



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 06:25 PM EDT

PDB ID : 1CIC
Title : IDIOTOPE-ANTI-IDIOTOPE FAB-FAB COMPLEX; D1.3-E225
Authors : Bentley, G.A.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

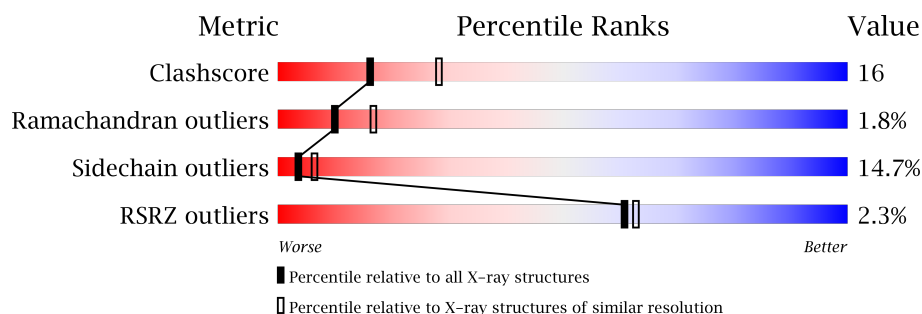
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 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 $\leq 5\%$. 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	<div> <div>2%</div> <div>48%</div> <div>42%</div> <div>9%</div> <div>.</div> </div>
2	B	217	<div> <div>3%</div> <div>63%</div> <div>28%</div> <div>9%</div> </div>
3	C	214	<div> <div>2%</div> <div>57%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
4	D	218	<div> <div>2%</div> <div>63%</div> <div>28%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6733 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 PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1668	1038	283	338	9			

- Molecule 2 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1629	1030	262	329	8			

- Molecule 3 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1665	1037	281	340	7			

- Molecule 4 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1643	1030	279	326	8			

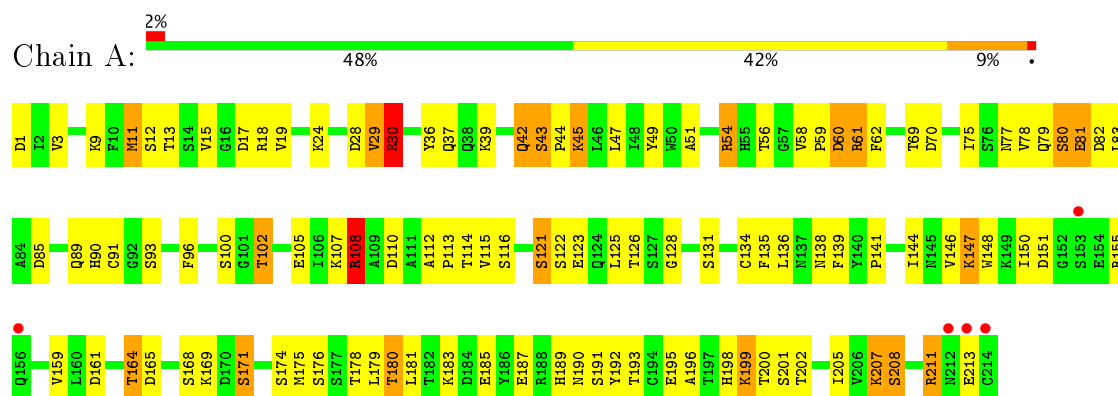
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	33	Total	O	0	0
			33	33		
5	C	34	Total	O	0	0
			34	34		
5	D	36	Total	O	0	0
			36	36		

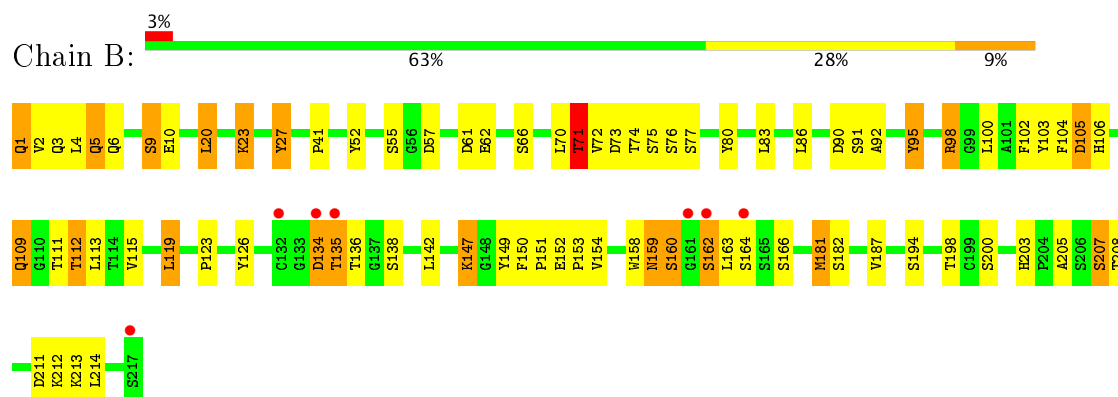
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

