



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:49 PM UTC

PDB ID : 2HFF / pdb_00002hff
Title : Crystal structure of CB2 Fab
Authors : Hymowitz, S.G.
Deposited on : 2006-06-23
Resolution : 1.95 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

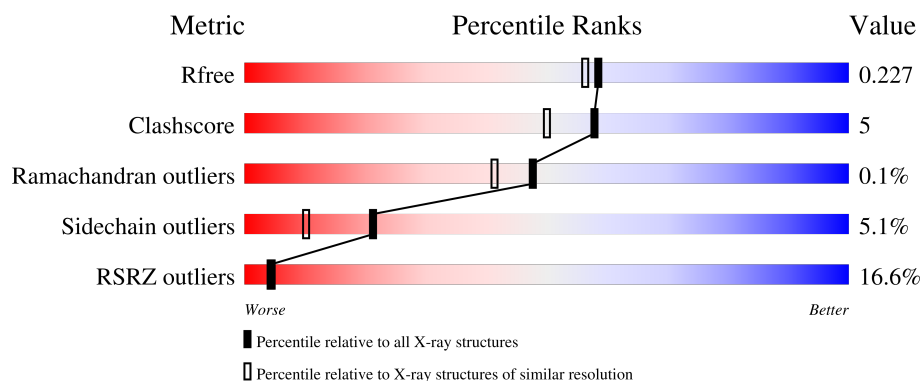
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	214	5% 84% 13% .
1	L	214	30% 87% 9% ..
2	B	232	8% 81% 9% . 8%
2	H	232	21% 82% 8% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6539 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 CB2 Fab, light chain.

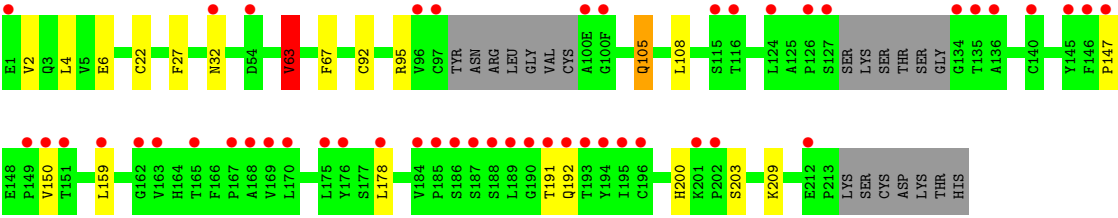
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1628	1019	273	330	6			
1	L	211	Total	C	N	O	S	0	0	0
			1617	1013	271	328	5			

- Molecule 2 is a protein called CB2 Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1581	994	267	313	7			
2	H	212	Total	C	N	O	S	0	0	0
			1563	982	265	310	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	56	Total	O	0	0
			56	56		
3	L	16	Total	O	0	0
			16	16		
3	H	41	Total	O	0	0
			41	41		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.71Å 72.98Å 89.92Å 109.42° 100.96° 96.10°	Depositor
Resolution (Å)	30.00 – 1.95 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-1.95) 97.6 (30.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.221 0.197 , 0.227	Depositor DCC
R_{free} test set	6425 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.52	0/1663	0.69	1/2259 (0.0%)
1	L	0.47	0/1652	0.65	0/2245
2	B	0.57	0/1617	0.71	3/2206 (0.1%)
2	H	0.53	0/1598	0.67	1/2180 (0.0%)
All	All	0.52	0/6530	0.68	5/8890 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	VAL	N-CA-CB	-6.64	104.43	112.33
2	B	63	VAL	N-CA-CB	-5.99	104.04	112.12
2	B	63	VAL	CB-CA-C	5.66	116.20	110.65
2	B	48	VAL	N-CA-C	5.04	115.98	111.90
1	A	66	GLY	N-CA-C	5.00	117.16	111.85

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	1628	0	1590	18	0
1	L	1617	0	1581	11	0
2	B	1581	0	1539	12	0
2	H	1563	0	1525	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	37	0	0	0	1
3	B	56	0	0	1	0
3	H	41	0	0	1	0
3	L	16	0	0	1	1
All	All	6539	0	6235	54	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 5.

