



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:30 PM UTC

PDB ID : 5D1Z / pdb_00005d1z
Title : IsdB NEAT1 bound by clone D4-10
Authors : Deng, X.
Deposited on : 2015-08-04
Resolution : 3.17 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

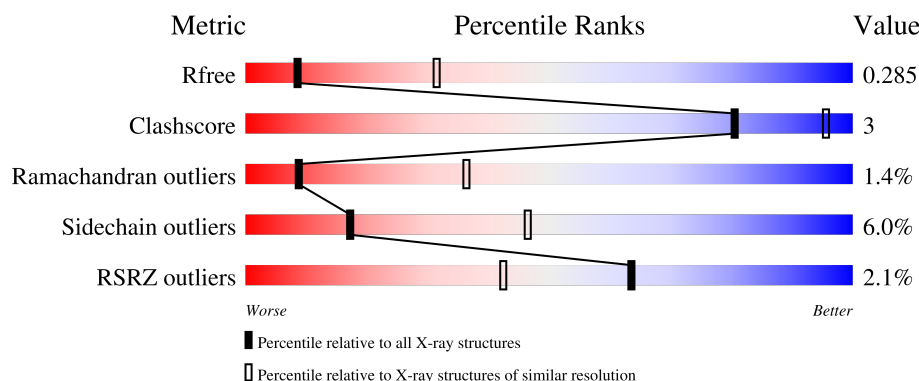
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	90% 9%
1	H	214	90% 10%
2	B	264	2% 73% 8% 17%
2	G	264	2% 69% 12% 16%
3	C	214	2% 79% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	214	2% 86% 14%
4	D	270	6% 70% 14% 15%
4	F	270	3% 65% 14% 17%
5	I	157	89% 6% 5%
5	J	157	% 83% 10% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15704 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 Y10 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1644	1033	275	331	5			
1	H	214	Total	C	N	O	S	0	0	0
			1650	1036	276	332	6			

- Molecule 2 is a protein called Y10 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1645	1041	279	319	6			
2	G	222	Total	C	N	O	S	0	0	0
			1668	1053	283	325	7			

- Molecule 3 is a protein called D4-10 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	208	Total	C	N	O	S	0	0	0
			1601	1004	268	325	4			
3	E	213	Total	C	N	O	S	0	0	0
			1635	1025	274	332	4			

- Molecule 4 is a protein called D4-10 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	230	Total	C	N	O	S	0	0	0
			1729	1090	289	343	7			
4	F	223	Total	C	N	O	S	0	0	0
			1680	1062	280	331	7			

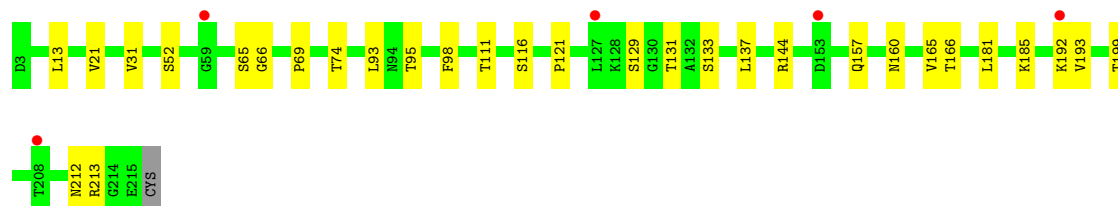
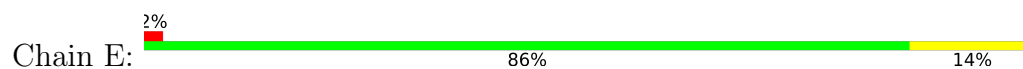
- Molecule 5 is a protein called Iron-regulated surface determinant protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	149	Total	C	N	O	S	0	0	0
			1226	787	204	233	2			
5	J	149	Total	C	N	O	S	0	0	0
			1226	787	204	233	2			