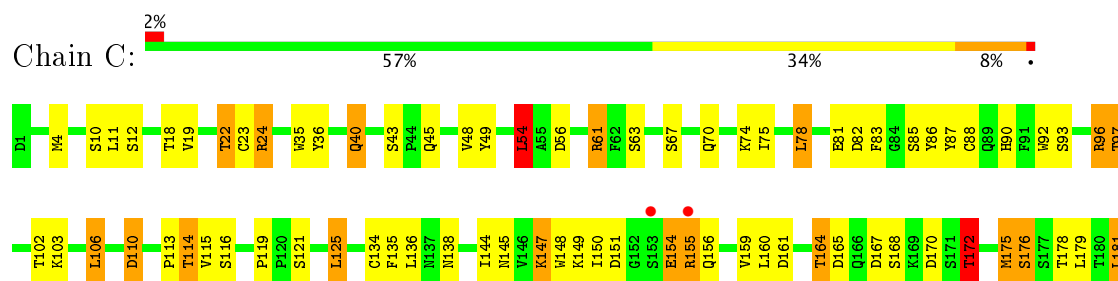
• Molecule 1: PROTEIN (IG HEAVY CHAIN V REGIONS)

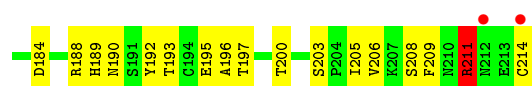


• Molecule 2: PROTEIN (IG HEAVY CHAIN V REGIONS)

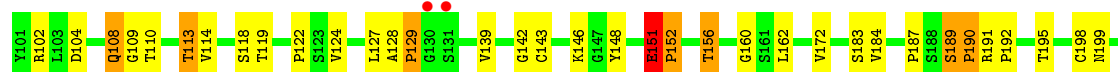


• Molecule 3: PROTEIN (IG HEAVY CHAIN V REGIONS)





• Molecule 4: PROTEIN (IG HEAVY CHAIN V REGIONS)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.11Å 77.65Å 96.75Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50 7.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 81.2 (7.00-2.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	203.33 (at 2.51Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.179 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6733	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	0.92	0/1707	1.71	28/2315 (1.2%)
2	B	1.01	0/1676	1.76	19/2294 (0.8%)
3	C	1.01	0/1705	1.77	25/2315 (1.1%)
4	D	1.03	0/1684	1.72	22/2300 (1.0%)
All	All	0.99	0/6772	1.74	94/9224 (1.0%)