All (54) 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:L:22:THR:HG23	3:L:214:HOH:O	1.85	0.76
2:H:22:CYS:HG	2:H:92:CYS:HG	0.86	0.76
1:A:133:CYS:HG	1:A:193:CYS:HG	0.93	0.74
2:B:95:ARG:NH2	3:B:252:HOH:O	2.20	0.73
2:H:95:ARG:NH2	3:H:239:HOH:O	2.26	0.69
1:A:4:MET:HE3	1:A:23:CYS:SG	2.35	0.67
2:B:105:GLN:HE21	2:B:105:GLN:H	1.40	0.66
2:B:6:GLU:H	2:B:105:GLN:HE22	1.43	0.65
1:A:188:HIS:O	1:A:210:ARG:NH1	2.29	0.65
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.78	0.64
1:L:4:MET:HE3	1:L:23:CYS:SG	2.39	0.62
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.64	0.62
2:H:6:GLU:H	2:H:105:GLN:HE22	1.48	0.62
2:B:147:PRO:O	2:B:200:HIS:HE1	1.84	0.60
2:H:147:PRO:O	2:H:200:HIS:HE1	1.84	0.60
1:A:90:GLN:HG3	1:A:97:THR:HG23	1.86	0.58
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.85	0.57
1:L:2:ILE:O	1:L:97:THR:HG21	2.07	0.54
2:B:199:ASN:HD21	2:B:206:LYS:HE3	1.72	0.54
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.89	0.54
1:A:106:ILE:H	1:A:165:GLN:HE22	1.54	0.54
1:A:2:ILE:O	1:A:97:THR:HG21	2.08	0.53
2:B:200:HIS:HD2	2:B:203:SER:OG	1.92	0.53
1:L:154:GLN:HB3	1:L:157:ASN:HD21	1.74	0.53
1:A:168:LYS:HG2	1:A:169:ASP:N	2.24	0.52
1:A:197:HIS:CD2	1:A:199:GLY:H	2.28	0.52
2:H:4:LEU:HD21	2:H:27:PHE:HZ	1.75	0.52
1:A:140:PRO:O	1:A:197:HIS:HE1	1.94	0.51
1:A:25:ALA:O	1:A:69:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:VAL:O	1:L:29:VAL:CG1	2.61	0.49
2:H:105:GLN:HE21	2:H:105:GLN:H	1.60	0.49
2:H:191:THR:OG1	2:H:192:GLN:N	2.45	0.49
2:H:105:GLN:H	2:H:105:GLN:NE2	2.12	0.48
2:H:2:VAL:HG13	2:H:27:PHE:HD1	1.79	0.48
1:L:106:ILE:H	1:L:165:GLN:HE22	1.61	0.47
1:A:154:GLN:HB3	1:A:157:ASN:HD21	1.80	0.47
2:B:143:LYS:NZ	2:B:171:GLN:HE22	2.12	0.47
2:H:178:LEU:C	2:H:178:LEU:HD12	2.39	0.47
1:A:189:LYS:NZ	1:A:213:CYS:SG	2.80	0.46
2:B:178:LEU:HD12	2:B:178:LEU:C	2.41	0.46
2:H:200:HIS:HD2	2:H:203:SER:OG	1.99	0.45
1:A:90:GLN:CG	1:A:97:THR:HG23	2.46	0.45
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.51	0.45
1:A:28:ASP:OD1	1:A:68:GLY:HA2	2.17	0.45
2:B:192:GLN:HG2	2:B:194:TYR:CZ	2.53	0.44
1:L:107:ARG:HD3	1:L:108:THR:O	2.18	0.44
1:A:107:ARG:HD3	1:A:108:THR:O	2.19	0.42
1:L:105:GLU:HG2	1:L:165:GLN:HE22	1.84	0.42
1:L:112:PRO:HD3	1:L:197:HIS:CD2	2.55	0.42
2:B:20:LEU:HG	2:B:82:MET:HE2	2.00	0.42
1:L:9:SER:HB3	1:L:100:GLN:HE22	1.85	0.42
1:A:139:TYR:CG	1:A:140:PRO:HA	2.55	0.41
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.86	0.40
2:B:22:CYS:HG	2:B:92:CYS:CB	2.28	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:232:HOH:O	3:L:221:HOH:O[1_554]	1.85	0.35