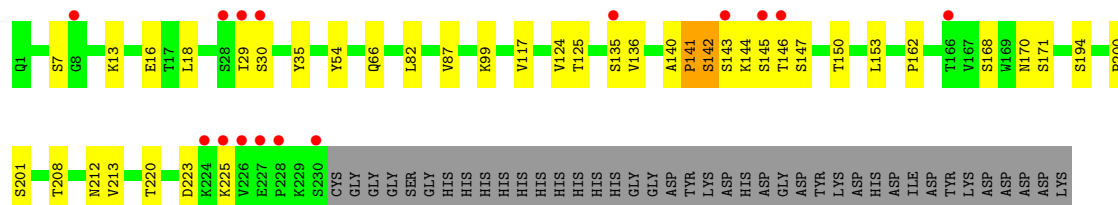
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	113	GLY	-	expression tag	UNP Q6GA86
I	114	PRO	-	expression tag	UNP Q6GA86
J	113	GLY	-	expression tag	UNP Q6GA86
J	114	PRO	-	expression tag	UNP Q6GA86

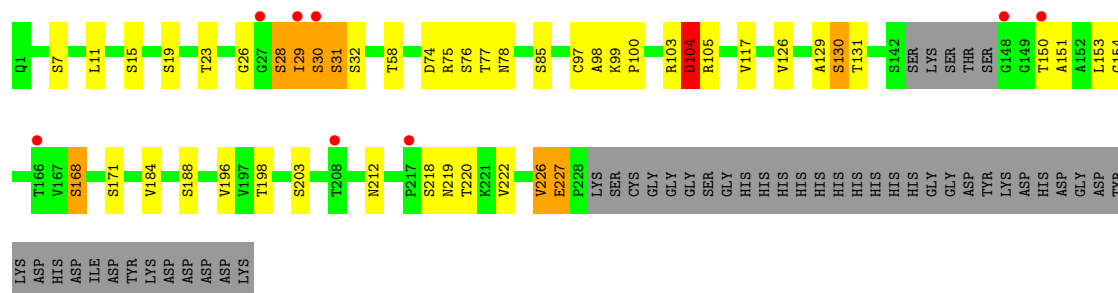
- Molecule 3: D4-10 Light Chain



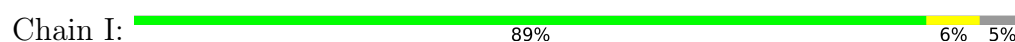
- Molecule 4: D4-10 Heavy Chain



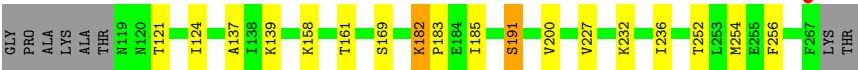
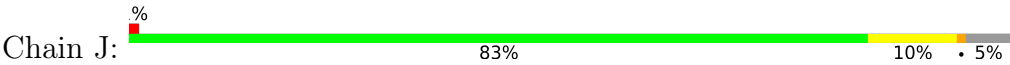
- Molecule 4: D4-10 Heavy Chain



- Molecule 5: Iron-regulated surface determinant protein B



- Molecule 5: Iron-regulated surface determinant protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	115.29Å 147.00Å 165.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 3.17 24.96 – 3.17	Depositor EDS
% Data completeness (in resolution range)	98.0 (24.96-3.17) 98.3 (24.96-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.233 , 0.287 0.233 , 0.285	Depositor DCC
R_{free} test set	2344 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 9.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15704	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5101e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