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	ARG	NE-CZ-NH2	-13.24	113.68	120.30
3	C	61	ARG	NE-CZ-NH2	11.06	125.83	120.30
4	D	99	ARG	NE-CZ-NH2	-10.81	114.89	120.30
4	D	6	GLU	CA-CB-CG	10.63	136.79	113.40
4	D	58	ASP	CB-CG-OD2	10.38	127.64	118.30
3	C	24	ARG	NE-CZ-NH1	10.35	125.47	120.30
3	C	61	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	A	54	ARG	NE-CZ-NH2	-9.54	115.53	120.30
2	B	105	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	61	ARG	CA-CB-CG	9.42	134.12	113.40
2	B	73	ASP	CB-CG-OD1	9.33	126.70	118.30
2	B	57	ASP	CB-CG-OD1	-9.26	109.97	118.30
1	A	151	ASP	CB-CG-OD2	8.68	126.12	118.30
3	C	49	TYR	CB-CG-CD2	8.53	126.11	121.00
3	C	181	LEU	CA-CB-CG	8.33	134.46	115.30
4	D	92	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	B	152	GLU	CA-CB-CG	8.01	131.01	113.40
3	C	164	THR	CA-CB-CG2	7.99	123.59	112.40
2	B	103	TYR	CB-CG-CD2	7.88	125.73	121.00
4	D	100	ASP	CB-CG-OD1	-7.84	111.25	118.30
4	D	38	ARG	NE-CZ-NH2	-7.71	116.45	120.30
2	B	103	TYR	CB-CG-CD1	-7.38	116.57	121.00
2	B	71	THR	N-CA-CB	-7.35	96.33	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	45	LEU	N-CA-CB	-7.35	95.70	110.40
3	C	172	THR	N-CA-CB	-7.32	96.39	110.30
2	B	61	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	61	ARG	NE-CZ-NH2	-7.05	116.77	120.30
3	C	87	TYR	CB-CG-CD2	-7.02	116.79	121.00
2	B	74	THR	CA-CB-CG2	6.93	122.10	112.40
3	C	81	GLU	CB-CA-C	-6.90	96.60	110.40
3	C	61	ARG	CD-NE-CZ	-6.87	113.98	123.60
4	D	99	ARG	NE-CZ-NH1	6.84	123.72	120.30
4	D	151	GLU	CG-CD-OE1	6.84	131.99	118.30
1	A	85	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	1	ASP	CB-CG-OD1	6.80	124.42	118.30
3	C	56	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	128	GLY	N-CA-C	6.70	129.86	113.10
1	A	49	TYR	CB-CG-CD1	-6.62	117.03	121.00
3	C	97	THR	CA-CB-CG2	6.59	121.63	112.40
1	A	108	ARG	NE-CZ-NH2	6.58	123.59	120.30
4	D	94	TYR	CB-CG-CD2	-6.51	117.09	121.00
3	C	24	ARG	CA-CB-CG	6.38	127.44	113.40
4	D	14	PRO	C-N-CA	6.35	137.58	121.70
2	B	106	HIS	CA-CB-CG	-6.26	102.95	113.60
1	A	138	ASN	N-CA-CB	-6.24	99.36	110.60
1	A	108	ARG	CA-CB-CG	6.24	127.12	113.40
3	C	147	LYS	N-CA-CB	6.19	121.75	110.60
3	C	22	THR	N-CA-CB	-6.15	98.61	110.30
1	A	11	MET	CA-CB-CG	6.11	123.69	113.30
2	B	3	GLN	CA-CB-CG	6.09	126.80	113.40
1	A	61	ARG	N-CA-CB	6.08	121.54	110.60
4	D	104	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	54	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	B	61	ASP	CB-CG-OD1	6.06	123.76	118.30
3	C	87	TYR	O-C-N	6.01	132.31	122.70
1	A	77	ASN	N-CA-CB	-5.96	99.86	110.60
2	B	27	TYR	CB-CG-CD2	-5.94	117.44	121.00
4	D	25	SER	N-CA-CB	-5.89	101.67	110.50
4	D	212	LYS	CA-CB-CG	5.86	126.29	113.40
1	A	108	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	A	29	VAL	N-CA-CB	-5.84	98.65	111.50
4	D	3	GLN	CA-CB-CG	5.83	126.22	113.40
3	C	176	SER	N-CA-CB	5.79	119.19	110.50
2	B	98	ARG	NH1-CZ-NH2	5.75	125.72	119.40
4	D	67	LEU	N-CA-CB	-5.68	99.05	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	42	GLN	CA-CB-CG	5.61	125.75	113.40
2	B	5	GLN	CA-CB-CG	5.56	125.64	113.40
3	C	110	ASP	CB-CG-OD1	5.56	123.30	118.30
4	D	16	GLN	C-N-CA	5.52	135.49	121.70
4	D	151	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	A	42	GLN	CB-CA-C	5.45	121.30	110.40
3	C	56	ASP	CA-CB-CG	5.43	125.34	113.40
3	C	167	ASP	CB-CG-OD1	5.41	123.17	118.30
2	B	111	THR	O-C-N	5.40	131.34	122.70
1	A	36	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	102	THR	O-C-N	5.36	131.28	122.70
1	A	30	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	C	114	THR	N-CA-C	-5.34	96.59	111.00
3	C	114	THR	CA-CB-CG2	5.31	119.83	112.40
4	D	88	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	93	SER	CB-CA-C	5.24	120.06	110.10
4	D	108	GLN	CA-CB-CG	5.21	124.87	113.40
2	B	20	LEU	N-CA-CB	-5.19	100.03	110.40
1	A	213	GLU	CA-CB-CG	5.17	124.77	113.40
3	C	164	THR	CA-CB-OG1	-5.16	98.17	109.00
1	A	3	VAL	O-C-N	5.14	130.92	122.70
3	C	97	THR	N-CA-CB	-5.09	100.64	110.30
2	B	95	TYR	CA-CB-CG	5.08	123.06	113.40
1	A	70	ASP	CB-CG-OD2	5.07	122.86	118.30
4	D	94	TYR	O-C-N	5.07	130.81	122.70
4	D	97	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	114	THR	N-CA-C	-5.05	97.37	111.00
3	C	54	LEU	N-CA-CB	-5.01	100.39	110.40

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	1668	0	1589	71	0
2	B	1629	0	1562	44	0
3	C	1665	0	1582	58	0
4	D	1643	0	1612	41	0
5	A	25	0	0	0	0
5	B	33	0	0	1	0
5	C	34	0	0	0	0
5	D	36	0	0	0	0
All	All	6733	0	6345	206	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 16.

