Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID	:	3DGS
Title	:	Changing the determinants of protein stability from covalent to non-covalent interactions by in-vitro evolution: a structural and energetic analysis
Authors	:	Jakob, R.P.; Kather, I.; Dobbek, H.; Schmid, F.X.
Deposited on	:	2008-06-16
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/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:

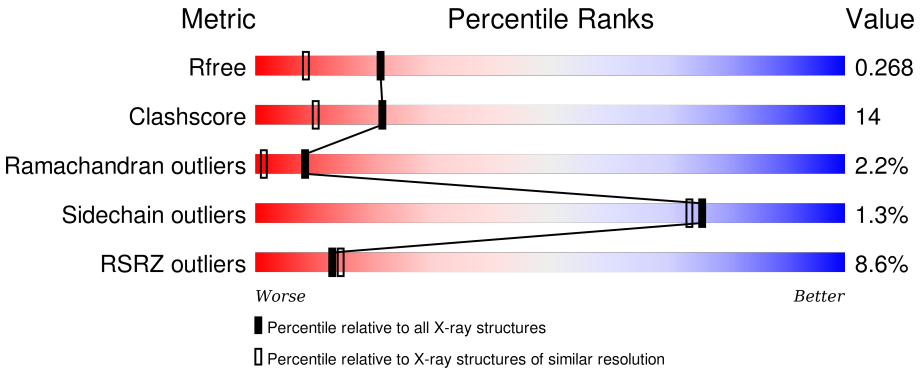
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	227	4% 64% 17% 18%
1	B	227	10% 63% 17% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3213 atoms, of which 2 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 Coat protein A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	H	N	O	S	4	0	0
			1483	955	1	238	287	2			
1	B	186	Total	C	H	N	O	S	15	0	0
			1472	947	1	237	285	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P03661
A	7	SER	CYS	ENGINEERED	UNP P03661
A	11	SER	PRO	ENGINEERED	UNP P03661
A	13	ILE	THR	ENGINEERED	UNP P03661
A	15	GLY	ASN	ENGINEERED	UNP P03661
A	29	TRP	ARG	ENGINEERED	UNP P03661
A	36	ILE	CYS	ENGINEERED	UNP P03661
A	39	LYS	ASN	ENGINEERED	UNP P03661
A	46	ILE	CYS	ENGINEERED	UNP P03661
A	53	VAL	CYS	ENGINEERED	UNP P03661
A	55	ALA	GLY	ENGINEERED	UNP P03661
A	56	ILE	THR	ENGINEERED	UNP P03661
A	60	VAL	ILE	ENGINEERED	UNP P03661
A	101	ILE	THR	ENGINEERED	UNP P03661
A	129	HIS	GLN	ENGINEERED	UNP P03661
A	138	GLY	ASN	ENGINEERED	UNP P03661
A	188	VAL	CYS	ENGINEERED	UNP P03661
A	199	LEU	PHE	ENGINEERED	UNP P03661
A	201	ALA	CYS	ENGINEERED	UNP P03661
A	207	LEU	SER	ENGINEERED	UNP P03661
A	209	TYR	ASP	ENGINEERED	UNP P03661
A	218	PRO	-	EXPRESSION TAG	UNP P03661
A	219	SER	-	EXPRESSION TAG	UNP P03661
A	220	GLY	-	EXPRESSION TAG	UNP P03661
A	221	HIS	-	EXPRESSION TAG	UNP P03661

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Chain	Residue	Modelled	Actual	Comment	Reference
A	222	HIS	-	EXPRESSION TAG	UNP P03661
A	223	HIS	-	EXPRESSION TAG	UNP P03661
A	224	HIS	-	EXPRESSION TAG	UNP P03661
A	225	HIS	-	EXPRESSION TAG	UNP P03661
A	226	HIS	-	EXPRESSION TAG	UNP P03661
B	0	MET	-	INITIATING METHIONINE	UNP P03661
B	7	SER	CYS	ENGINEERED	UNP P03661
B	11	SER	PRO	ENGINEERED	UNP P03661
B	13	ILE	THR	ENGINEERED	UNP P03661
B	15	GLY	ASN	ENGINEERED	UNP P03661
B	29	TRP	ARG	ENGINEERED	UNP P03661
B	36	ILE	CYS	ENGINEERED	UNP P03661
B	39	LYS	ASN	ENGINEERED	UNP P03661
B	46	ILE	CYS	ENGINEERED	UNP P03661
B	53	VAL	CYS	ENGINEERED	UNP P03661
B	55	ALA	GLY	ENGINEERED	UNP P03661
B	56	ILE	THR	ENGINEERED	UNP P03661
B	60	VAL	ILE	ENGINEERED	UNP P03661
B	101	ILE	THR	ENGINEERED	UNP P03661
B	129	HIS	GLN	ENGINEERED	UNP P03661
B	138	GLY	ASN	ENGINEERED	UNP P03661
B	188	VAL	CYS	ENGINEERED	UNP P03661
B	199	LEU	PHE	ENGINEERED	UNP P03661
B	201	ALA	CYS	ENGINEERED	UNP P03661
B	207	LEU	SER	ENGINEERED	UNP P03661
B	209	TYR	ASP	ENGINEERED	UNP P03661
B	218	PRO	-	EXPRESSION TAG	UNP P03661
B	219	SER	-	EXPRESSION TAG	UNP P03661
B	220	GLY	-	EXPRESSION TAG	UNP P03661
B	221	HIS	-	EXPRESSION TAG	UNP P03661
B	222	HIS	-	EXPRESSION TAG	UNP P03661
B	223	HIS	-	EXPRESSION TAG	UNP P03661
B	224	HIS	-	EXPRESSION TAG	UNP P03661
B	225	HIS	-	EXPRESSION TAG	UNP P03661
B	226	HIS	-	EXPRESSION TAG	UNP P03661