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	1.22	2/1682 (0.1%)	1.07	0/2288
1	H	1.27	3/1688 (0.2%)	1.08	4/2296 (0.2%)
2	B	1.23	1/1686 (0.1%)	1.15	3/2294 (0.1%)
2	G	1.19	3/1709 (0.2%)	1.16	7/2325 (0.3%)
3	C	1.19	3/1635 (0.2%)	1.08	2/2223 (0.1%)
3	E	1.23	2/1670 (0.1%)	1.12	3/2271 (0.1%)
4	D	1.24	4/1772 (0.2%)	1.18	3/2415 (0.1%)
4	F	1.25	2/1722 (0.1%)	1.19	8/2348 (0.3%)
5	I	1.18	2/1257 (0.2%)	1.10	2/1695 (0.1%)
5	J	1.17	2/1257 (0.2%)	1.10	2/1695 (0.1%)
All	All	1.22	24/16078 (0.1%)	1.13	34/21850 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	120	PRO	CA-C	7.76	1.57	1.52
2	G	144	THR	N-CA	7.66	1.55	1.46
2	G	210	LYS	N-CA	6.99	1.51	1.46
5	I	182	LYS	CA-C	5.99	1.57	1.52
1	H	60	VAL	CA-C	5.95	1.58	1.53
4	D	145	SER	CA-C	5.91	1.60	1.52
1	H	8	GLN	N-CA	5.68	1.53	1.46
1	A	120	PHE	CA-C	5.50	1.57	1.52
4	F	226	VAL	CA-C	5.49	1.59	1.52
5	J	124	ILE	CA-CB	5.45	1.59	1.53
2	B	144	THR	N-CA	5.39	1.53	1.46
4	D	200	PRO	CA-C	5.32	1.58	1.52
3	E	193	VAL	N-CA	5.31	1.52	1.46
5	J	158	LYS	CA-C	5.29	1.59	1.52
4	F	28	SER	CA-C	5.28	1.57	1.53
4	D	150	THR	CA-C	5.23	1.59	1.52
3	E	121	PRO	CA-C	5.23	1.57	1.52
1	A	207	VAL	N-CA	5.18	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	170	SER	CA-C	5.18	1.59	1.52
1	H	207	VAL	N-CA	5.17	1.52	1.46
4	D	29	ILE	CA-CB	5.15	1.59	1.54
5	I	208	PRO	CA-C	5.09	1.57	1.52
3	C	141	TYR	CA-C	5.02	1.58	1.52
3	C	172	SER	CA-C	5.01	1.60	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	149	ARG	N-CA-C	7.69	115.05	108.13
4	D	140	ALA	CA-C-N	6.38	126.34	120.21
4	D	140	ALA	C-N-CA	6.38	126.34	120.21
1	H	68	GLY	N-CA-C	6.31	117.94	111.95
4	F	28	SER	N-CA-C	6.09	118.37	108.08
4	F	154	GLY	N-CA-C	5.83	119.27	110.18
2	G	193	VAL	CB-CA-C	5.82	115.03	109.33
4	F	227	GLU	N-CA-C	5.61	122.21	109.81
3	E	69	PRO	N-CA-C	5.54	119.94	111.34
2	G	143	GLY	N-CA-C	5.53	122.15	113.86
4	F	104	ASP	N-CA-C	5.47	117.95	111.33
1	H	8	GLN	N-CA-C	5.41	117.22	108.34
5	J	191	SER	CA-C-N	5.40	125.94	120.00
5	J	191	SER	C-N-CA	5.40	125.94	120.00
2	G	170	SER	N-CA-C	5.37	118.30	109.76
3	E	212	ASN	N-CA-C	5.35	119.01	111.52
2	G	40	GLN	N-CA-C	5.35	116.14	107.32
2	B	74	ASP	N-CA-C	-5.31	99.49	110.80
1	H	60	VAL	N-CA-C	5.28	114.13	108.95
3	C	187	TYR	N-CA-C	5.26	116.87	111.03
2	B	97	CYS	N-CA-C	-5.24	102.73	110.48
1	H	188	TYR	N-CA-C	5.19	117.02	111.36
4	F	98	ALA	N-CA-C	5.15	116.81	109.14
4	D	141	PRO	N-CA-C	5.13	118.40	111.22
2	G	144	THR	N-CA-C	5.08	116.67	108.34
3	C	138	ASN	N-CA-C	5.05	117.56	111.40
4	F	31	SER	N-CA-C	-5.04	102.02	109.83
2	B	88	ARG	N-CA-C	5.03	117.51	109.81
3	E	185	LYS	N-CA-C	5.03	116.76	111.28
2	G	209	HIS	CA-C-N	5.02	125.40	119.83
2	G	209	HIS	C-N-CA	5.02	125.40	119.83
4	F	103	ARG	CA-C-N	5.02	127.25	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	103	ARG	C-N-CA	5.02	127.25	120.38
5	I	185	ILE	N-CA-C	5.01	115.06	107.75