All (206) 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:C:4:MET:HG2	3:C:97:THR:HG22	1.24	1.15
4:D:195:THR:HG23	4:D:212:LYS:HE3	1.21	1.09
4:D:187:PRO:O	4:D:190:PRO:HD2	1.57	1.05
1:A:193:THR:HG22	1:A:208:SER:HB3	1.47	0.96
2:B:119:LEU:HD12	2:B:119:LEU:H	1.33	0.94
3:C:4:MET:HG2	3:C:97:THR:CG2	2.02	0.89
3:C:4:MET:CG	3:C:97:THR:HG22	2.03	0.89
1:A:190:ASN:HA	1:A:211:ARG:HB2	1.54	0.87
3:C:145:ASN:HB2	3:C:197:THR:HB	1.62	0.81
3:C:189:HIS:O	3:C:211:ARG:HD3	1.81	0.80
1:A:193:THR:HG22	1:A:208:SER:CB	2.13	0.78
4:D:195:THR:HG23	4:D:212:LYS:CE	2.10	0.78
4:D:67:LEU:HD11	4:D:80:LEU:HD11	1.66	0.78
1:A:207:LYS:HA	1:A:207:LYS:NZ	1.99	0.76
2:B:119:LEU:HD12	2:B:119:LEU:N	1.99	0.76
4:D:195:THR:CG2	4:D:212:LYS:HE3	2.10	0.76
2:B:160:SER:HB2	2:B:162:SER:OG	1.86	0.75
2:B:10:GLU:HB2	2:B:113:LEU:HD12	1.69	0.74
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.67	0.74
4:D:187:PRO:HG2	4:D:190:PRO:HG2	1.69	0.73
3:C:150:ILE:HD11	3:C:179:LEU:HD21	1.73	0.71
1:A:9:LYS:HD2	1:A:9:LYS:N	2.06	0.69
3:C:138:ASN:HA	3:C:172:THR:HG23	1.75	0.68
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.76	0.67
2:B:159:ASN:HD22	2:B:163:LEU:HD23	1.59	0.67
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:PRO:HG3	3:C:144:ILE:HD11	1.77	0.66
2:B:147:LYS:HB2	2:B:147:LYS:NZ	2.10	0.66
3:C:170:ASP:OD1	3:C:172:THR:HB	1.96	0.66
4:D:86:HIS:O	4:D:114:VAL:HG11	1.97	0.65
3:C:205:ILE:H	3:C:205:ILE:HD12	1.62	0.65
1:A:91:CYS:HB3	2:B:102:PHE:HB3	1.80	0.64
1:A:59:PRO:HG2	1:A:62:PHE:CD2	2.32	0.64
3:C:190:ASN:ND2	3:C:211:ARG:HB2	2.12	0.64
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.79	0.64
2:B:86:LEU:HA	2:B:90:ASP:OD2	1.99	0.63
1:A:189:HIS:O	1:A:211:ARG:HD3	1.98	0.62
3:C:40:GLN:HE21	3:C:165:ASP:HB3	1.66	0.61
2:B:119:LEU:CD1	2:B:119:LEU:H	2.07	0.60
2:B:147:LYS:CB	2:B:147:LYS:NZ	2.64	0.60
2:B:198:THR:HG23	2:B:213:LYS:HG2	1.83	0.60
1:A:136:LEU:HD13	1:A:175:MET:HE1	1.83	0.60
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.84	0.59
2:B:159:ASN:HD22	2:B:163:LEU:CD2	2.16	0.59
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.85	0.59
1:A:44:PRO:O	1:A:45:LYS:HD2	2.04	0.58
1:A:207:LYS:HA	1:A:207:LYS:HZ3	1.68	0.58
3:C:190:ASN:HA	3:C:211:ARG:HG3	1.86	0.57
4:D:187:PRO:HG2	4:D:190:PRO:CG	2.34	0.57
2:B:71:THR:HG22	2:B:80:TYR:HB2	1.85	0.57
1:A:159:VAL:HA	1:A:178:THR:O	2.04	0.57
2:B:181:MET:HG2	2:B:182:SER:N	2.18	0.57
2:B:91:SER:O	2:B:92:ALA:HB2	2.05	0.57
2:B:147:LYS:HB2	2:B:147:LYS:HZ1	1.70	0.56
