wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2021 – 04:31 PM EDT

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 X-ray Structure Validation Summary 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 (i) symbol.

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

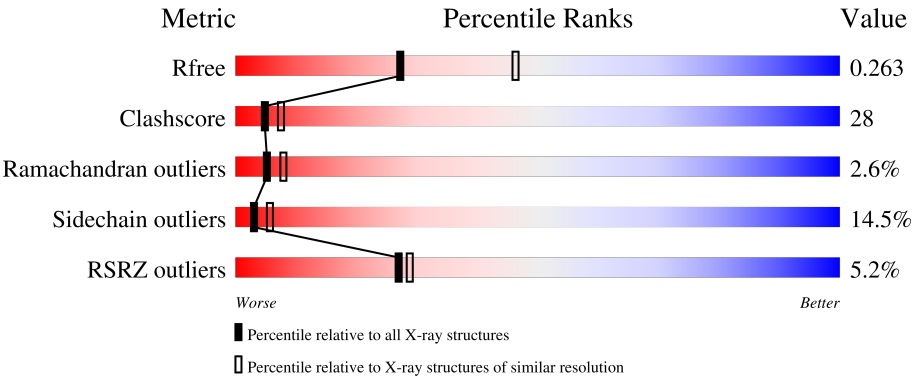
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	14	21% 29% 50%
1	C	14	7% 50% 43%
1	E	14	36% 43% 21%
1	G	14	21% 36% 43%
2	B	14	7% 36% 57%

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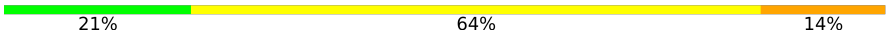
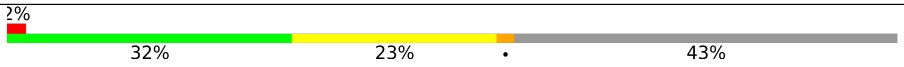
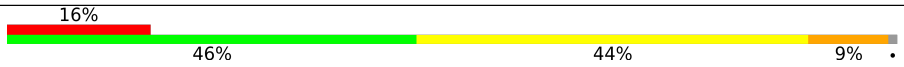
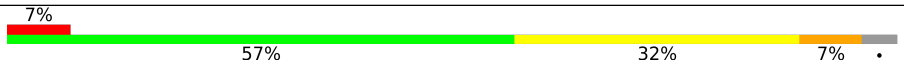
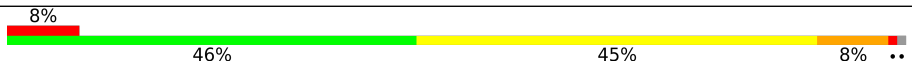
Mol	Chain	Length	Quality of chain
2	D	14	
2	F	14	
2	H	14	
3	I	151	
3	J	151	
3	K	151	
3	L	151	
3	M	151	
3	N	151	
3	O	151	
3	P	151	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10089 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 DNA chain called 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*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	conflict	UNP Q14863
I	172	MSE	LEU	conflict	UNP Q14863
I	186	SER	CYS	engineered mutation	UNP Q14863
I	267	MSE	ILE	conflict	UNP Q14863
I	283	SER	CYS	engineered mutation	UNP Q14863
J	144	MSE	LEU	conflict	UNP Q14863
J	172	MSE	LEU	conflict	UNP Q14863
J	186	SER	CYS	engineered mutation	UNP Q14863
J	267	MSE	ILE	conflict	UNP Q14863
J	283	SER	CYS	engineered mutation	UNP Q14863
K	144	MSE	LEU	conflict	UNP Q14863
K	172	MSE	LEU	conflict	UNP Q14863
K	186	SER	CYS	engineered mutation	UNP Q14863
K	267	MSE	ILE	conflict	UNP Q14863
K	283	SER	CYS	engineered mutation	UNP Q14863
L	144	MSE	LEU	conflict	UNP Q14863
L	172	MSE	LEU	conflict	UNP Q14863
L	186	SER	CYS	engineered mutation	UNP Q14863
L	267	MSE	ILE	conflict	UNP Q14863
L	283	SER	CYS	engineered mutation	UNP Q14863
M	144	MSE	LEU	conflict	UNP Q14863
M	172	MSE	LEU	conflict	UNP Q14863
M	186	SER	CYS	engineered mutation	UNP Q14863
M	267	MSE	ILE	conflict	UNP Q14863
M	283	SER	CYS	engineered mutation	UNP Q14863
N	144	MSE	LEU	conflict	UNP Q14863
N	172	MSE	LEU	conflict	UNP Q14863
N	186	SER	CYS	engineered mutation	UNP Q14863
N	267	MSE	ILE	conflict	UNP Q14863