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	1644	0	1592	6	0
1	H	1650	0	1596	11	0
2	B	1645	0	1599	10	0
2	G	1668	0	1621	15	0
3	C	1601	0	1553	14	0
3	E	1635	0	1593	7	0
4	D	1729	0	1700	11	0
4	F	1680	0	1646	13	0
5	I	1226	0	1204	1	0
5	J	1226	0	1204	9	0
All	All	15704	0	15308	82	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 3.

All (82) 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:H:87:THR:HG22	1:H:105:ARG:HG3	1.82	0.61
4:F:58:THR:HG21	5:J:169:SER:HB2	1.83	0.60
4:D:170:ASN:O	4:D:212:ASN:ND2	2.36	0.59
4:F:99:LYS:HE3	4:F:117:VAL:HG22	1.85	0.59
1:A:165:VAL:HG22	1:A:177:LEU:HD12	1.84	0.59
1:A:147:LYS:HE2	1:A:149:GLN:OE1	2.03	0.58
4:D:35:TYR:HB3	4:D:54:TYR:CD1	2.39	0.58
4:F:11:LEU:CD2	4:F:131:THR:HB	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD13	2:B:108:TYR:CE1	2.40	0.57
3:C:9:PRO:HG2	3:C:12:LEU:HD13	1.87	0.57
4:D:99:LYS:HE3	4:D:117:VAL:HG12	1.88	0.55
2:G:89:ALA:O	2:G:92:THR:HG23	2.07	0.55
2:B:31:ASN:O	2:B:54:VAL:HG13	2.06	0.55
4:D:142:SER:OG	4:D:147:SER:OG	2.19	0.53
2:G:84:MET:HE1	2:G:118:VAL:HG11	1.93	0.51
4:D:136:VAL:HG21	4:D:213:VAL:HG11	1.91	0.51
5:J:185:ILE:HD13	5:J:256:PHE:CZ	2.46	0.51
2:G:12:VAL:HG11	2:G:155:PHE:HE1	1.76	0.50
2:B:170:SER:HB2	4:F:104:ASP:HB3	1.94	0.50
4:F:58:THR:HG23	5:J:191:SER:OG	2.11	0.50
4:D:146:THR:HG22	4:D:146:THR:O	2.11	0.49
2:B:65:VAL:HG13	2:B:69:PHE:HB2	1.93	0.49
5:J:254:MET:HE2	5:J:256:PHE:CE1	2.47	0.49
3:E:13:LEU:CD2	3:E:21:VAL:HG13	2.43	0.49
1:A:40:GLN:HE22	2:B:40:GLN:HE22	1.59	0.48
4:F:28:SER:O	4:F:32:SER:OG	2.28	0.48
3:C:211:ASN:N	3:C:211:ASN:OD1	2.46	0.48
2:G:223:LYS:NZ	1:H:124:ASP:OD2	2.47	0.48
2:B:33:PHE:O	2:B:73:ARG:NH2	2.48	0.47
4:D:141:PRO:HG3	4:D:153:LEU:CB	2.45	0.47
3:E:13:LEU:HD21	3:E:21:VAL:HG13	1.96	0.46
2:B:3:VAL:HG13	2:B:28:PHE:CD1	2.51	0.46
1:H:87:THR:HG22	1:H:105:ARG:CG	2.45	0.46
5:J:200:VAL:HG22	5:J:236:ILE:HG12	1.98	0.46
1:A:94:ASN:HD22	1:A:95:THR:HG23	1.81	0.46
2:B:35:MET:CB	2:B:80:LEU:HD13	2.46	0.46
4:D:18:LEU:CD1	4:D:124:VAL:HG11	2.45	0.46
2:B:89:ALA:O	2:B:92:THR:HG23	2.16	0.45
3:C:124:GLU:N	3:C:124:GLU:OE2	2.50	0.45
2:G:33:PHE:O	2:G:73:ARG:NH2	2.50	0.45
5:J:182:LYS:HG2	5:J:183:PRO:HD2	1.99	0.45
1:H:93:LEU:HA	1:H:98:TYR:CD1	2.52	0.45
1:H:94:ASN:OD1	5:J:139:LYS:HE3	2.17	0.45