3:C:205:ILE:HD12	3:C:205:ILE:N	2.21	0.56
3:C:24:ARG:HG3	3:C:24:ARG:HH11	1.70	0.55
1:A:17:ASP:O	1:A:78:VAL:HG23	2.07	0.55
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.37	0.55
1:A:125:LEU:HD22	1:A:183:LYS:HG3	1.88	0.54
1:A:207:LYS:HA	1:A:207:LYS:HZ2	1.71	0.54
3:C:151:ASP:OD2	3:C:189:HIS:HB3	2.07	0.54
3:C:85:SER:HA	3:C:102:THR:O	2.08	0.54
3:C:78:LEU:HD13	3:C:106:LEU:HD12	1.90	0.54
1:A:39:LYS:HD2	1:A:42:GLN:NE2	2.23	0.53
3:C:149:LYS:HB2	3:C:193:THR:HB	1.91	0.53
4:D:1:GLN:OE1	4:D:1:GLN:HA	2.08	0.53
1:A:205:ILE:H	1:A:205:ILE:HD12	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:O	1:A:155:ARG:N	2.41	0.53
3:C:149:LYS:O	3:C:193:THR:N	2.42	0.52
2:B:1:GLN:OE1	2:B:1:GLN:N	2.43	0.52
3:C:90:HIS:HD2	3:C:92:TRP:H	1.57	0.52
4:D:195:THR:HA	4:D:212:LYS:NZ	2.25	0.52
1:A:28:ASP:OD1	1:A:30:ARG:HD2	2.09	0.51
3:C:148:TRP:O	3:C:154:GLU:HA	2.11	0.51
4:D:189:SER:CB	4:D:190:PRO:HD3	2.41	0.51
2:B:142:LEU:HB3	2:B:214:LEU:HD22	1.93	0.51
2:B:6:GLN:O	2:B:109:GLN:NE2	2.43	0.51
1:A:121:SER:HB2	1:A:123:GLU:OE1	2.10	0.50
2:B:134:ASP:O	2:B:135:THR:OG1	2.26	0.50
3:C:195:GLU:HG2	3:C:206:VAL:HG23	1.92	0.50
1:A:181:LEU:HD22	1:A:185:GLU:CD	2.32	0.50
2:B:198:THR:HG23	2:B:212:LYS:C	2.32	0.50
2:B:198:THR:HA	2:B:212:LYS:O	2.12	0.50
3:C:184:ASP:HB2	3:C:188:ARG:HH21	1.76	0.50
1:A:181:LEU:HD22	1:A:185:GLU:OE2	2.12	0.50
3:C:61:ARG:NH1	3:C:82:ASP:OD2	2.45	0.50
3:C:119:PRO:HB3	3:C:209:PHE:CE2	2.47	0.49
4:D:18:LEU:HD21	4:D:20:ILE:HD11	1.94	0.49
2:B:76:SER:O	2:B:77:SER:HB2	2.12	0.49
4:D:122:PRO:HD2	4:D:207:THR:HG21	1.94	0.49
1:A:59:PRO:HG2	1:A:62:PHE:CE2	2.47	0.49
4:D:187:PRO:HG2	4:D:190:PRO:CD	2.43	0.49
1:A:125:LEU:O	1:A:183:LYS:HD3	2.12	0.49
3:C:155:ARG:HE	3:C:179:LEU:HD11	1.77	0.49
1:A:116:SER:O	1:A:134:CYS:HA	2.12	0.49
1:A:131:SER:OG	1:A:180:THR:HG23	2.13	0.48
2:B:158:TRP:HB2	2:B:163:LEU:O	2.13	0.48
3:C:36:TYR:O	3:C:86:TYR:HA	2.13	0.48
4:D:11:LEU:HA	4:D:113:THR:O	2.14	0.48
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.48	0.48
3:C:116:SER:O	3:C:134:CYS:HA	2.14	0.48
3:C:145:ASN:N	3:C:197:THR:O	2.45	0.48
3:C:93:SER:O	3:C:96:ARG:HD2	2.13	0.48
3:C:160:LEU:HD22	4:D:172:VAL:HG11	1.96	0.48
2:B:198:THR:CG2	2:B:213:LYS:HG2	2.44	0.48
2:B:83:LEU:HB3	2:B:86:LEU:HD21	1.96	0.47
1:A:110:ASP:OD2	1:A:199:LYS:HE2	2.13	0.47
4:D:119:THR:HG21	4:D:204:ALA:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:VAL:HB	4:D:209:VAL:HG11	1.97	0.47
1:A:89:GLN:HE21	1:A:96:PHE:HB3	1.78	0.47