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Chain	Residue	Modelled	Actual	Comment	Reference
N	283	SER	CYS	engineered mutation	UNP Q14863
O	144	MSE	LEU	conflict	UNP Q14863
O	172	MSE	LEU	conflict	UNP Q14863
O	186	SER	CYS	engineered mutation	UNP Q14863
O	267	MSE	ILE	conflict	UNP Q14863
O	283	SER	CYS	engineered mutation	UNP Q14863
P	144	MSE	LEU	conflict	UNP Q14863
P	172	MSE	LEU	conflict	UNP Q14863
P	186	SER	CYS	engineered mutation	UNP Q14863
P	267	MSE	ILE	conflict	UNP Q14863
P	283	SER	CYS	engineered mutation	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 3 3	0	0

3 Residue-property plots (i)

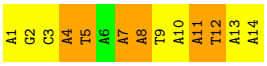
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

Chain A:

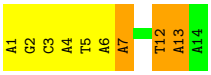
• Molecule 1: 5'-D(*DAP*DGP*DCP*DAP*DTP*DAP*DAP*DAP*DTP*DAP*DAP*DTP*DAP*DA)-3'

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*DC P*DT)-3'

Chain D:

• Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DC P*DT)-3'

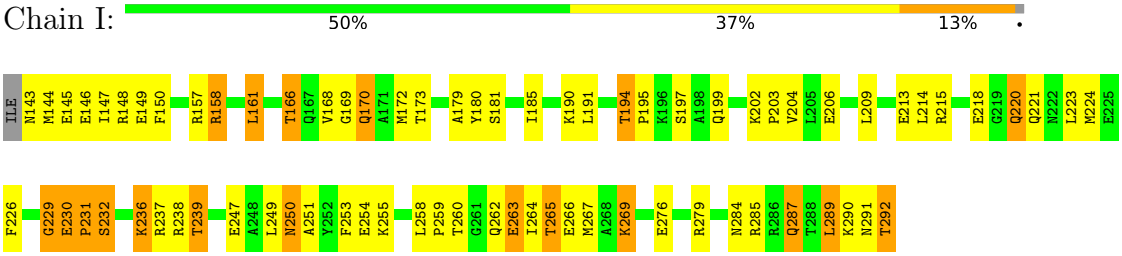
Chain F:

• Molecule 2: 5'-D(*DTP*DTP*DAP*DTP*DTP*DAP*DTP*DTP*DTP*DAP*DTP*DGP*DC P*DT)-3'

Chain H:

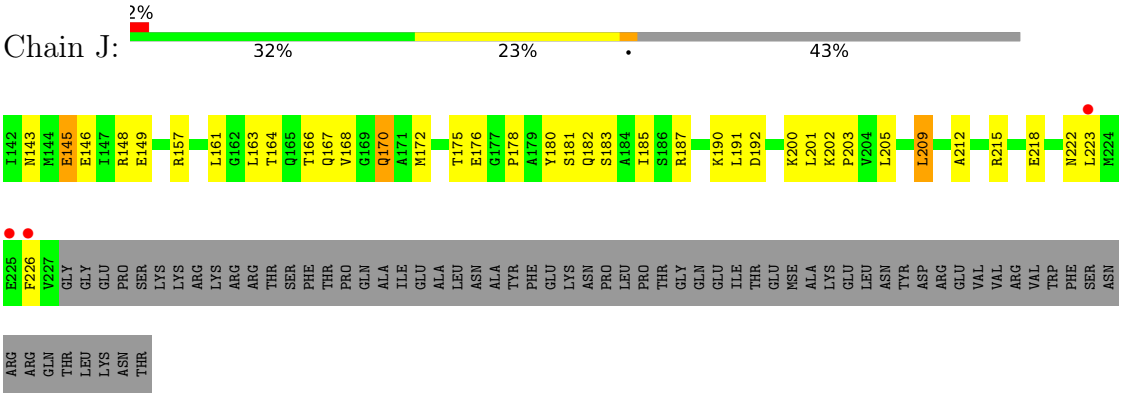
• Molecule 3: POU domain, class 6, transcription factor 1