- Molecule 2 is water.

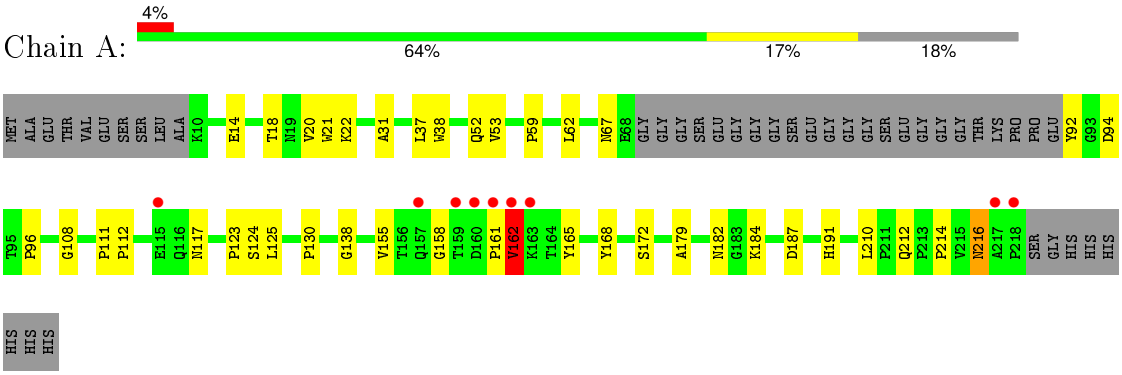
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	151	Total O 151 151	0	0
2	B	107	Total O 107 107	0	0

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 errors 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.

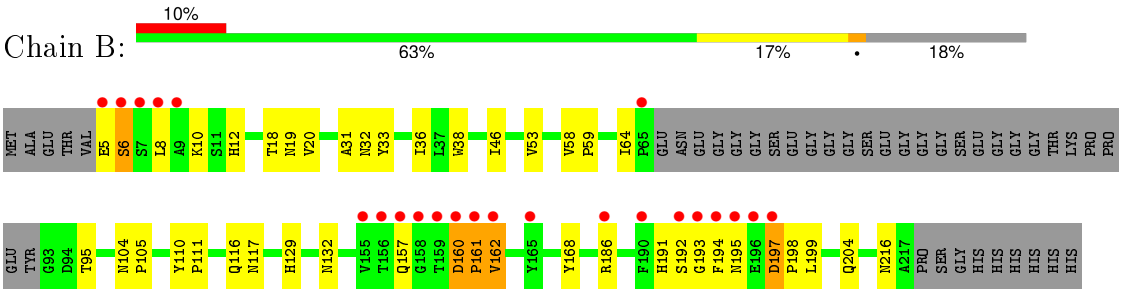
- Molecule 1: Coat protein A

Chain A:



- Molecule 1: Coat protein A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.86Å 92.21Å 94.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 100.0 (19.63-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.263 0.222 , 0.268	Depositor DCC
R_{free} test set	1715 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	EDS
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 40229 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3213	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.43	0/1533	0.63	0/2105
1	B	0.42	0/1520	0.65	0/2086
All	All	0.43	0/3053	0.64	0/4191

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	1482	1	1383	38	1
1	B	1471	1	1381	42	1
2	A	151	0	0	5	0
2	B	107	0	0	4	0
All	All	3211	2	2764	80	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 14.