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	L	209/214 (98%)	201 (96%)	7 (3%)	1 (0%)	24	16
2	B	208/232 (90%)	206 (99%)	2 (1%)	0	100	100
2	H	206/232 (89%)	202 (98%)	4 (2%)	0	100	100
All	All	834/892 (94%)	813 (98%)	20 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	155	SER

5.3.2 Protein sidechains ⓘ

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	187/188 (100%)	178 (95%)	9 (5%)	23	12
1	L	186/188 (99%)	176 (95%)	10 (5%)	20	9
2	B	175/192 (91%)	164 (94%)	11 (6%)	16	6
2	H	173/192 (90%)	166 (96%)	7 (4%)	28	17
All	All	721/760 (95%)	684 (95%)	37 (5%)	21	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	97	THR
1	A	100	GLN
1	A	107	ARG
1	A	121	ASP
1	A	124	LEU
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	168	LYS
1	A	213	CYS
2	B	3	GLN
2	B	12	VAL
2	B	48	VAL
2	B	63	VAL
2	B	105	GLN
2	B	108	LEU
2	B	150	VAL
2	B	159	LEU
2	B	170	LEU
2	B	178	LEU
2	B	199	ASN
1	L	3	GLN
1	L	29	VAL
1	L	69	THR
1	L	90	GLN
1	L	97	THR
1	L	100	GLN
1	L	103	LYS
1	L	107	ARG
1	L	157	ASN
1	L	168	LYS
2	H	32	ASN
2	H	63	VAL
2	H	105	GLN
2	H	108	LEU
2	H	150	VAL
2	H	159	LEU
2	H	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	27	GLN
1	A	37	GLN
1	A	38	GLN
1	A	79	GLN
1	A	157	ASN
1	A	165	GLN
1	A	197	HIS

