-CG-OD1	7.12	124.70	118.30
1	B	90	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	719	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	125	ARG	NE-CZ-NH2	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	90	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	657	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	125	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	450	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	572	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	90	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	719	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	246	LYS	CB-CA-C	-5.95	98.49	110.40
1	A	450	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	360	VAL	CB-CA-C	-5.91	100.17	111.40
1	B	719	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	572	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	806	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	572	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	572	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	481	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	620	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	326	GLU	CB-CA-C	-5.58	99.23	110.40
1	A	431	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	620	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	263	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	B	696	LYS	CD-CE-NZ	5.41	124.15	111.70
1	A	320	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	B	185	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	727	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	620	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	620	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	798	VAL	CB-CA-C	5.33	121.52	111.40
1	B	582	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	582	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	57	ARG	CG-CD-NE	-5.25	100.76	111.80
1	A	744	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	360	VAL	CB-CA-C	-5.14	101.62	111.40
1	B	361	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	B	320	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	6422	0	6186	39	0
1	B	6422	0	6186	35	0
2	A	455	0	0	1	0
2	B	465	0	0	6	0
All	All	13764	0	12372	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 3.

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:B:167:ASP:OD2	1:B:169:ARG:HD3	1.66	0.96
1:B:582:ARG:NH1	1:B:583:ASP:OD1	2.01	0.93
1:B:407:GLN:HB3	2:B:1292:HOH:O	1.74	0.88
1:A:226:ARG:NH2	1:A:228:ASP:OD1	2.18	0.76
1:A:514:ASN:HD22	1:A:514:ASN:H	1.35	0.72
1:B:50:ASN:HD21	1:B:196:VAL:H	1.37	0.71
1:A:167:ASP:OD1	1:A:167:ASP:N	2.26	0.69
1:A:648:TRP:HB2	1:A:730:VAL:CG1	2.29	0.62
1:A:262:VAL:HG12	1:A:279:GLN:NE2	2.15	0.62
1:B:494:ASN:HD22	1:B:497:ILE:H	1.46	0.61
1:B:649:ASN:HD21	1:B:733:ALA:H	1.48	0.61
1:A:453:ASN:C	1:A:453:ASN:HD22	2.05	0.60
1:B:246:LYS:HE2	1:B:263:GLU:OE1	2.03	0.58
1:B:262:VAL:HG12	1:B:279:GLN:NE2	2.19	0.58
1:A:648:TRP:HB2	1:A:730:VAL:HG12	1.85	0.57
1:A:514:ASN:H	1:A:514:ASN:ND2	2.01	0.56
1:B:375:ILE:HB	1:B:397:ILE:HD13	1.88	0.56
1:A:376:ARG:HH22	1:A:446:ASN:ND2	2.05	0.54
1:B:167:ASP:N	1:B:167:ASP:OD1	2.41	0.54
1:B:582:ARG:NH2	1:B:694:GLU:OE2	2.41	0.54
1:B:585:LYS:HG2	1:B:688:TRP:CZ3	2.43	0.53
1:B:405:TRP:CD2	1:B:448:ILE:HG21	2.44	0.53
1:A:136:ASN:HA	1:A:150:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TRP:CD2	1:A:448:ILE:HG21	2.45	0.52
1:B:582:ARG:HH11	1:B:582:ARG:HG2	1.73	0.52
1:A:376:ARG:HH22	1:A:446:ASN:HD22	1.56	0.52
1:B:582:ARG:NH2	2:B:901:HOH:O	2.39	0.51
1:A:375:ILE:HB	1:A:397:ILE:HD13	1.92	0.51
1:B:45:ARG:NH1	1:B:311:ASP:OD2	2.44	0.50
1:B:585:LYS:HG2	1:B:688:TRP:CE3	2.47	0.50
1:B:489:ASN:HB2	2:B:1250:HOH:O	2.11	0.49
1:A:296:ARG:HD3	2:A:1180:HOH:O	2.13	0.49
1:A:246:LYS:HG3	1:A:266:GLU:HG2	1.95	0.49
1:B:45:ARG:NH2	2:B:913:HOH:O	2.46	0.49
1:A:453:ASN:ND2	1:A:456:GLY:H	2.12	0.48
1:B:340:HIS:HB3	1:B:636:TRP:CE3	2.49	0.48
1:A:167:ASP:OD2	1:A:169:ARG:HD3	2.13	0.47
1:B:136:ASN:HA	1:B:150:PRO:HA	1.95	0.47
1:A:167:ASP:OD2	1:A:169:ARG:CD	2.63	0.47
1:B:320:ARG:HD3	1:B:320:ARG:O	2.14	0.47
1:A:53:TRP:NE1	1:A:81:LEU:HD22	2.30	0.46
1:B:645:LEU:HB2	1:B:646:PRO:HA	1.98	0.46
1:A:738:SER:HA	1:A:835:LEU:HB3	1.97	0.45
1:A:185:ARG:HD3	1:A:403:ASP:OD2	2.16	0.45
1:A:327:ASN:HD22	1:A:520:HIS:HE1	1.64	0.45
1:A:377:VAL:HG22	1:A:380:ASN:O	2.16	0.45
1:B:320:ARG:HD3	1:B:320:ARG:C	2.36	0.45
1:A:608:SER:O	1:A:609:TYR:C	2.53	0.45
1:B:78:LYS:HE3	1:B:78:LYS:HB2	1.57	0.45
1:B:608:SER:O	1:B:609:TYR:C	2.55	0.44
1:A:493:ILE:HG22	1:A:494:ASN:O	2.17	0.44
1:A:243:LYS:HD3	1:A:243:LYS:HA	1.87	0.44
1:B:243:LYS:HD3	1:B:243:LYS:HA	1.82	0.44
1:B:378:THR:HA	1:B:379:HIS:HA	1.88	0.43
1:A:106:GLY:H	1:A:181:GLN:NE2	2.16	0.43
1:A:165:TYR:CB	1:A:169:ARG:HG3	2.48	0.43
1:A:517:ASP:O	1:A:520:HIS:HB3	2.18	0.43
1:A:666:LYS:HB3	1:A:680:ASN:HB3	1.99	0.43
1:B:50:ASN:ND2	1:B:196:VAL:H	2.09	0.43
1:B:193:TYR:CE2	1:B:194:ARG:HG3	2.53	0.43
1:A:100:GLU:OE1	1:A:410:LYS:NZ	2.52	0.43
1:A:645:LEU:HB2	1:A:646:PRO:HA	2.00	0.43
1:A:193:TYR:CE2	1:A:194:ARG:HG3	2.54	0.42
1:B:45:ARG:NH1	1:B:311:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:C	1:A:453:ASN:ND2	2.72	0.42
1:A:185:ARG:NH1	1:A:403:ASP:OD1	2.52	0.42
1:A:320:ARG:O	1:A:320:ARG:HD3	2.20	0.41
1:A:611:ALA:HA	1:A:796:SER:HA	2.01	0.41
1:A:493:ILE:HG12	1:A:519:TYR:CZ	2.56	0.41
1:B:165:TYR:HA	2:B:903:HOH:O	2.20	0.41
1:A:340:HIS:HB3	1:A:636:TRP:CE3	2.55	0.41
1:B:38:SER:N	2:B:928:HOH:O	2.53	0.41
1:B:169:ARG:H	1:B:169:ARG:HG2	1.74	0.40
1:B:517:ASP:O	1:B:520:HIS:HB3	2.21	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	808/810 (100%)	777 (96%)	30 (4%)	1 (0%)	51	73
1	B	808/810 (100%)	777 (96%)	30 (4%)	1 (0%)	51	73
All	All	1616/1620 (100%)	1554 (96%)	60 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	SER
1	B	534	SER

