Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 01:30 PM EDT

PDB ID	:	1IGI
Title	:	26-10 FAB:DIGOXIN COMPLEX-AFFINITY AND SPECIFICITY DUE TO SURFACE COMPLEMENTARITY
Authors	:	Jeffrey, P.D.; Sheriff, S.
Deposited on	:	1993-02-19
Resolution	:	2.70 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:

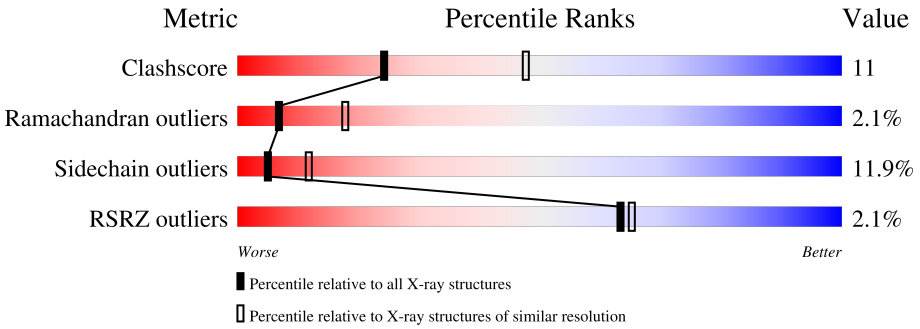
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	L	219	61% 32% 6%
2	H	218	4% 65% 29% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3298 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 IGG2A-KAPPA 26-10 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	218	1676	1046	286	338	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	THR	SER	conflict	PIR S52028
L	27B	LEU	ILE	conflict	PIR S52028
L	34	ASN	GLU	conflict	PIR S52028
L	40	ALA	PRO	conflict	PIR S52028
L	85	ILE	VAL	conflict	PIR S52028
L	87	PHE	TYR	conflict	PIR S52028
L	89	SER	PHE	conflict	PIR S52028
L	91	THR	GLY	conflict	PIR S52028
L	92	THR	SER	conflict	PIR S52028
L	103	LYS	ASN	conflict	PIR S52028

- Molecule 2 is a protein called IGG2A-KAPPA 26-10 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1622	1024	264	325	9	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	LYS	ARG	conflict	PIR S38950
H	19	ARG	LYS	conflict	PIR S38950
H	20	MET	ILE	conflict	PIR S38950
H	24	SER	ALA	conflict	PIR S38950
H	28	ILE	THR	conflict	PIR S38950
H	32	PHE	TYR	conflict	PIR S38950

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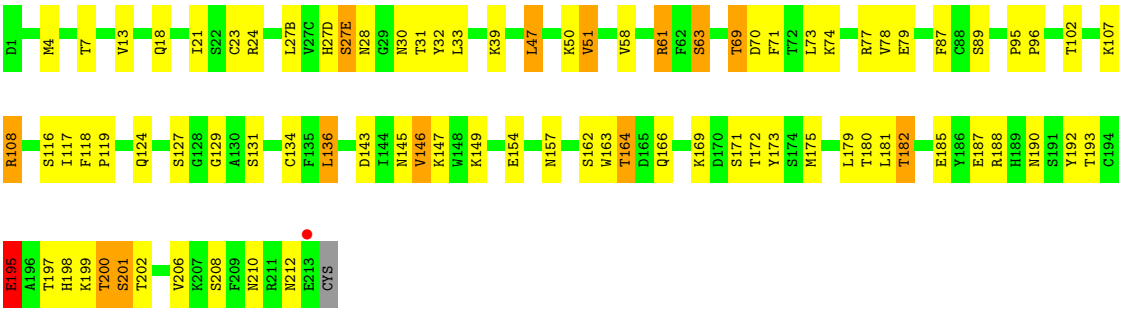
Chain	Residue	Modelled	Actual	Comment	Reference
H	34	MET	ILE	conflict	PIR S38950
H	35	ASN	HIS	conflict	PIR S38950
H	38	ARG	LYS	conflict	PIR S38950
H	40	SER	ARG	conflict	PIR S38950
H	41	HIS	PRO	conflict	PIR S38950
H	43	LYS	GLU	conflict	PIR S38950
H	44	SER	GLY	conflict	PIR S38950
H	46	ASP	GLU	conflict	PIR S38950
H	47	TYR	TRP	conflict	PIR S38950
H	50	TYR	TRP	conflict	PIR S38950
H	52	SER	TYR	conflict	PIR S38950
H	53	TYR	GLY	conflict	PIR S38950
H	56	VAL	ASN	conflict	PIR S38950
H	58	GLY	LYS	conflict	PIR S38950
H	61	GLN	GLU	conflict	PIR S38950
H	73	LYS	THR	conflict	PIR S38950
H	81	GLU	GLN	conflict	PIR S38950
H	82A	ARG	SER	conflict	PIR S38950
H	91	TYR	PHE	conflict	PIR S38950
H	94	GLY	-	insertion	PIR S38950
H	95	SER	-	insertion	PIR S38950
H	96	SER	ARG	conflict	PIR S38950
H	98	ASN	GLY	conflict	PIR S38950
H	100	TRP	PHE	conflict	PIR S38950
H	105	HIS	GLN	conflict	PIR S38950
H	107	ALA	THR	conflict	PIR S38950