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Mol	Chain	Res	Type
1	A	198	GLN
1	A	209	ASN
2	B	13	GLN
2	B	39	GLN
2	B	105	GLN
2	B	171	GLN
2	B	199	ASN
2	B	200	HIS
1	L	6	GLN
1	L	38	GLN
1	L	79	GLN
1	L	100	GLN
1	L	136	ASN
1	L	157	ASN
1	L	165	GLN
1	L	197	HIS
1	L	209	ASN
2	H	13	GLN
2	H	39	GLN
2	H	105	GLN
2	H	164	HIS
2	H	171	GLN
2	H	192	GLN
2	H	199	ASN
2	H	200	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 oligosaccharides 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 [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	213/214 (99%)	0.71	10 (4%) 36 42	29, 37, 49, 67	0
1	L	211/214 (98%)	1.62	64 (30%) 1 1	30, 39, 47, 51	0
2	B	214/232 (92%)	0.72	18 (8%) 17 19	30, 37, 49, 70	0
2	H	212/232 (91%)	1.28	49 (23%) 2 2	30, 38, 49, 68	0
All	All	850/892 (95%)	1.08	141 (16%) 4 4	29, 38, 48, 70	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	97	CYS	6.5
1	A	213	CYS	5.8
1	L	163	THR	5.7
1	L	139	TYR	5.5
1	L	172	TYR	4.9
1	L	171	THR	4.8
1	L	183	ALA	4.8
1	L	110	ALA	4.8
1	A	155	SER	4.7
2	H	190	GLY	4.6
1	L	199	GLY	4.6
1	L	149	VAL	4.5
1	L	162	VAL	4.5
2	H	192	GLN	4.5
1	L	187	LYS	4.4
1	L	173	SER	4.4
2	H	134	GLY	4.3
1	L	113	SER	4.3
2	B	97	CYS	4.3
1	L	167	SER	4.3
2	B	134	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	161	SER	4.1
1	L	170	SER	4.1
2	H	176	TYR	4.1
1	L	174	LEU	4.1
2	H	191	THR	4.0
2	B	98	TYR	4.0
2	H	96	VAL	3.9
2	B	196	CYS	3.9
2	H	150	VAL	3.8
2	H	146	PHE	3.8
2	H	189	LEU	3.8
2	H	136	ALA	3.7
2	H	147	PRO	3.7
2	H	168	ALA	3.6
1	L	166	ASP	3.6
2	H	188	SER	3.6
1	L	135	LEU	3.6
1	L	153	LEU	3.6
1	L	152	ALA	3.6
1	L	121	ASP	3.6
1	L	124	LEU	3.5
2	B	190	GLY	3.5
2	H	162	GLY	3.5
2	H	100(E)	ALA	3.4
1	L	164	GLU	3.4
1	L	208	PHE	3.4
1	L	127	GLY	3.3
2	H	127	SER	3.3
2	H	186	SER	3.3
2	H	187	SER	3.3
2	H	169	VAL	3.3
2	H	185	PRO	3.3
2	H	201	LYS	3.1
1	L	200	LEU	3.1
2	B	214	LYS	3.1
1	L	138	PHE	3.1
2	H	202	PRO	3.1
2	B	1	GLU	3.1
1	L	147	TRP	3.0
1	L	1	ASP	3.0
2	H	100(F)	GLY	3.0
1	L	111	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	149	PRO	3.0
2	H	193	THR	2.9
2	H	140	CYS	2.9
1	L	134	LEU	2.9
2	H	184	VAL	2.9
1	L	202	SER	2.9
2	H	170	LEU	2.8
1	L	140	PRO	2.8
2	B	100(E)	ALA	2.8
1	L	88	CYS	2.8
2	H	212	GLU	2.8
2	H	115	SER	2.8
2	B	140	CYS	2.8
2	H	151	THR	2.8
2	B	186	SER	2.7
2	H	163	VAL	2.7
1	A	212	GLU	2.7
1	L	193	CYS	2.7
2	H	196	CYS	2.7
1	L	97	THR	2.7
1	L	209	ASN	2.7
2	H	116	THR	2.7
1	L	143	ALA	2.6
1	A	211	GLY	2.6
1	L	186	GLU	2.6
1	L	151	ASN	2.6
1	L	201	SER	2.6
2	H	126	PRO	2.5
2	B	100(F)	GLY	2.5
1	L	165	GLN	2.5
2	H	167	PRO	2.5
2	H	195	ILE	2.5
1	L	169	ASP	2.4
1	L	114	VAL	2.4
1	L	119	PRO	2.4
1	L	148	LYS	2.4
2	H	135	THR	2.3
1	A	168	LYS	2.3
1	L	128	THR	2.3
1	L	115	PHE	2.3
2	H	175	LEU	2.3
1	A	108	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	136	ASN	2.3
2	B	135	THR	2.3
1	A	156	GLY	2.3
1	L	175	SER	2.3
2	B	18	LEU	2.3
2	H	145	TYR	2.2
1	L	126	SER	2.2
2	B	161	SER	2.2
1	L	141	ARG	2.2
1	L	157	ASN	2.2
2	H	124	LEU	2.2
1	L	150	ASP	2.2
1	L	197	HIS	2.2
2	B	2	VAL	2.2
2	B	193	THR	2.2
1	L	80	PRO	2.2
2	H	32	ASN	2.1
1	L	191	TYR	2.1
2	H	194	TYR	2.1
1	L	198	GLN	2.1
2	H	165	THR	2.1
1	A	126	SER	2.1
1	L	112	PRO	2.1
2	H	178	LEU	2.1
1	L	137	ASN	2.1
1	L	12	SER	2.1
2	B	127	SER	2.1
2	H	1	GLU	2.1
2	H	54	ASP	2.1
1	L	181	SER	2.1
2	B	213	PRO	2.1
1	L	60	SER	2.0
1	A	23	CYS	2.0
2	H	159	LEU	2.0
1	L	168	LYS	2.0
1	A	12	SER	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 [i](#)

There are no oligosaccharides 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.