2:B:159:ASN:HB3	2:B:163:LEU:HG	1.96	0.47
1:A:150:ILE:HG23	1:A:192:TYR:CE1	2.50	0.47
2:B:163:LEU:CD1	2:B:187:VAL:HG11	2.45	0.47
1:A:112:ALA:HB2	1:A:200:THR:HB	1.97	0.47
1:A:37:GLN:O	1:A:44:PRO:HA	2.15	0.47
2:B:23:LYS:HD3	2:B:23:LYS:C	2.35	0.47
4:D:203:PRO:O	4:D:205:SER:N	2.47	0.46
4:D:151:GLU:OE1	4:D:152:PRO:HA	2.15	0.46
1:A:136:LEU:HD13	1:A:175:MET:CE	2.46	0.46
1:A:139:PHE:CZ	1:A:144:ILE:HG21	2.51	0.46
1:A:15:VAL:HA	1:A:78:VAL:O	2.16	0.46
3:C:136:LEU:HD23	3:C:196:ALA:HB2	1.98	0.46
1:A:198:HIS:CD2	1:A:200:THR:OG1	2.67	0.46
1:A:164:THR:HB	1:A:174:SER:O	2.16	0.45
1:A:122:SER:O	1:A:126:THR:HG23	2.16	0.45
2:B:86:LEU:HB3	2:B:115:VAL:HG21	1.98	0.45
2:B:160:SER:C	2:B:162:SER:H	2.20	0.45
3:C:214:CYS:SG	4:D:216:ARG:CZ	3.05	0.45
2:B:150:PHE:CG	2:B:151:PRO:HA	2.51	0.45
3:C:113:PRO:HG3	3:C:144:ILE:CD1	2.44	0.45
3:C:193:THR:HG23	3:C:206:VAL:HG23	1.98	0.45
4:D:205:SER:O	4:D:206:SER:HB2	2.16	0.45
1:A:112:ALA:HB2	1:A:200:THR:CB	2.47	0.45
1:A:169:LYS:HA	1:A:169:LYS:HD3	1.83	0.45
3:C:161:ASP:HB3	3:C:175:MET:CE	2.47	0.45
4:D:162:LEU:HG	4:D:184:VAL:HG21	1.98	0.44
1:A:205:ILE:N	1:A:205:ILE:HD12	2.32	0.44
3:C:24:ARG:NH1	3:C:24:ARG:HG3	2.30	0.44
1:A:13:THR:OG1	1:A:17:ASP:HB2	2.17	0.44
3:C:192:TYR:HB2	3:C:209:PHE:CE1	2.52	0.44
3:C:48:VAL:HG22	3:C:54:LEU:HD12	2.00	0.44
4:D:122:PRO:HB3	4:D:148:TYR:HB3	2.00	0.44
1:A:30:ARG:HH22	4:D:54:ASP:CG	2.21	0.43
2:B:203:HIS:CE1	2:B:205:ALA:HB3	2.53	0.43
2:B:98:ARG:HD2	2:B:105:ASP:OD1	2.19	0.43
4:D:71:LYS:NZ	4:D:73:ASN:HD21	2.15	0.43
3:C:135:PHE:CE2	4:D:183:SER:HB3	2.54	0.43
3:C:145:ASN:O	3:C:196:ALA:HA	2.18	0.43
4:D:34:VAL:HG21	4:D:78:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:TYR:O	4:D:109:GLY:HA2	2.18	0.43
3:C:161:ASP:HB3	3:C:175:MET:HE1	2.00	0.43
1:A:54:ARG:NH2	1:A:60:ASP:HB3	2.33	0.43
3:C:121:SER:O	3:C:125:LEU:HD22	2.18	0.43
3:C:196:ALA:HB3	3:C:205:ILE:HB	1.99	0.43
3:C:190:ASN:CG	3:C:211:ARG:HB2	2.38	0.43
4:D:156:THR:HG23	4:D:160:GLY:N	2.34	0.43
4:D:214:VAL:HA	4:D:215:PRO:HD3	1.84	0.43
4:D:128:ALA:HA	4:D:129:PRO:HD3	1.79	0.42
1:A:43:SER:HA	1:A:44:PRO:HD3	1.92	0.42
2:B:150:PHE:CE1	2:B:151:PRO:HB3	2.55	0.42
2:B:159:ASN:HB3	2:B:163:LEU:HB2	2.02	0.42
2:B:1:GLN:CA	2:B:1:GLN:OE1	2.68	0.42
1:A:43:SER:HB3	2:B:95:TYR:CE2	2.54	0.42
4:D:189:SER:N	4:D:190:PRO:CD	2.81	0.42
1:A:61:ARG:CZ	1:A:79:GLN:HG3	2.49	0.42
4:D:22:CYS:HB2	4:D:36:TRP:CH2	2.55	0.42
1:A:168:SER:HB2	1:A:169:LYS:NZ	2.35	0.42