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.

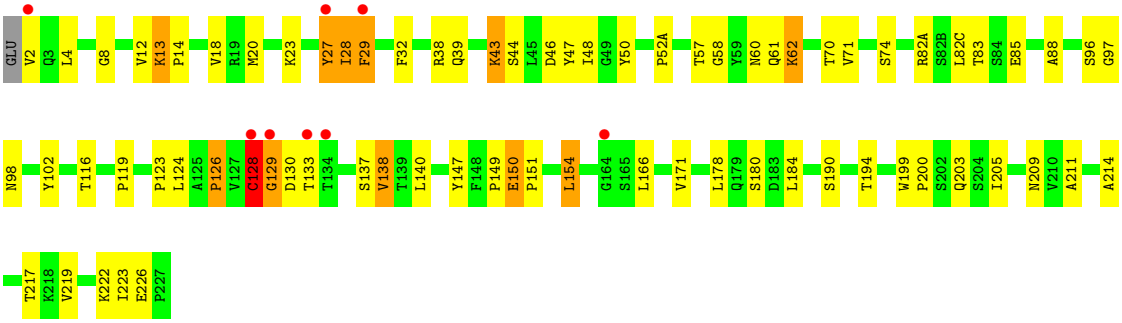
• Molecule 1: IGG2A-KAPPA 26-10 FAB (LIGHT CHAIN)

Chain L:



• Molecule 2: IGG2A-KAPPA 26-10 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.78Å 89.25Å 59.24Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 31.17 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.70) 65.3 (31.17-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.72Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available) 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 120.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3298	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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

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	L	0.71	0/1713	1.54	17/2326 (0.7%)
2	H	0.71	0/1664	1.62	17/2268 (0.7%)
All	All	0.71	0/3377	1.58	34/4594 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	150	GLU	N-CA-CB	-8.38	95.51	110.60
2	H	29	PHE	CA-C-N	-7.70	100.26	117.20
2	H	28	ILE	CA-C-N	-7.43	100.84	117.20
1	L	180	THR	CA-CB-CG2	-6.79	102.90	112.40
2	H	150	GLU	CB-CA-C	6.66	123.73	110.40
2	H	47	TYR	CB-CG-CD1	-6.36	117.19	121.00
2	H	226	GLU	O-C-N	6.26	133.00	121.10
1	L	47	LEU	CA-CB-CG	6.26	129.69	115.30
1	L	201	SER	CA-C-N	-6.19	103.59	117.20
1	L	89	SER	CA-CB-OG	6.17	127.85	111.20
2	H	129	GLY	CA-C-N	-6.12	103.72	117.20
1	L	61	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	H	29	PHE	O-C-N	5.87	132.09	122.70
1	L	201	SER	O-C-N	5.82	132.01	122.70
2	H	27	TYR	CA-C-N	-5.68	104.69	117.20
2	H	154	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	192	TYR	CB-CG-CD1	-5.62	117.63	121.00
2	H	28	ILE	O-C-N	5.61	131.68	122.70
1	L	50	LYS	C-N-CA	5.59	135.67	121.70
1	L	162	SER	N-CA-CB	-5.51	102.24	110.50
1	L	195	GLU	CA-CB-CG	5.49	125.47	113.40
1	L	188	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	L	164	THR	N-CA-CB	-5.43	99.98	110.30
2	H	60	ASN	N-CA-C	-5.42	96.36	111.00
1	L	175	MET	CA-CB-CG	5.42	122.51	113.30
1	L	146	VAL	CA-CB-CG2	-5.36	102.86	110.90
2	H	226	GLU	CA-C-N	-5.32	102.21	117.10
2	H	57	THR	N-CA-CB	5.27	120.32	110.30
2	H	20	MET	CG-SD-CE	-5.27	91.77	100.20
2	H	129	GLY	O-C-N	5.16	130.95	122.70
2	H	128	CYS	CA-CB-SG	5.14	123.25	114.00
1	L	108	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	L	107	LYS	CB-CG-CD	-5.04	98.51	111.60
1	L	195	GLU	CA-C-N	-5.03	106.13	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	8	GLY	Peptide

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	L	1676	0	1621	39	0
2	H	1622	0	1566	38	0
All	All	3298	0	3187	71	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 11.

