



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 4KUC / pdb_00004kuc
Title : Crystal structure of ricin-A chain in complex with the antibody 6C2
Authors : Zhu, Y.; Li, X.; Teng, M.
Deposited on : 2013-05-21
Resolution : 2.79 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

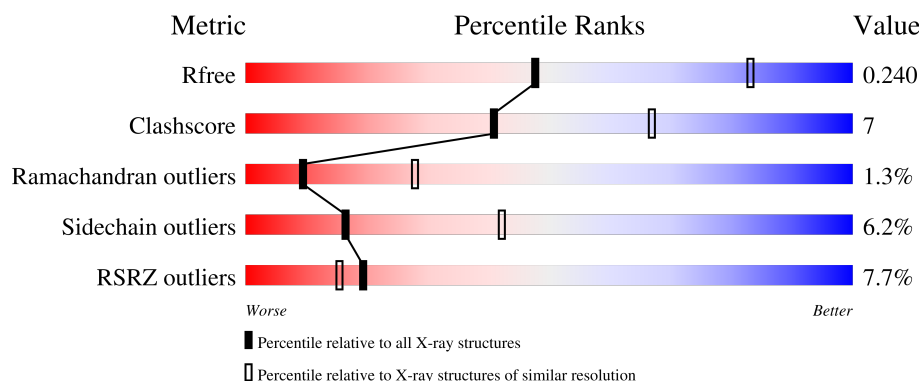
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 $\leq 5\%$. 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	267	82% 14% .
1	I	267	83% 13% .
2	D	231	10% 70% 17% . 10%
2	E	231	10% 35% 10% . 53%
3	F	237	8% 42% 8% . 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	237	8% 70% 14% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8287 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 Ricin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1987	1259	353	370	5			
1	I	259	Total	C	N	O	S	0	0	0
			1989	1260	353	371	5			

- Molecule 2 is a protein called mAb6c2 fab-Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total	C	N	O	S	0	0	0
			1397	881	240	272	4			
2	E	109	Total	C	N	O	S	0	0	0
			732	463	130	137	2			

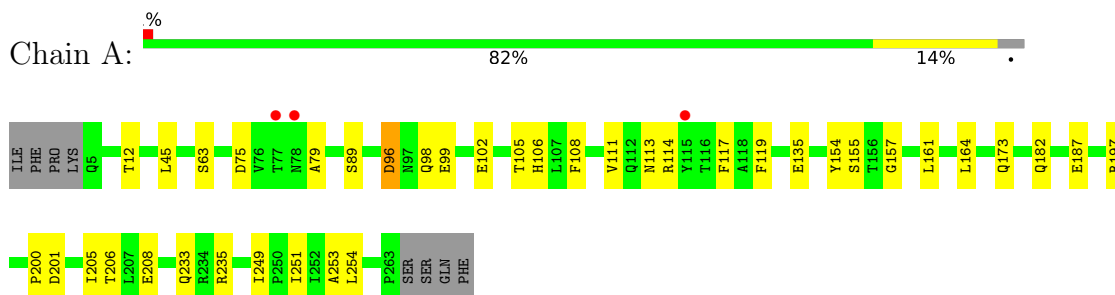
- Molecule 3 is a protein called mAb6c2 fab-Light chain.

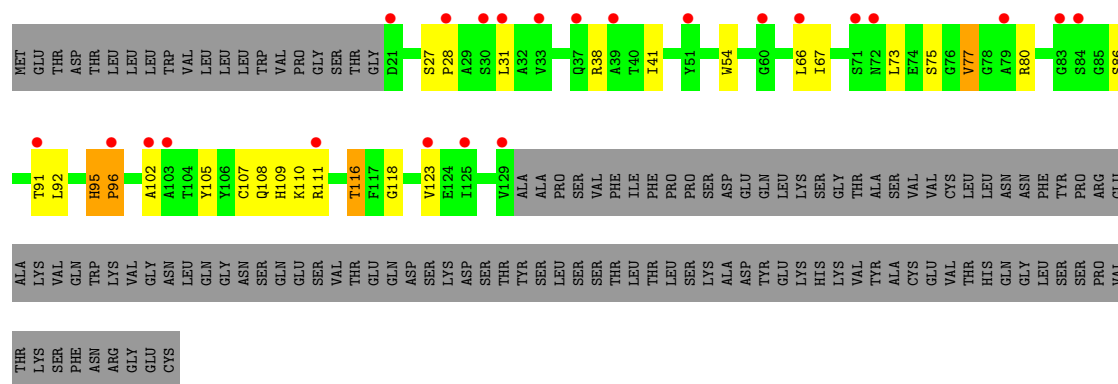
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	202	Total	C	N	O	S	0	0	0
			1361	879	224	254	4			
3	F	119	Total	C	N	O	S	0	0	0
			821	526	135	158	2			