3:E:160:ASN:HB2	3:E:181:LEU:HD12	1.98	0.44
4:F:99:LYS:NZ	4:F:100:PRO:O	2.49	0.44
3:E:144:ARG:NH2	3:E:165:VAL:HG13	2.33	0.44
2:G:23:CYS:HB3	2:G:80:LEU:HB3	1.99	0.44
2:G:65:VAL:HG13	2:G:69:PHE:HB2	1.99	0.44
3:E:137:LEU:HD21	4:F:196:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MET:HE1	2:B:118:VAL:HG21	1.99	0.43
2:G:107:GLY:C	1:H:93:LEU:CD2	2.91	0.43
3:C:159:ASN:HD22	3:C:159:ASN:N	2.16	0.43
4:F:29:ILE:O	4:F:31:SER:N	2.52	0.43
2:G:12:VAL:HG11	2:G:155:PHE:CE1	2.53	0.43
4:F:226:VAL:O	4:F:226:VAL:HG23	2.18	0.43
4:F:168:SER:O	4:F:212:ASN:N	2.51	0.43
2:G:107:GLY:HA3	1:H:93:LEU:CD2	2.49	0.43
4:F:74:ASP:CG	4:F:77:THR:HG22	2.44	0.42
2:G:40:GLN:HE22	1:H:40:GLN:HE22	1.66	0.42
3:C:92:LEU:HA	3:C:97:PHE:CD1	2.54	0.42
3:C:151:VAL:HG22	3:C:190:HIS:CD2	2.54	0.42
3:C:181:THR:O	3:C:182:LEU:HD12	2.19	0.42
3:C:32:SER:OG	3:C:68:PRO:HB3	2.20	0.42
2:G:107:GLY:HA3	1:H:93:LEU:HD22	2.02	0.42
3:E:66:GLY:HA2	3:E:74:THR:O	2.19	0.42
2:G:106:SER:HB2	5:J:137:ALA:HB2	2.01	0.42
1:H:151:LYS:HB2	1:H:195:ALA:HB3	2.01	0.42
4:D:18:LEU:HD12	4:D:124:VAL:HG11	2.00	0.42
3:C:192:VAL:HA	3:C:211:ASN:HB3	2.01	0.41
4:D:168:SER:O	4:D:212:ASN:HB2	2.20	0.41
3:C:35:ALA:HA	3:C:49:ILE:O	2.20	0.41
4:D:13:LYS:HB2	4:D:16:GLU:HG3	2.02	0.41
3:C:114:PRO:HB3	3:C:140:PHE:HB3	2.03	0.41
5:I:200:VAL:HG23	5:I:209:ILE:HD11	2.03	0.41
3:C:12:LEU:HD21	3:C:20:VAL:HG13	2.03	0.41
4:F:58:THR:HG21	5:J:169:SER:CB	2.49	0.41
3:C:7:GLN:HE21	3:C:89:CYS:HB2	1.85	0.40
1:A:6:MET:HE1	1:A:27:ALA:HB2	2.03	0.40
3:C:194:ALA:HA	3:C:209:SER:HB3	2.02	0.40
3:E:93:LEU:HA	3:E:98:PHE:CD1	2.56	0.40
2:G:108:TYR:CE1	1:H:93:LEU:HD13	2.56	0.40
2:G:73:ARG:NH1	2:G:75:ASN:OD1	2.53	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	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
1	H	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	24	57
2	B	214/264 (81%)	202 (94%)	10 (5%)	2 (1%)	14	45
2	G	218/264 (83%)	205 (94%)	10 (5%)	3 (1%)	9	36
3	C	204/214 (95%)	186 (91%)	15 (7%)	3 (2%)	8	35
3	E	211/214 (99%)	196 (93%)	13 (6%)	2 (1%)	14	45
4	D	228/270 (84%)	198 (87%)	24 (10%)	6 (3%)	4	23
4	F	219/270 (81%)	190 (87%)	18 (8%)	11 (5%)	1	11
5	I	147/157 (94%)	134 (91%)	13 (9%)	0	100	100
5	J	147/157 (94%)	139 (95%)	8 (5%)	0	100	100
All	All	2011/2238 (90%)	1848 (92%)	135 (7%)	28 (1%)	9	36