All (71) 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)
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.61	0.82
2:H:38:ARG:HB2	2:H:48:ILE:HD11	1.72	0.72
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.72	0.71
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.79	0.64
1:L:21:ILE:HG12	1:L:102:THR:HG21	1.80	0.63
1:L:95:PRO:HG3	2:H:62:LYS:NZ	2.14	0.63
1:L:119:PRO:HD3	2:H:128:CYS:HB3	1.82	0.62
2:H:205:ILE:H	2:H:222:LYS:HZ3	1.47	0.60
2:H:211:ALA:HA	2:H:217:THR:O	2.01	0.60
1:L:145:ASN:HB3	1:L:197:THR:HB	1.85	0.58
1:L:117:ILE:O	2:H:128:CYS:SG	2.62	0.58
2:H:126:PRO:HD3	2:H:140:LEU:HD23	1.86	0.58
1:L:116:SER:O	1:L:134:CYS:HA	2.05	0.57
2:H:12:VAL:HG11	2:H:18:VAL:HB	1.87	0.57
1:L:13:VAL:HG21	1:L:78:VAL:HG11	1.87	0.57
2:H:52(A):PRO:HA	2:H:71:VAL:HG11	1.88	0.56
1:L:4:MET:HE3	1:L:23:CYS:SG	2.45	0.56
1:L:166:GLN:NE2	1:L:171:SER:HB3	2.21	0.56
2:H:140:LEU:HD22	2:H:223:ILE:HG21	1.89	0.55
2:H:27:TYR:HE2	2:H:96:SER:HG	1.55	0.55
2:H:2:VAL:HG22	2:H:27:TYR:HB2	1.88	0.53
1:L:33:LEU:HD13	1:L:71:PHE:CD2	2.44	0.52
1:L:163:TRP:HE1	1:L:173:TYR:HB3	1.75	0.52
2:H:126:PRO:HA	2:H:128:CYS:SG	2.50	0.52
1:L:28:ASN:ND2	1:L:30:ASN:HD22	2.08	0.51
1:L:198:HIS:HD1	1:L:200:THR:HG1	1.58	0.51
1:L:28:ASN:HD21	1:L:30:ASN:HD22	1.59	0.50
1:L:149:LYS:HB2	1:L:193:THR:HB	1.92	0.50
1:L:193:THR:HG22	1:L:195:GLU:HB3	1.94	0.50
2:H:50:TYR:CZ	2:H:58:GLY:HA3	2.47	0.50
2:H:154:LEU:HA	2:H:209:ASN:O	2.11	0.49
2:H:178:LEU:HA	2:H:184:LEU:O	2.12	0.49
2:H:126:PRO:HG3	2:H:138:VAL:HG12	1.96	0.48
1:L:190:ASN:O	1:L:210:ASN:HA	2.13	0.48
2:H:116:THR:HG21	2:H:214:ALA:O	2.13	0.48
1:L:95:PRO:HD3	2:H:61:GLN:OE1	2.14	0.48
2:H:38:ARG:HG2	2:H:39:GLN:N	2.30	0.46
1:L:131:SER:HA	1:L:179:LEU:O	2.15	0.46
2:H:126:PRO:O	2:H:128:CYS:SG	2.67	0.46
1:L:24:ARG:HA	1:L:69:THR:O	2.15	0.46
1:L:63:SER:O	1:L:73:LEU:HD12	2.15	0.46
1:L:95:PRO:HG3	2:H:62:LYS:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HH11	1:L:172:THR:HG23	1.81	0.45
2:H:4:LEU:HA	2:H:23:LYS:O	2.17	0.45
1:L:182:THR:HB	1:L:185:GLU:H	1.80	0.45
2:H:2:VAL:HG21	2:H:102:TYR:CZ	2.52	0.45
1:L:4:MET:CE	1:L:23:CYS:SG	3.04	0.45
2:H:123:PRO:O	2:H:124:LEU:HD23	2.17	0.45
2:H:205:ILE:H	2:H:222:LYS:NZ	2.13	0.44
1:L:61:ARG:HG2	1:L:77:ARG:NH1	2.32	0.44
2:H:28:ILE:HG22	2:H:29:PHE:CD2	2.53	0.44
1:L:30:ASN:HB2	1:L:32:TYR:CE2	2.53	0.44
2:H:128:CYS:SG	2:H:129:GLY:N	2.91	0.43
1:L:124:GLN:O	1:L:127:SER:HB3	2.18	0.43
1:L:136:LEU:HD11	1:L:146:VAL:HG21	1.99	0.43
1:L:87:PHE:HE2	2:H:43:LYS:O	2.01	0.43
1:L:193:THR:HG23	1:L:206:VAL:HG13	2.01	0.43
2:H:126:PRO:C	2:H:128:CYS:SG	2.97	0.42
2:H:61:GLN:H	2:H:61:GLN:CD	2.23	0.42
2:H:199:TRP:CZ2	2:H:223:ILE:HG22	2.55	0.42
2:H:52(A):PRO:HB3	2:H:71:VAL:HG21	2.02	0.42
1:L:27(B):LEU:HB2	1:L:31:THR:HG23	2.02	0.41
1:L:124:GLN:HG2	1:L:129:GLY:O	2.20	0.41
2:H:13:LYS:HD3	2:H:13:LYS:HA	1.89	0.41
1:L:163:TRP:HD1	1:L:164:THR:O	2.03	0.41
2:H:38:ARG:HD2	2:H:88:ALA:HB3	2.03	0.41
1:L:27(D):HIS:ND1	1:L:27(E):SER:N	2.69	0.41
2:H:171:VAL:HA	2:H:190:SER:O	2.21	0.41
1:L:39:LYS:HB3	1:L:39:LYS:HE3	1.88	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.88	0.40
1:L:147:LYS:HD3	1:L:154:GLU:HG3	2.02	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	L	216/219 (99%)	200 (93%)	13 (6%)	3 (1%)	11 28
2	H	215/218 (99%)	187 (87%)	22 (10%)	6 (3%)	5 11
All	All	431/437 (99%)	387 (90%)	35 (8%)	9 (2%)	7 18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	212	ASN
2	H	98	ASN
2	H	128	CYS
2	H	133	THR
2	H	97	GLY
1	L	51	VAL
1	L	169	LYS
2	H	130	ASP
2	H	180	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	L	193/196 (98%)	171 (89%)	22 (11%)	5 13
2	H	184/187 (98%)	161 (88%)	23 (12%)	4 10
All	All	377/383 (98%)	332 (88%)	45 (12%)	5 12