3:C:150:ILE:HD13	3:C:192:TYR:HE1	1.83	0.42
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.55	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB2	1.60	0.42
1:A:11:MET:HE2	1:A:102:THR:HG21	2.01	0.42
1:A:80:SER:O	1:A:83:LEU:HB2	2.20	0.42
4:D:71:LYS:CE	4:D:73:ASN:HD21	2.33	0.42
1:A:161:ASP:HA	1:A:176:SER:O	2.20	0.42
1:A:59:PRO:HG2	1:A:62:PHE:HD2	1.78	0.42
3:C:159:VAL:HA	3:C:178:THR:O	2.20	0.42
4:D:99:ARG:O	4:D:102:ARG:HG2	2.19	0.42
1:A:24:LYS:HA	1:A:69:THR:O	2.20	0.41
2:B:52:TYR:HD2	2:B:55:SER:OG	2.03	0.41
3:C:19:VAL:O	3:C:74:LYS:HA	2.20	0.41
3:C:110:ASP:HB3	3:C:200:THR:CG2	2.49	0.41
4:D:127:LEU:HB2	4:D:142:GLY:C	2.40	0.41
1:A:19:VAL:HG12	1:A:75:ILE:HB	2.03	0.41
3:C:115:VAL:HA	3:C:135:PHE:O	2.20	0.41
1:A:115:VAL:HA	1:A:135:PHE:O	2.20	0.41
1:A:89:GLN:HG2	1:A:90:HIS:N	2.36	0.41
1:A:121:SER:OG	2:B:126:TYR:HB3	2.20	0.41
2:B:9:SER:HA	2:B:112:THR:O	2.20	0.41
3:C:18:THR:HA	3:C:75:ILE:O	2.20	0.41
1:A:113:PRO:HG3	1:A:144:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG12	1:A:207:LYS:HG3	2.03	0.41
1:A:141:PRO:O	1:A:198:HIS:HE1	2.04	0.41
4:D:127:LEU:HB2	4:D:142:GLY:CA	2.51	0.41
4:D:203:PRO:C	4:D:205:SER:H	2.24	0.41
3:C:136:LEU:CD2	3:C:196:ALA:HB2	2.51	0.41
1:A:108:ARG:HG3	1:A:171:SER:HB2	2.03	0.41
1:A:146:VAL:HG21	1:A:175:MET:HE1	2.03	0.41
3:C:83:PHE:CE1	3:C:168:SER:HA	2.56	0.41
1:A:193:THR:HG22	1:A:208:SER:OG	2.20	0.40
3:C:214:CYS:HG	4:D:218:CYS:CB	2.25	0.40
3:C:175:MET:HG2	3:C:176:SER:N	2.36	0.40
3:C:61:ARG:HH11	3:C:61:ARG:HD2	1.34	0.40
1:A:147:LYS:HG2	1:A:195:GLU:HB3	2.02	0.40
2:B:9:SER:HB3	5:B:229:HOH:O	2.21	0.40
1:A:9:LYS:CD	1:A:9:LYS:N	2.81	0.40
4:D:192:PRO:HB3	4:D:215:PRO:HG3	2.04	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	212/214 (99%)	192 (91%)	15 (7%)	5 (2%)	7	11
2	B	215/217 (99%)	199 (93%)	11 (5%)	5 (2%)	7	11
3	C	212/214 (99%)	199 (94%)	11 (5%)	2 (1%)	20	36
4	D	216/218 (99%)	204 (94%)	9 (4%)	3 (1%)	13	23
All	All	855/863 (99%)	794 (93%)	46 (5%)	15 (2%)	10	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
2	B	134	ASP
2	B	159	ASN
3	C	211	ARG
4	D	129	PRO
1	A	30	ARG
1	A	199	LYS
4	D	204	ALA
2	B	135	THR
3	C	40	GLN
2	B	207	SER
1	A	81	GLU
4	D	190	PRO
1	A	60	ASP
2	B	41	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	191/191 (100%)	167 (87%)	24 (13%)	5	10
2	B	186/186 (100%)	154 (83%)	32 (17%)	2	4
3	C	189/189 (100%)	161 (85%)	28 (15%)	3	6
4	D	190/190 (100%)	163 (86%)	27 (14%)	4	7
All	All	756/756 (100%)	645 (85%)	111 (15%)	3	6