All (80) 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:132:ASN:OD1	1:B:193:GLY:N	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:H	1:A:216:ASN:HD21	1.10	0.91
1:A:162:VAL:HG22	2:A:344:HOH:O	1.68	0.91
1:A:155:VAL:HG13	1:A:165:TYR:HB2	1.52	0.89
1:B:132:ASN:ND2	1:B:192:SER:HA	1.96	0.81
1:B:197:ASP:HB3	1:B:198:PRO:HD2	1.63	0.80
1:A:125:LEU:HD12	1:A:155:VAL:HG11	1.61	0.80
1:B:5:GLU:HG3	2:B:325:HOH:O	1.85	0.76
1:B:132:ASN:OD1	1:B:192:SER:C	2.31	0.68
1:B:132:ASN:CG	1:B:192:SER:HA	2.13	0.68
1:B:8:LEU:HB3	1:B:59:PRO:HB2	1.76	0.68
1:B:129:HIS:HD2	1:B:168:TYR:OH	1.76	0.68
1:A:20:VAL:HG21	1:A:53:VAL:HG23	1.79	0.65
1:B:191:HIS:CG	1:B:199:LEU:HD11	2.32	0.65
1:A:52:GLN:HE22	1:A:212:GLN:HE22	1.45	0.64
1:B:5:GLU:HG2	1:B:6:SER:H	1.63	0.64
1:A:18:THR:N	1:A:216:ASN:HD21	1.90	0.63
1:A:158:GLY:HA3	1:A:162:VAL:O	1.98	0.63
1:B:160:ASP:HA	1:B:161:PRO:O	2.01	0.61
1:A:18:THR:H	1:A:216:ASN:ND2	1.92	0.59
1:A:125:LEU:N	1:A:125:LEU:HD22	2.18	0.59
1:B:10:LYS:HE2	1:B:36:ILE:CD1	2.35	0.56
1:B:197:ASP:HB3	1:B:198:PRO:CD	2.34	0.56
1:A:52:GLN:NE2	1:A:212:GLN:HE22	2.04	0.55
1:A:111:PRO:O	1:A:117:ASN:HB3	2.06	0.55
1:A:52:GLN:NE2	1:A:214:PRO:HB3	2.22	0.55
1:A:155:VAL:CG1	1:A:165:TYR:HB2	2.31	0.54
1:A:21:TRP:CD2	1:A:67:ASN:HB3	2.42	0.54
1:B:20:VAL:HG21	1:B:53:VAL:HG23	1.90	0.54
1:B:132:ASN:OD1	1:B:192:SER:CA	2.56	0.54
1:B:5:GLU:HG2	1:B:6:SER:N	2.24	0.52
1:A:124:SER:C	1:A:125:LEU:HD22	2.30	0.52
1:A:92:TYR:HA	2:A:323:HOH:O	2.09	0.52
1:A:125:LEU:HD12	1:A:155:VAL:CG1	2.36	0.52
1:B:32:ASN:HD21	1:B:64:ILE:H	1.57	0.51
1:B:186:ARG:HG2	2:B:340:HOH:O	2.12	0.50
1:B:111:PRO:O	1:B:117:ASN:HB3	2.11	0.50
1:B:132:ASN:ND2	1:B:193:GLY:H	2.10	0.50
1:B:33:TYR:HB3	1:B:38:TRP:NE1	2.26	0.50
1:B:6:SER:C	1:B:8:LEU:H	2.14	0.50
1:B:132:ASN:HD21	1:B:192:SER:HA	1.73	0.49
1:B:132:ASN:CG	1:B:193:GLY:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HD22	1:A:216:ASN:H	1.61	0.49
1:B:193:GLY:O	1:B:194:PHE:HB3	2.13	0.48
1:A:125:LEU:CD1	1:A:155:VAL:HG11	2.37	0.48
1:A:22:LYS:NZ	1:A:138:GLY:O	2.47	0.47
1:A:52:GLN:HE21	1:A:214:PRO:HB3	1.79	0.47
1:A:38:TRP:CZ3	1:A:59:PRO:HD3	2.49	0.47
1:B:32:ASN:ND2	1:B:64:ILE:H	2.11	0.47
1:A:20:VAL:HG12	1:A:31:ALA:HB2	1.95	0.47
1:B:20:VAL:HG12	1:B:31:ALA:HB2	1.97	0.47
1:B:132:ASN:OD1	1:B:192:SER:HA	2.15	0.46
1:A:179:ALA:HA	1:A:184:LYS:HD2	1.97	0.46
1:B:204:GLN:HB3	2:B:283:HOH:O	2.14	0.46
1:B:10:LYS:O	1:B:59:PRO:HG3	2.16	0.46
1:B:12:HIS:CD2	1:B:58:VAL:HG12	2.50	0.46
1:B:160:ASP:HA	1:B:161:PRO:C	2.35	0.46
1:B:46:ILE:HG12	1:B:53:VAL:HG22	1.98	0.46
1:B:194:PHE:CG	1:B:194:PHE:O	2.70	0.45
1:A:112:PRO:HA	1:A:117:ASN:O	2.17	0.45
1:A:96:PRO:HA	1:A:210:LEU:O	2.16	0.45
1:A:182:ASN:HB2	2:A:251:HOH:O	2.16	0.45
1:A:14:GLU:OE1	2:A:288:HOH:O	2.21	0.45
1:A:216:ASN:HD22	1:A:216:ASN:N	2.13	0.44
1:A:22:LYS:HD3	2:A:361:HOH:O	2.16	0.44
1:B:18:THR:HG22	1:B:216:ASN:OD1	2.18	0.44
1:A:125:LEU:N	1:A:125:LEU:CD2	2.81	0.44
1:B:162:VAL:O	1:B:162:VAL:HG13	2.18	0.44
1:B:104:ASN:HA	1:B:105:PRO:HD3	1.88	0.43
1:A:130:PRO:HD2	1:A:168:TYR:CE1	2.54	0.43
1:B:18:THR:HG23	1:B:19:ASN:ND2	2.34	0.43
1:A:108:GLY:HA2	1:A:172:SER:HB2	2.01	0.43
1:A:37:LEU:HB2	1:A:62:LEU:O	2.19	0.42
1:A:187:ASP:O	1:A:191:HIS:HE1	2.01	0.42
1:B:110:TYR:CD1	1:B:116:GLN:HG2	2.54	0.42
1:A:18:THR:HG22	1:A:216:ASN:ND2	2.34	0.42
1:A:155:VAL:HG13	1:A:155:VAL:O	2.19	0.42
1:B:95:THR:HG23	2:B:254:HOH:O	2.20	0.41
1:B:132:ASN:CG	1:B:193:GLY:N	2.69	0.40
1:B:5:GLU:O	1:B:6:SER:CB	2.70	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)
1:A:123:PRO:O	1:B:192:SER:OG[3_555]	2.14	0.06