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	685/685 (100%)	651 (95%)	34 (5%)	24	46
1	B	685/685 (100%)	658 (96%)	27 (4%)	32	57
All	All	1370/1370 (100%)	1309 (96%)	61 (4%)	27	51

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	78	LYS
1	A	81	LEU
1	A	85	TRP
1	A	92	ASN
1	A	122	LYS
1	A	166	LYS
1	A	167	ASP
1	A	169	ARG
1	A	243	LYS
1	A	284	LYS
1	A	316	LYS
1	A	320	ARG
1	A	360	VAL
1	A	377	VAL
1	A	450	ASP
1	A	453	ASN
1	A	514	ASN
1	A	538	ARG
1	A	608	SER
1	A	612	LYS
1	A	638	LYS
1	A	645	LEU
1	A	652	GLU
1	A	655	LYS
1	A	659	LEU
1	A	666	LYS
1	A	730	VAL
1	A	798	VAL
1	A	805	LYS
1	A	822	LEU
1	A	836	SER
1	A	839	SER

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Mol	Chain	Res	Type
1	A	846	THR
1	B	60	ASN
1	B	78	LYS
1	B	85	TRP
1	B	163	LYS
1	B	167	ASP
1	B	169	ARG
1	B	190	SER
1	B	241	GLU
1	B	243	LYS
1	B	246	LYS
1	B	316	LYS
1	B	320	ARG
1	B	360	VAL
1	B	450	ASP
1	B	510	ASN
1	B	538	ARG
1	B	582	ARG
1	B	608	SER
1	B	612	LYS
1	B	638	LYS
1	B	645	LEU
1	B	651	LYS
1	B	655	LYS
1	B	685	GLN
1	B	805	LYS
1	B	806	ARG
1	B	836	SER

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

Mol	Chain	Res	Type
1	A	52	ASN
1	A	92	ASN
1	A	179	ASN
1	A	181	GLN
1	A	260	GLN
1	A	280	ASN
1	A	327	ASN
1	A	363	GLN
1	A	446	ASN
1	A	453	ASN

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Mol	Chain	Res	Type
1	A	462	ASN
1	A	514	ASN
1	A	607	ASN
1	B	50	ASN
1	B	181	GLN
1	B	230	ASN
1	B	280	ASN
1	B	462	ASN
1	B	494	ASN
1	B	510	ASN
1	B	522	GLN
1	B	551	GLN
1	B	559	GLN
1	B	649	ASN
1	B	794	ASN

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)

There are no ligands in this entry.

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	810/810 (100%)	-0.60	7 (0%)	84	86	15, 26, 52, 81	0
1	B	810/810 (100%)	-0.54	16 (1%)	65	68	17, 28, 55, 89	0
All	All	1620/1620 (100%)	-0.57	23 (1%)	75	77	15, 27, 54, 89	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	ASP	3.5
1	B	847	PRO	3.5
1	A	60	ASN	3.2
1	B	271	ALA	3.1
1	A	721	ASN	2.9
1	B	42	ASP	2.8
1	B	60	ASN	2.7
1	A	224	GLU	2.5
1	B	168	GLY	2.5
1	B	166	LYS	2.4
1	A	651	LYS	2.4
1	B	40	SER	2.4
1	B	270	ALA	2.3
1	B	38	SER	2.3
1	B	255	ALA	2.2
1	A	42	ASP	2.2
1	B	241	GLU	2.2
1	A	40	SER	2.1
1	B	651	LYS	2.1
1	B	119	GLU	2.1
1	B	240	ALA	2.1
1	B	846	THR	2.1
1	A	847	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.