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	18	ARG
1	A	29	VAL
1	A	43	SER
1	A	45	LYS
1	A	56	THR
1	A	80	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	81	GLU
1	A	100	SER
1	A	105	GLU
1	A	108	ARG
1	A	121	SER
1	A	147	LYS
1	A	164	THR
1	A	165	ASP
1	A	171	SER
1	A	180	THR
1	A	187	GLU
1	A	191	SER
1	A	201	SER
1	A	202	THR
1	A	207	LYS
1	A	208	SER
1	A	211	ARG
2	B	1	GLN
2	B	4	LEU
2	B	5	GLN
2	B	9	SER
2	B	20	LEU
2	B	23	LYS
2	B	62	GLU
2	B	66	SER
2	B	70	LEU
2	B	71	THR
2	B	72	VAL
2	B	75	SER
2	B	100	LEU
2	B	104	PHE
2	B	109	GLN
2	B	112	THR
2	B	119	LEU
2	B	136	THR
2	B	138	SER
2	B	147	LYS
2	B	153	PRO
2	B	154	VAL
2	B	160	SER
2	B	162	SER
2	B	164	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	166	SER
2	B	181	MET
2	B	194	SER
2	B	200	SER
2	B	207	SER
2	B	208	THR
2	B	211	ASP
3	C	10	SER
3	C	11	LEU
3	C	12	SER
3	C	22	THR
3	C	23	CYS
3	C	43	SER
3	C	45	GLN
3	C	54	LEU
3	C	63	SER
3	C	67	SER
3	C	70	GLN
3	C	78	LEU
3	C	96	ARG
3	C	103	LYS
3	C	106	LEU
3	C	114	THR
3	C	125	LEU
3	C	147	LYS
3	C	154	GLU
3	C	155	ARG
3	C	156	GLN
3	C	164	THR
3	C	172	THR
3	C	175	MET
3	C	181	LEU
3	C	203	SER
3	C	208	SER
3	C	211	ARG
4	D	3	GLN
4	D	6	GLU
4	D	25	SER
4	D	38	ARG
4	D	45	LEU
4	D	48	LEU
4	D	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	64	LYS
4	D	74	SER
4	D	97	ARG
4	D	108	GLN
4	D	110	THR
4	D	113	THR
4	D	118	SER
4	D	139	VAL
4	D	143	CYS
4	D	146	LYS
4	D	151	GLU
4	D	152	PRO
4	D	156	THR
4	D	189	SER
4	D	191	ARG
4	D	198	CYS
4	D	199	ASN
4	D	211	LYS
4	D	212	LYS
4	D	218	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	198	HIS
1	A	212	ASN
2	B	3	GLN
2	B	5	GLN
2	B	159	ASN
2	B	168	HIS
3	C	40	GLN
3	C	45	GLN
3	C	90	HIS
3	C	137	ASN
3	C	156	GLN
4	D	73	ASN
4	D	83	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 carbohydrates 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 ⓘ

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	214/214 (100%)	-0.42	5 (2%) 61 63	11, 42, 83, 112	0
2	B	217/217 (100%)	-0.71	7 (3%) 48 51	10, 31, 64, 80	0
3	C	214/214 (100%)	-0.60	4 (1%) 67 69	9, 30, 83, 112	0
4	D	218/218 (100%)	-0.81	4 (1%) 69 70	7, 27, 63, 99	0
All	All	863/863 (100%)	-0.64	20 (2%) 61 63	7, 33, 77, 112	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	CYS	5.2
2	B	134	ASP	5.1
1	A	213	GLU	4.6
3	C	212	ASN	4.4
2	B	135	THR	4.2
3	C	214	CYS	4.0
1	A	156	GLN	3.7
1	A	153	SER	3.7
4	D	130	GLY	3.6
3	C	153	SER	3.3
2	B	132	CYS	3.0
2	B	162	SER	2.8
2	B	217	SER	2.8
1	A	212	ASN	2.5
3	C	155	ARG	2.4
4	D	217	ASP	2.3
4	D	131	SER	2.2
2	B	161	GLY	2.2
4	D	218	CYS	2.2
2	B	164	SER	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 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.