



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:50 PM GMT

PDB ID : 3D1N
Title : Structure of human Brn-5 transcription factor in complex with corticotrophin
-releasing hormone gene promoter
Authors : Pereira, J.H.; Ha, S.C.; Kim, S.-H.
Deposited on : 2008-05-06
Resolution : 2.51 Å (reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

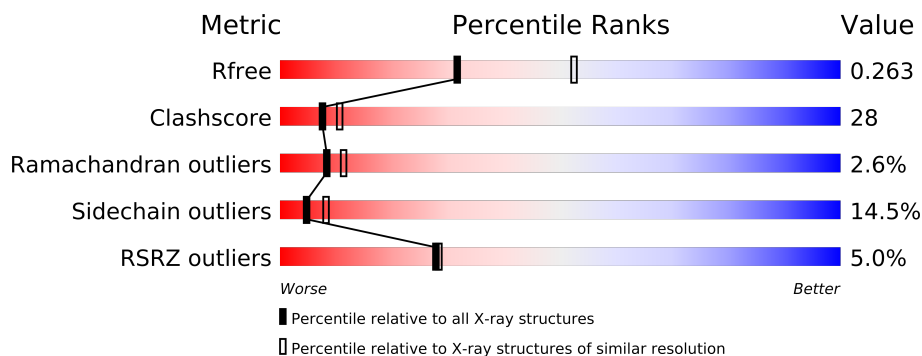
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.51 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	14	
1	C	14	
1	E	14	
1	G	14	
2	B	14	
2	D	14	
2	F	14	
2	H	14	
3	I	151	
3	J	151	
3	K	151	
3	L	151	
3	M	151	
3	N	151	

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Mol	Chain	Length	Quality of chain
3	O	151	
3	P	151	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10089 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	C	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	E	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			
1	G	14	Total	C	N	O	P	0	0	0
			287	139	59	76	13			

- Molecule 2 is a DNA chain called 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DCP*DT)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	D	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	F	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			
2	H	14	Total	C	N	O	P	0	0	0
			281	139	41	88	13			

- Molecule 3 is a protein called POU domain, class 6, transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	150	Total	C	N	O	Se	0	0	0
			1192	746	216	226	4			
3	J	86	Total	C	N	O	Se	0	0	0
			666	420	114	129	3			
3	K	150	Total	C	N	O	Se	0	0	0
			1100	689	194	213	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	145	Total	C	N	O	Se	0	0	0
			1130	708	203	215	4			
3	M	150	Total	C	N	O	Se	0	0	0
			1188	742	215	227	4			
3	N	85	Total	C	N	O	Se	0	0	0
			658	414	113	128	3			
3	O	150	Total	C	N	O	Se	0	0	0
			1166	730	209	223	4			
3	P	82	Total	C	N	O	Se	0	0	0
			620	390	108	119	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	144	MSE	LEU	ENGINEERED	UNP Q14863
I	172	MSE	LEU	ENGINEERED	UNP Q14863
I	186	SER	CYS	ENGINEERED	UNP Q14863
I	267	MSE	ILE	ENGINEERED	UNP Q14863
I	283	SER	CYS	ENGINEERED	UNP Q14863
J	144	MSE	LEU	ENGINEERED	UNP Q14863
J	172	MSE	LEU	ENGINEERED	UNP Q14863
J	186	SER	CYS	ENGINEERED	UNP Q14863
J	267	MSE	ILE	ENGINEERED	UNP Q14863
J	283	SER	CYS	ENGINEERED	UNP Q14863
K	144	MSE	LEU	ENGINEERED	UNP Q14863
K	172	MSE	LEU	ENGINEERED	UNP Q14863
K	186	SER	CYS	ENGINEERED	UNP Q14863
K	267	MSE	ILE	ENGINEERED	UNP Q14863
K	283	SER	CYS	ENGINEERED	UNP Q14863
L	144	MSE	LEU	ENGINEERED	UNP Q14863
L	172	MSE	LEU	ENGINEERED	UNP Q14863
L	186	SER	CYS	ENGINEERED	UNP Q14863
L	267	MSE	ILE	ENGINEERED	UNP Q14863
L	283	SER	CYS	ENGINEERED	UNP Q14863
M	144	MSE	LEU	ENGINEERED	UNP Q14863
M	172	MSE	LEU	ENGINEERED	UNP Q14863
M	186	SER	CYS	ENGINEERED	UNP Q14863
M	267	MSE	ILE	ENGINEERED	UNP Q14863
M	283	SER	CYS	ENGINEERED	UNP Q14863
N	144	MSE	LEU	ENGINEERED	UNP Q14863
N	172	MSE	LEU	ENGINEERED	UNP Q14863
N	186	SER	CYS	ENGINEERED	UNP Q14863
N	267	MSE	ILE	ENGINEERED	UNP Q14863