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: Ricin





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.52Å 151.80Å 208.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.44 – 2.79 36.44 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.6 (36.44-2.79) 93.6 (36.44-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.289 0.240 , 0.240	Depositor DCC
R_{free} test set	2025 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	1.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.4	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	0.91	EDS
Total number of atoms	8287	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.60	1/2031 (0.0%)	0.91	4/2769 (0.1%)
1	I	0.58	0/2033	0.89	3/2772 (0.1%)
2	D	0.70	0/1430	1.00	5/1967 (0.3%)
2	E	0.49	0/749	0.89	4/1026 (0.4%)
3	F	0.48	0/844	0.82	0/1161
3	H	0.68	0/1398	1.01	4/1929 (0.2%)
All	All	0.61	1/8485 (0.0%)	0.93	20/11624 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	ILE	CA-CB	5.22	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ILE	CA-C-N	-8.57	111.06	121.00
1	A	249	ILE	C-N-CA	-8.57	111.06	121.00
2	E	95	HIS	CA-C-N	-6.37	111.88	119.84
2	E	95	HIS	C-N-CA	-6.37	111.88	119.84
2	E	77	VAL	CA-C-N	6.20	125.88	119.92
2	E	77	VAL	C-N-CA	6.20	125.88	119.92
2	D	156	ASN	N-CA-C	5.88	119.64	110.17
3	H	225	LYS	CA-C-N	5.67	126.17	120.04
3	H	225	LYS	C-N-CA	5.67	126.17	120.04
1	A	251	ILE	N-CA-C	5.58	116.35	111.56
2	D	95	HIS	CA-C-N	-5.45	113.03	119.84
2	D	95	HIS	C-N-CA	-5.45	113.03	119.84
3	H	183	SER	N-CA-C	5.40	126.13	111.00
1	I	249	ILE	CB-CA-C	-5.38	108.65	114.35
1	I	228	SER	CA-C-N	-5.37	115.05	120.31
1	I	228	SER	C-N-CA	-5.37	115.05	120.31
2	D	220	SER	CA-C-N	5.30	126.13	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	220	SER	C-N-CA	5.30	126.13	119.98
1	A	249	ILE	CB-CA-C	-5.07	108.98	114.35
3	H	139	SER	N-CA-C	5.01	117.31	108.75

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	1987	0	1898	23	0
1	I	1989	0	1903	23	0
2	D	1397	0	1166	27	0
2	E	732	0	627	13	0
3	F	821	0	660	8	0
3	H	1361	0	1124	20	0
All	All	8287	0	7378	102	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 7.