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	THR
4	F	30	SER
4	F	130	SER
2	B	54	VAL
4	D	142	SER
4	F	129	ALA
4	F	150	THR
4	F	219	ASN
2	G	125	THR
2	G	224	SER
1	H	145	GLU
4	D	143	SER
4	F	29	ILE
4	F	151	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	155	LEU
4	D	66	GLN
4	D	144	LYS
3	E	129	SER
4	F	15	SER
4	D	30	SER
3	E	213	ARG
4	F	75	ARG
4	F	26	GLY
4	F	227	GLU
2	G	211	PRO
3	C	84	VAL
3	C	69	GLY
4	D	162	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	186/187 (100%)	176 (95%)	10 (5%)	20	50
1	H	187/187 (100%)	181 (97%)	6 (3%)	34	62
2	B	182/220 (83%)	176 (97%)	6 (3%)	33	62
2	G	185/220 (84%)	168 (91%)	17 (9%)	8	31
3	C	183/188 (97%)	170 (93%)	13 (7%)	13	41
3	E	187/188 (100%)	175 (94%)	12 (6%)	16	44
4	D	199/232 (86%)	187 (94%)	12 (6%)	17	46
4	F	192/232 (83%)	170 (88%)	22 (12%)	5	22
5	I	135/140 (96%)	132 (98%)	3 (2%)	45	68
5	J	135/140 (96%)	129 (96%)	6 (4%)	25	55
All	All	1771/1934 (92%)	1664 (94%)	107 (6%)	17	46