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Chain	Residue	Modelled	Actual	Comment	Reference
N	283	SER	CYS	ENGINEERED	UNP Q14863
O	144	MSE	LEU	ENGINEERED	UNP Q14863
O	172	MSE	LEU	ENGINEERED	UNP Q14863
O	186	SER	CYS	ENGINEERED	UNP Q14863
O	267	MSE	ILE	ENGINEERED	UNP Q14863
O	283	SER	CYS	ENGINEERED	UNP Q14863
P	144	MSE	LEU	ENGINEERED	UNP Q14863
P	172	MSE	LEU	ENGINEERED	UNP Q14863
P	186	SER	CYS	ENGINEERED	UNP Q14863
P	267	MSE	ILE	ENGINEERED	UNP Q14863
P	283	SER	CYS	ENGINEERED	UNP Q14863

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	10	Total O 10 10	0	0
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0
4	E	9	Total O 9 9	0	0
4	F	10	Total O 10 10	0	0
4	G	4	Total O 4 4	0	0
4	H	5	Total O 5 5	0	0
4	I	8	Total O 8 8	0	0
4	J	6	Total O 6 6	0	0
4	L	1	Total O 1 1	0	0
4	M	10	Total O 10 10	0	0
4	N	6	Total O 6 6	0	0
4	O	10	Total O 10 10	0	0

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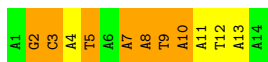
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

Chain A: 



- Molecule 1: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

Chain C: 



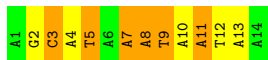
- Molecule 1: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

Chain E: 



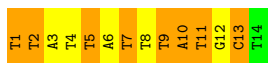
- Molecule 1: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

Chain G: 



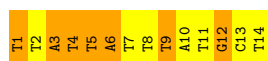
- Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DCP*DT)-3'

Chain B: 



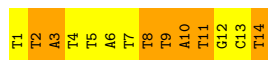
- Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DCP*DT)-3'

Chain D: 



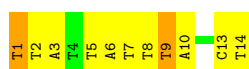
- Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*D CP*DT)-3'

Chain F:



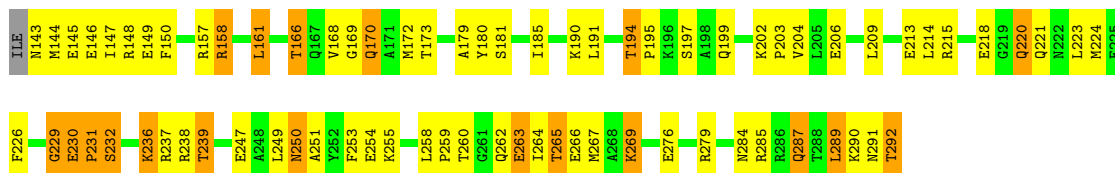
- Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*D CP*DT)-3'

Chain H:



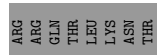
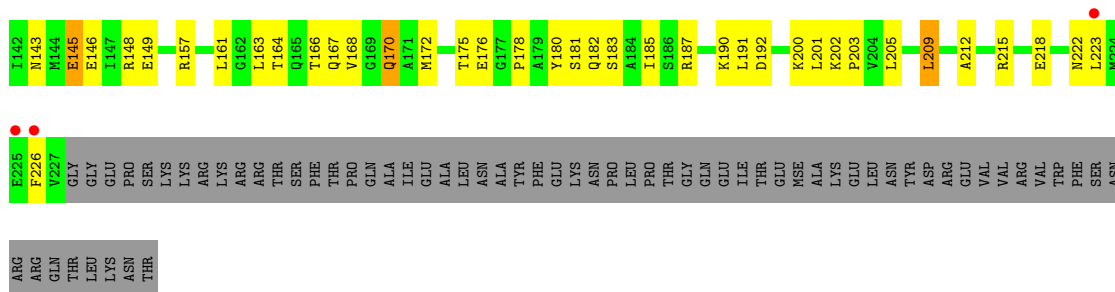
- Molecule 3: POU domain, class 6, transcription factor 1

Chain I:



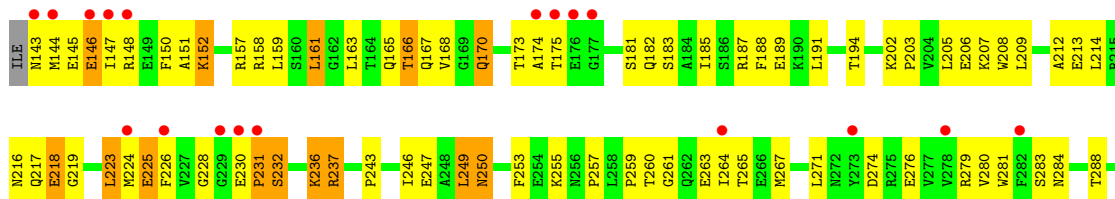
- Molecule 3: POU domain, class 6, transcription factor 1

Chain J:



- Molecule 3: POU domain, class 6, transcription factor 1

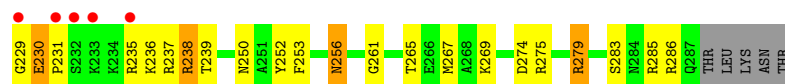
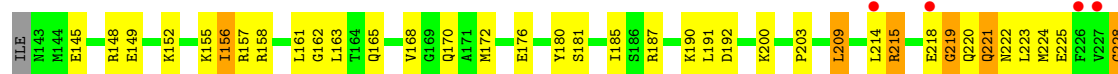
Chain K:





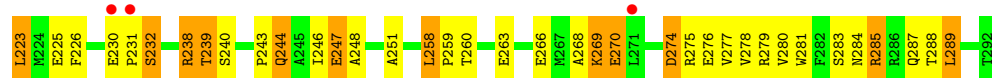
- Molecule 3: POU domain, class 6, transcription factor 1

Chain L:



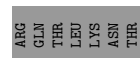
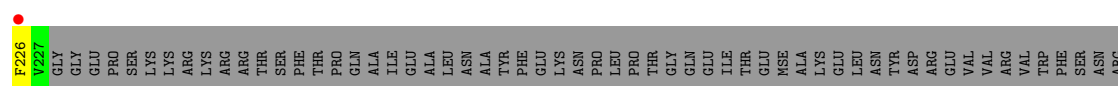
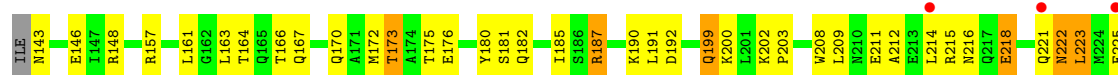
- Molecule 3: POU domain, class 6, transcription factor 1

Chain M:



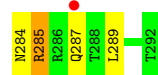
- Molecule 3: POU domain, class 6, transcription factor 1

Chain N:



- Molecule 3: POU domain, class 6, transcription factor 1

Chain O:



- Molecule 3: POU domain, class 6, transcription factor 1

Chain P:

THR	PRO	GLN	ALA	ILE	GLU	ALA	LEU	ASN	ALA	TYR	PHE	GLU	GLY	LYS	ASN	PRO	LEU	PRO	THR	GLY	GLN	GLU	ILE	THR	GLU	NSE	ALA	LYS	GLU	LEU	ASN	TYR	ASP	ARG	GLU	VAL	ARG	VAL	TRP	PHE	SER	ASN	ARG	ARG	GLN	THR	LEU	LYS	ASN	THR
M143	M144	I147	K155	I156	R157	R158	L161	G162	L163	T164	Q165	T166	Q167	V168	M172	T173	A174	T175	E176	G177	P178	Q182	K190	K202	P203	L209	L214	R215	N216	L223	M224	GLU	PHE	VAL	GLY	GLY	GLY	PRO	SER	LYS	LYS	ARG	LYS	ARG	ARG	THR	SER	PHE		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.30Å 112.06Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.51 48.91 – 2.51	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.91-2.51) 74.7 (48.91-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	65.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.270 0.207 , 0.263	Depositor DCC
R_{free} test set	2670 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 52734 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.80	0/324	1.84	11/498 (2.2%)
1	C	0.79	0/324	1.89	13/498 (2.6%)
1	E	0.95	0/324	1.93	13/498 (2.6%)
1	G	0.87	0/324	1.89	12/498 (2.4%)
2	B	0.83	0/312	1.95	13/480 (2.7%)
2	D	0.85	0/312	2.17	15/480 (3.1%)
2	F	0.85	0/312	2.19	21/480 (4.4%)
2	H	0.96	0/312	2.03	10/480 (2.1%)
3	I	0.42	0/1208	0.59	0/1622
3	J	0.41	0/672	0.57	0/900
3	K	0.29	0/1114	0.52	0/1507
3	L	0.36	0/1146	0.55	0/1540
3	M	0.42	0/1204	0.65	0/1620
3	N	0.41	0/664	0.60	0/889
3	O	0.36	0/1182	0.55	0/1593
3	P	0.38	0/625	0.55	0/836
All	All	0.54	0/10359	1.15	108/14419 (0.7%)

There are no bond length outliers.

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	DT	O4'-C1'-N1	-13.05	98.87	108.00
2	D	9	DT	O4'-C1'-N1	13.04	117.13	108.00
2	D	12	DG	O4'-C1'-N9	-11.20	100.16	108.00
2	D	5	DT	O4'-C1'-N1	-10.91	100.36	108.00
1	A	5	DT	O4'-C1'-N1	10.16	115.11	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	287	0	159	13	0
1	C	287	0	159	7	0
1	E	287	0	159	8	0
1	G	287	0	159	8	0
2	B	281	0	165	14	0
2	D	281	0	165	18	0
2	F	281	0	165	21	0
2	H	281	0	165	11	0
3	I	1192	0	1174	65	0
3	J	666	0	654	28	0
3	K	1100	0	1017	68	0
3	L	1130	0	1090	62	0
3	M	1188	0	1157	81	0
3	N	658	0	643	39	0
3	O	1166	0	1120	80	0
3	P	620	0	606	22	0
4	A	9	0	0	5	0
4	B	10	0	0	2	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
4	E	9	0	0	2	0
4	F	10	0	0	3	0
4	G	4	0	0	0	0
4	H	5	0	0	0	0
4	I	8	0	0	2	0
4	J	6	0	0	1	0
4	L	1	0	0	0	0
4	M	10	0	0	1	0
4	N	6	0	0	2	0
4	O	10	0	0	0	0
4	P	3	0	0	1	0
All	All	10089	0	8757	512	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 512 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:265:THR:HG22	3:L:275:ARG:HE	1.09	1.15
3:L:238:ARG:HG2	3:L:238:ARG:HH11	1.03	1.15
3:M:238:ARG:HH11	3:M:238:ARG:HG2	1.18	1.06
3:K:250:ASN:HA	3:K:253:PHE:HB3	1.38	1.03
2:F:9:DT:OP2	3:N:166:THR:HG23	1.59	1.03