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	182/227 (80%)	168 (92%)	12 (7%)	2 (1%)	17 6
1	B	182/227 (80%)	164 (90%)	12 (7%)	6 (3%)	5 0
All	All	364/454 (80%)	332 (91%)	24 (7%)	8 (2%)	8 1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	6	SER
1	B	161	PRO
1	B	162	VAL
1	B	197	ASP
1	A	162	VAL
1	B	195	ASN
1	B	160	ASP

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	159/185 (86%)	156 (98%)	3 (2%)	65 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	158/185 (85%)	157 (99%)	1 (1%)	90 90
All	All	317/370 (86%)	313 (99%)	4 (1%)	76 73

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	162	VAL
1	A	216	ASN
1	B	157	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	52	GLN
1	A	116	GLN
1	A	167	GLN
1	A	191	HIS
1	A	195	ASN
1	A	206	GLN
1	A	216	ASN
1	B	19	ASN
1	B	32	ASN
1	B	129	HIS
1	B	167	GLN
1	B	206	GLN

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

There are no ligands in this entry.

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	186/227 (81%)	-0.01	9 (4%) 34 37	14, 23, 62, 124	1 (0%)
1	B	186/227 (81%)	0.52	23 (12%) 5 5	12, 26, 86, 136	6 (3%)
All	All	372/454 (81%)	0.26	32 (8%) 13 14	12, 24, 79, 136	7 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	PHE	20.5
1	B	159	THR	11.3
1	B	195	ASN	8.4
1	B	161	PRO	7.2
1	A	159	THR	6.6
1	B	196	GLU	6.2
1	B	5	GLU	5.5
1	B	8	LEU	4.5
1	B	193	GLY	4.2
1	B	7	SER	3.9
1	B	9	ALA	3.9
1	A	161	PRO	3.9
1	A	157	GLN	3.8
1	B	158	GLY	3.7
1	A	218	PRO	3.4
1	B	156	THR	3.2
1	B	190	PHE	3.2
1	B	197	ASP	3.1
1	A	160	ASP	2.7
1	B	65	PRO	2.7
1	B	165	TYR	2.6
1	B	160	ASP	2.6
1	B	192	SER	2.5
1	A	163	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	162	VAL	2.5
1	B	155	VAL	2.4
1	B	186	ARG	2.3
1	A	162	VAL	2.3
1	A	115	GLU	2.3
1	B	6	SER	2.2
1	B	157	GLN	2.1
1	A	217	ALA	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.