All (102) 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)
3:H:183:SER:HB2	3:H:184:GLY:CA	1.58	1.31
3:H:183:SER:CB	3:H:184:GLY:HA2	1.62	1.28
1:A:98:GLN:HE22	3:H:119:VAL:HG13	1.32	0.94
3:H:184:GLY:HA3	3:H:185:ALA:HB2	1.46	0.94
3:H:183:SER:CB	3:H:184:GLY:CA	2.34	0.83
1:I:12:THR:HG22	1:I:63:SER:HB2	1.64	0.79
1:A:187:GLU:OE2	1:A:235:ARG:NH2	2.24	0.71
2:E:54:TRP:HB2	2:E:67:ILE:HB	1.73	0.70
3:H:183:SER:HB2	3:H:184:GLY:HA2	0.74	0.67
1:A:12:THR:HG22	1:A:63:SER:HB2	1.77	0.67
3:H:189:HIS:HB2	3:H:206:VAL:HG13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:HIS:HB2	2:D:108:GLN:HB3	1.79	0.65
2:D:95:HIS:CG	2:D:96:PRO:HD3	2.32	0.64
3:F:126:ALA:HB3	3:F:127:LEU:HA	1.80	0.62
2:E:95:HIS:CG	2:E:96:PRO:HD3	2.37	0.59
1:A:96:ASP:OD1	1:A:96:ASP:N	2.24	0.59
1:I:105:THR:HG22	2:E:111:ARG:NH2	2.19	0.58
3:F:125:SER:OG	3:F:127:LEU:CB	2.52	0.57
1:I:105:THR:HG22	2:E:111:ARG:HH21	1.70	0.57
1:A:108:PHE:O	1:A:111:VAL:HG22	2.04	0.56
1:A:114:ARG:HH21	2:D:111:ARG:HH22	1.54	0.56
2:D:68:TYR:CE1	3:H:126:ALA:HB2	2.40	0.56
1:I:99:GLU:CD	3:F:76:ARG:HH21	2.14	0.55
3:F:105:LEU:HD22	3:F:109:ASP:HB3	1.88	0.55
3:H:184:GLY:HA3	3:H:185:ALA:CB	2.17	0.55
1:A:98:GLN:NE2	3:H:119:VAL:HG13	2.14	0.54
2:D:170:GLY:HA2	2:D:208:VAL:HB	1.88	0.54
2:E:41:ILE:HD12	2:E:92:LEU:HD23	1.90	0.54
1:A:45:LEU:HD21	1:A:254:LEU:HD13	1.91	0.53
1:A:102:GLU:OE1	1:A:106:HIS:NE2	2.39	0.53
1:I:182:GLN:HG3	1:I:253:ALA:HB2	1.92	0.52
1:A:173:GLN:NE2	1:A:208:GLU:OE2	2.42	0.52
1:I:48:ARG:HH22	1:I:97:ASN:HD21	1.58	0.52
1:I:151:LEU:HD12	1:I:164:LEU:HD12	1.92	0.51
1:I:117:PHE:HB3	1:I:119:PHE:CE1	2.46	0.51
2:D:99:GLU:C	2:D:101:ASP:H	2.19	0.51
2:D:111:ARG:O	2:D:111:ARG:NH2	2.43	0.51
1:I:64:ASN:HB2	1:I:145:GLU:CD	2.37	0.50
2:D:102:ALA:HA	2:D:123:VAL:HG13	1.94	0.50
1:A:154:TYR:CE2	1:A:164:LEU:HD22	2.46	0.50
2:E:66:LEU:HD22	2:E:105:TYR:HE2	1.77	0.49
3:H:72:PRO:HB3	3:H:91:VAL:HG21	1.94	0.49
2:E:28:PRO:HG2	2:E:31:LEU:HB2	1.93	0.49
3:H:59:ARG:HG2	3:H:111:ALA:HB2	1.95	0.48
2:D:54:TRP:HB2	2:D:67:ILE:HB	1.94	0.48
1:A:75:ASP:O	1:A:79:ALA:N	2.42	0.48
2:E:107:CYS:O	2:E:118:GLY:N	2.46	0.48
2:D:68:TYR:CD1	3:H:126:ALA:HB2	2.49	0.48
1:A:197:ARG:O	1:A:197:ARG:HG3	2.13	0.48
2:D:132:PRO:HB3	2:D:158:PHE:HB3	1.95	0.48
3:H:182:GLY:N	3:H:183:SER:HA	2.28	0.48
1:I:96:ASP:OD1	1:I:96:ASP:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:PRO:HG2	1:I:205:ILE:HD11	1.96	0.47
2:E:102:ALA:HA	2:E:123:VAL:HG13	1.96	0.47
1:A:102:GLU:OE2	3:H:76:ARG:NH1	2.47	0.47
3:H:146:PRO:HB3	3:H:172:TYR:HB3	1.96	0.47
1:A:201:ASP:CG	1:A:235:ARG:HG2	2.39	0.47
1:I:197:ARG:O	1:I:197:ARG:HG3	2.14	0.47
1:I:99:GLU:OE2	3:F:76:ARG:NH2	2.45	0.45
1:A:200:PRO:HG2	1:A:205:ILE:HD11	1.98	0.45
1:A:182:GLN:HG3	1:A:253:ALA:HB2	1.99	0.45
3:F:39:LEU:HD22	3:F:134:THR:HG21	1.98	0.44
2:D:216:GLN:O	2:D:218:LEU:N	2.50	0.44
2:D:155:LEU:HB2	2:D:192:LEU:HB3	2.00	0.44
1:I:11:PHE:HB2	1:I:24:PHE:CD1	2.53	0.44
1:I:173:GLN:NE2	1:I:208:GLU:OE2	2.49	0.44
2:E:27:SER:HA	2:E:28:PRO:HA	1.77	0.44
2:E:75:SER:C	2:E:77:VAL:H	2.26	0.44
1:A:12:THR:HA	1:A:63:SER:O	2.18	0.43
2:D:85:GLY:HA3	2:D:90:PHE:HA	2.00	0.43
1:I:44:VAL:HG22	1:I:255:MET:HE3	2.01	0.43
2:E:108:GLN:HG2	2:E:116:THR:O	2.18	0.43
2:D:67:ILE:CD1	2:D:92:LEU:HD13	2.49	0.43
1:I:161:LEU:HB3	1:I:162:PRO:HD3	2.00	0.43
2:D:67:ILE:HD12	2:D:92:LEU:HD13	2.00	0.43
2:D:181:THR:OG1	2:D:191:SER:HB2	2.18	0.43
1:I:171:CYS:O	1:I:175:ILE:HG12	2.19	0.43
1:A:206:THR:HG21	1:A:233:GLN:N	2.34	0.43
2:D:215:HIS:CG	2:D:216:GLN:N	2.87	0.43
1:I:91:TYR:OH	1:I:155:SER:HA	2.19	0.43
2:D:108:GLN:NE2	2:D:109:HIS:O	2.51	0.42
2:D:111:ARG:HA	2:D:111:ARG:HD2	1.65	0.42
3:F:56:VAL:HG11	3:F:64:LEU:HG	2.01	0.42
2:D:129:VAL:HG21	2:D:216:GLN:OE1	2.18	0.42
3:H:31:VAL:HG11	3:H:105:LEU:HD12	2.01	0.42
1:A:89:SER:HA	1:A:113:ASN:O	2.20	0.42
1:A:105:THR:HG22	2:D:111:ARG:NH2	2.34	0.42
2:D:192:LEU:HD23	2:D:193:SER:N	2.35	0.42
2:D:79:ALA:C	2:D:81:PHE:H	2.27	0.42
3:H:58:GLN:HG3	3:H:63:GLY:O	2.20	0.41
3:H:166:GLY:HA2	3:H:205:SER:O	2.20	0.41
1:I:154:TYR:CE1	1:I:164:LEU:HD22	2.55	0.41
2:D:183:GLN:HB2	2:D:190:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:HB3	1:A:119:PHE:CE1	2.55	0.41
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.91	0.41
2:D:99:GLU:C	2:D:101:ASP:N	2.78	0.41
2:D:156:ASN:OD1	3:H:206:VAL:HG21	2.21	0.41
1:I:48:ARG:HH22	1:I:97:ASN:ND2	2.18	0.41
2:E:107:CYS:SG	2:E:118:GLY:HA3	2.61	0.41
3:F:121:GLY:O	3:F:123:PHE:N	2.41	0.40
1:I:161:LEU:HA	1:I:161:LEU:HD12	1.87	0.40
1:I:206:THR:HG21	1:I:233:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