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	
3	I	148/151 (98%)	123 (83%)	17 (12%)	8 (5%)	3	2
3	J	84/151 (56%)	78 (93%)	6 (7%)	0	100	100
3	K	148/151 (98%)	119 (80%)	22 (15%)	7 (5%)	4	3
3	L	143/151 (95%)	122 (85%)	16 (11%)	5 (4%)	6	7
3	M	148/151 (98%)	136 (92%)	10 (7%)	2 (1%)	16	27
3	N	83/151 (55%)	79 (95%)	3 (4%)	1 (1%)	19	32
3	O	148/151 (98%)	127 (86%)	19 (13%)	2 (1%)	16	27
3	P	80/151 (53%)	70 (88%)	9 (11%)	1 (1%)	18	29
All	All	982/1208 (81%)	854 (87%)	102 (10%)	26 (3%)	8	11

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	230	GLU
3	I	231	PRO
3	I	232	SER
3	K	218	GLU
3	N	218	GLU

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	
3	I	125/129 (97%)	103 (82%)	22 (18%)	3	4
3	J	69/129 (54%)	63 (91%)	6 (9%)	15	27
3	K	105/129 (81%)	89 (85%)	16 (15%)	4	7
3	L	115/129 (89%)	105 (91%)	10 (9%)	15	27
3	M	124/129 (96%)	96 (77%)	28 (23%)	1	2
3	N	68/129 (53%)	63 (93%)	5 (7%)	20	35
3	O	119/129 (92%)	98 (82%)	21 (18%)	3	4
3	P	62/129 (48%)	56 (90%)	6 (10%)	12	21
All	All	787/1032 (76%)	673 (86%)	114 (14%)	5	8

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	279	ARG
3	M	197	SER
3	O	269	LYS
3	L	286	ARG
3	M	170	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	287	GLN
3	N	199	GLN
3	P	199	GLN
3	N	170	GLN
3	N	216	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	14/14 (100%)	0.02	0	100	100	36, 43, 52, 53	0
1	C	14/14 (100%)	-0.15	0	100	100	42, 48, 57, 58	0
1	E	14/14 (100%)	-0.08	0	100	100	33, 37, 49, 53	0
1	G	14/14 (100%)	-0.11	0	100	100	35, 41, 59, 59	0
2	B	14/14 (100%)	-0.14	0	100	100	34, 46, 58, 59	0
2	D	14/14 (100%)	-0.20	0	100	100	43, 50, 54, 55	0
2	F	14/14 (100%)	-0.07	0	100	100	33, 41, 45, 55	0
2	H	14/14 (100%)	-0.20	0	100	100	37, 44, 48, 52	0
3	I	150/151 (99%)	-0.06	0	100	100	34, 68, 103, 131	0
3	J	86/151 (56%)	0.09	3 (3%)	42	43	37, 60, 97, 105	0
3	K	150/151 (99%)	0.96	20 (13%)	4	3	51, 107, 137, 146	0
3	L	145/151 (96%)	0.36	9 (6%)	20	20	46, 68, 115, 142	0
3	M	150/151 (99%)	-0.01	3 (2%)	62	64	33, 58, 92, 123	0
3	N	85/151 (56%)	0.23	4 (4%)	30	31	38, 58, 92, 106	0
3	O	150/151 (99%)	0.39	14 (9%)	9	8	40, 79, 123, 136	0
3	P	82/151 (54%)	0.11	3 (3%)	39	41	43, 73, 103, 119	0
All	All	1110/1320 (84%)	0.24	56 (5%)	28	28	33, 67, 121, 146	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	175	THR	8.6
3	K	292	THR	8.4
3	K	174	ALA	6.4
3	K	282	PHE	5.0
3	K	273	TYR	4.8

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.