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	THR
1	L	18	GLN
1	L	27(E)	SER
1	L	51	VAL
1	L	63	SER
1	L	69	THR
1	L	70	ASP

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Mol	Chain	Res	Type
1	L	74	LYS
1	L	79	GLU
1	L	96	PRO
1	L	136	LEU
1	L	143	ASP
1	L	157	ASN
1	L	181	LEU
1	L	182	THR
1	L	187	GLU
1	L	195	GLU
1	L	199	LYS
1	L	200	THR
1	L	201	SER
1	L	202	THR
1	L	208	SER
2	H	13	LYS
2	H	14	PRO
2	H	32	PHE
2	H	43	LYS
2	H	44	SER
2	H	46	ASP
2	H	62	LYS
2	H	70	THR
2	H	74	SER
2	H	82(A)	ARG
2	H	83	THR
2	H	85	GLU
2	H	126	PRO
2	H	137	SER
2	H	138	VAL
2	H	149	PRO
2	H	150	GLU
2	H	151	PRO
2	H	166	LEU
2	H	194	THR
2	H	200	PRO
2	H	203	GLN
2	H	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	30	ASN
1	L	124	GLN
1	L	138	ASN

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 monosaccharides 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	L	218/219 (99%)	-0.53	1 (0%)	91	92	2, 13, 28, 34	0
2	H	217/218 (99%)	-0.19	8 (3%)	41	41	3, 19, 44, 60	0
All	All	435/437 (99%)	-0.36	9 (2%)	63	65	2, 15, 35, 60	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	29	PHE	7.3
2	H	129	GLY	4.2
2	H	128	CYS	3.3
2	H	134	THR	3.0
2	H	133	THR	2.5
2	H	164	GLY	2.5
1	L	213	GLU	2.2
2	H	27	TYR	2.1
2	H	2	VAL	2.0

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.