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	257/267 (96%)	248 (96%)	8 (3%)	1 (0%)	30	57
1	I	257/267 (96%)	247 (96%)	9 (4%)	1 (0%)	30	57
2	D	206/231 (89%)	183 (89%)	18 (9%)	5 (2%)	4	15
2	E	107/231 (46%)	96 (90%)	9 (8%)	2 (2%)	6	19
3	F	117/237 (49%)	101 (86%)	14 (12%)	2 (2%)	7	22
3	H	196/237 (83%)	176 (90%)	16 (8%)	4 (2%)	6	18
All	All	1140/1470 (78%)	1051 (92%)	74 (6%)	15 (1%)	9	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	96	PRO
2	D	146	SER
2	D	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	228	ASN
3	F	122	ASN
2	D	217	GLY
3	H	143	THR
3	H	185	ALA
1	I	157	GLY
2	E	80	ARG
2	E	96	PRO
2	D	171	ASN
3	F	123	PHE
1	A	157	GLY
3	H	146	PRO

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	200/226 (88%)	196 (98%)	4 (2%)	48	77
1	I	201/226 (89%)	199 (99%)	2 (1%)	68	86
2	D	118/201 (59%)	106 (90%)	12 (10%)	7	21
2	E	59/201 (29%)	52 (88%)	7 (12%)	5	15
3	F	67/201 (33%)	59 (88%)	8 (12%)	5	15
3	H	114/201 (57%)	100 (88%)	14 (12%)	4	14
All	All	759/1256 (60%)	712 (94%)	47 (6%)	16	42