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	58	SER
1	A	65	SER
1	A	72	GLU
1	A	107	GLU
1	A	128	LYS
1	A	161	SER
1	A	169	ASP
1	A	204	SER
1	A	207	VAL
2	B	64	SER
2	B	65	VAL
2	B	78	ASN
2	B	92	THR
2	B	122	SER
2	B	215	LYS
3	C	23	THR
3	C	54	THR
3	C	61	SER
3	C	70	THR
3	C	82	GLU
3	C	110	THR
3	C	124	GLU
3	C	133	VAL
3	C	157	SER
3	C	159	ASN
3	C	169	SER
3	C	190	HIS
3	C	211	ASN
4	D	7	SER
4	D	82	LEU
4	D	87	VAL
4	D	125	THR
4	D	135	SER
4	D	171	SER
4	D	194	SER
4	D	201	SER
4	D	208	THR
4	D	220	THR
4	D	223	ASP
4	D	225	LYS
5	I	158	LYS
5	I	232	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	263	SER
3	E	31	VAL
3	E	52	SER
3	E	65	SER
3	E	95	THR
3	E	111	THR
3	E	116	SER
3	E	131	THR
3	E	133	SER
3	E	157	GLN
3	E	166	THR
3	E	192	LYS
3	E	199	THR
4	F	7	SER
4	F	19	SER
4	F	23	THR
4	F	30	SER
4	F	76	SER
4	F	78	ASN
4	F	85	SER
4	F	97	CYS
4	F	104	ASP
4	F	105	ARG
4	F	126	VAL
4	F	130	SER
4	F	153	LEU
4	F	168	SER
4	F	171	SER
4	F	184	VAL
4	F	188	SER
4	F	198	THR
4	F	203	SER
4	F	218	SER
4	F	220	THR
4	F	222	VAL
2	G	7	GLU
2	G	13	VAL
2	G	29	THR
2	G	64	SER
2	G	65	VAL
2	G	69	PHE
2	G	92	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	119	THR
2	G	126	LYS
2	G	144	THR
2	G	178	VAL
2	G	182	SER
2	G	187	LEU
2	G	198	LEU
2	G	212	SER
2	G	214	THR
2	G	223	LYS
1	H	9	SER
1	H	32	THR
1	H	106	LEU
1	H	133	SER
1	H	176	SER
1	H	204	SER
5	J	121	THR
5	J	161	THR
5	J	182	LYS
5	J	227	VAL
5	J	232	LYS
5	J	252	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	94	ASN
2	B	83	GLN
2	B	208	ASN
3	C	80	GLN
3	C	148	GLN
3	C	159	ASN
3	C	190	HIS
4	D	179	HIS
4	D	212	ASN
4	D	215	HIS
5	I	147	ASN
5	I	262	ASN
3	E	39	GLN
3	E	139	ASN
4	F	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	170	ASN
4	F	179	HIS
4	F	207	GLN
4	F	215	HIS
1	H	39	GLN
1	H	40	GLN
1	H	149	GLN
1	H	162	GLN
5	J	120	ASN
5	J	147	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 [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	213/214 (99%)	0.18	1 (0%) 87 75	34, 53, 66, 72	0
1	H	214/214 (100%)	0.15	1 (0%) 87 75	35, 51, 67, 75	0
2	B	218/264 (82%)	0.08	2 (0%) 81 64	30, 43, 62, 89	0
2	G	222/264 (84%)	0.16	5 (2%) 61 40	23, 42, 60, 84	2 (0%)
3	C	208/214 (97%)	0.16	4 (1%) 66 45	26, 40, 93, 108	0
3	E	213/214 (99%)	0.32	5 (2%) 61 40	28, 49, 92, 102	0
4	D	230/270 (85%)	0.52	15 (6%) 25 14	27, 49, 87, 96	6 (2%)
4	F	223/270 (82%)	0.40	8 (3%) 46 27	30, 55, 83, 95	0
5	I	149/157 (94%)	-0.08	0 100 100	26, 38, 61, 78	0
5	J	149/157 (94%)	-0.01	1 (0%) 84 69	29, 40, 66, 80	0
All	All	2039/2238 (91%)	0.21	42 (2%) 63 42	23, 46, 82, 108	8 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	230	SER	9.3
4	D	226	VAL	8.5
2	G	141	SER	7.6
4	D	224	LYS	7.0
4	D	225	LYS	6.6
4	D	227	GLU	6.0
2	G	142	GLY	4.6
1	H	216	CYS	3.6
4	D	28	SER	3.4
4	D	145	SER	3.4
4	F	30	SER	3.3
4	D	228	PRO	3.3
3	C	125	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	148	GLY	3.1
3	C	214	GLU	3.1
2	B	142	GLY	3.0
4	F	29	ILE	3.0
4	D	146	THR	2.8
4	D	143	SER	2.8
3	C	191	LYS	2.8
4	D	135	SER	2.7
3	C	123	ASP	2.6
4	F	150	THR	2.6
3	E	59	GLY	2.6
4	F	27	GLY	2.6
2	G	1	ALA	2.6
3	E	153	ASP	2.5
3	E	127	LEU	2.4
4	F	208	THR	2.4
5	J	267	PHE	2.3
2	G	208	ASN	2.3
1	A	145	GLU	2.3
4	F	217	PRO	2.2
2	B	204	ILE	2.2
4	D	29	ILE	2.2
2	G	107	GLY	2.2
4	D	166	THR	2.1
4	F	166	THR	2.1
4	D	8	GLY	2.1
3	E	192	LYS	2.1
3	E	208	THR	2.1
4	D	30	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 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.