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	99	GLU
1	A	135	GLU
1	A	155	SER
2	D	42	SER
2	D	66	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	73	LEU
2	D	108	GLN
2	D	109	HIS
2	D	111	ARG
2	D	116	THR
2	D	152	VAL
2	D	154	LEU
2	D	169	VAL
2	D	181	THR
2	D	184	ASP
3	H	30	LEU
3	H	31	VAL
3	H	36	SER
3	H	47	THR
3	H	64	LEU
3	H	74	SER
3	H	94	SER
3	H	98	VAL
3	H	102	VAL
3	H	179	VAL
3	H	195	LEU
3	H	206	VAL
3	H	208	THR
3	H	220	CYS
1	I	96	ASP
1	I	135	GLU
2	E	38	ARG
2	E	73	LEU
2	E	86	SER
2	E	91	THR
2	E	109	HIS
2	E	110	LYS
2	E	116	THR
3	F	31	VAL
3	F	37	VAL
3	F	47	THR
3	F	90	THR
3	F	93	THR
3	F	94	SER
3	F	102	VAL
3	F	105	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	23	ASN
1	A	98	GLN
1	A	113	ASN
1	A	136	ASN
1	A	231	GLN
2	D	55	ASN
3	H	221	ASN
1	I	19	GLN
1	I	23	ASN
1	I	47	ASN
1	I	141	ASN
1	I	182	GLN
3	F	69	ASN
3	F	78	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 oligosaccharides 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 ⓘ

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, 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	259/267 (97%)	0.16	3 (1%) 76 70	27, 42, 57, 68	2 (0%)
1	I	259/267 (97%)	0.22	3 (1%) 76 70	30, 45, 60, 87	1 (0%)
2	D	208/231 (90%)	0.64	22 (10%) 11 9	34, 51, 84, 96	0
2	E	109/231 (47%)	1.28	23 (21%) 2 2	46, 75, 114, 147	0
3	F	119/237 (50%)	1.15	20 (16%) 4 3	47, 72, 96, 107	0
3	H	202/237 (85%)	0.53	18 (8%) 15 12	29, 46, 63, 76	0
All	All	1156/1470 (78%)	0.53	89 (7%) 19 15	27, 48, 89, 147	3 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	124	ASP	5.5
2	E	129	VAL	5.3
3	F	85	ASN	4.9
3	F	125	SER	4.4
2	D	175	ASN	4.2
3	F	135	SER	3.8
3	F	126	ALA	3.6
2	E	71	SER	3.6
2	E	37	GLN	3.6
3	H	182	GLY	3.6
3	H	124	ASP	3.5
2	E	72	ASN	3.4
1	I	263	PRO	3.4
2	D	154	LEU	3.3
2	E	96	PRO	3.2
2	E	51	TYR	3.1
1	I	262	PRO	3.1
2	E	91	THR	3.1
2	D	150	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	39	ALA	3.0
2	D	174	GLY	2.9
1	A	77	THR	2.9
3	H	117	ARG	2.9
3	F	123	PHE	2.9
2	E	125	ILE	2.9
2	D	208	VAL	2.9
2	E	30	SER	2.8
3	H	214	LEU	2.8
3	H	129	TYR	2.8
2	E	31	LEU	2.8
2	D	220	SER	2.8
2	E	103	ALA	2.8
3	F	114	TYR	2.8
3	F	104	SER	2.7
3	F	122	ASN	2.7
2	D	66	LEU	2.7
2	E	102	ALA	2.7
2	E	60	GLY	2.7
3	F	45	GLY	2.7
3	H	126	ALA	2.7
3	F	132	GLN	2.6
2	E	79	ALA	2.6
2	D	171	ASN	2.6
3	H	227	SER	2.6
3	H	162	THR	2.6
3	H	133	GLY	2.6
3	H	204	SER	2.5
3	F	137	THR	2.5
2	D	167	TRP	2.5
3	H	61	GLY	2.5
3	F	113	PHE	2.5
3	F	32	ARG	2.4
3	F	108	GLU	2.4
2	D	209	TYR	2.4
2	E	111	ARG	2.4
2	E	66	LEU	2.4
2	D	170	GLY	2.4
2	D	214	THR	2.4
3	H	125	SER	2.4
2	E	33	VAL	2.3
2	D	201	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	67	ILE	2.3
3	F	28	SER	2.3
3	H	145	GLY	2.3
3	F	86	LYS	2.3
3	H	45	GLY	2.3
3	F	43	ALA	2.2
2	D	78	GLY	2.2
2	D	177	GLN	2.2
3	F	106	THR	2.2
1	A	78	ASN	2.2
2	D	223	THR	2.1
3	H	46	TYR	2.1
2	D	125	ILE	2.1
2	D	169	VAL	2.1
2	E	21	ASP	2.1
1	I	257	TYR	2.1
2	D	180	VAL	2.1
2	D	219	SER	2.1
2	E	84	SER	2.1
2	E	28	PRO	2.1
2	E	123	VAL	2.1
3	H	213	SER	2.0
2	D	37	GLN	2.0
3	H	62	GLN	2.0
2	E	83	GLY	2.0
1	A	115	TYR	2.0
3	H	171	ASP	2.0
2	D	217	GLY	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 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.