Chain I:



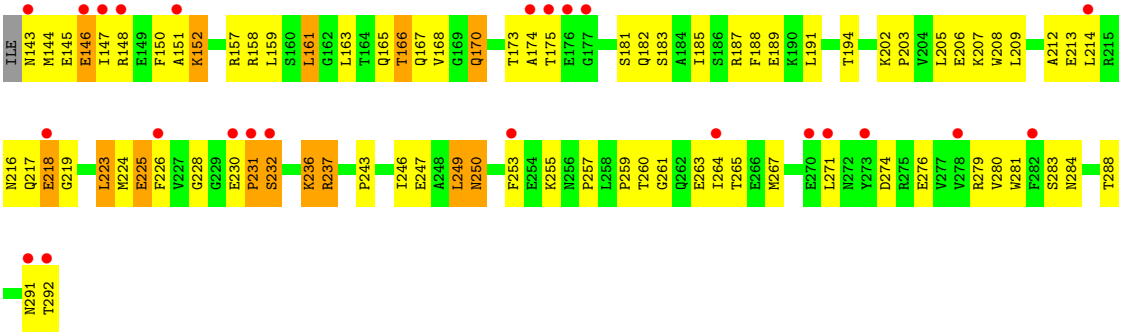
• Molecule 3: POU domain, class 6, transcription factor 1

Chain J:

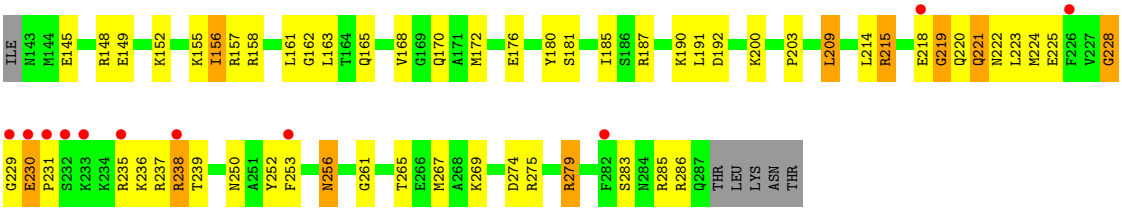


• Molecule 3: POU domain, class 6, transcription factor 1

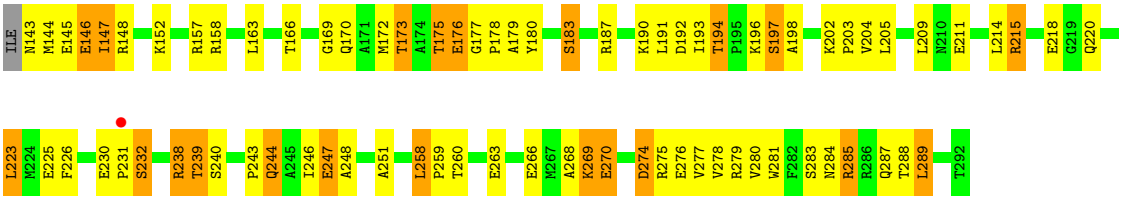
Chain K:



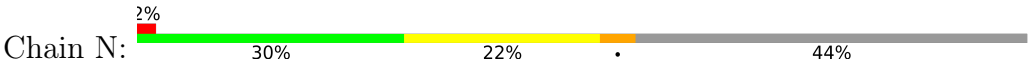
• Molecule 3: POU domain, class 6, transcription factor 1

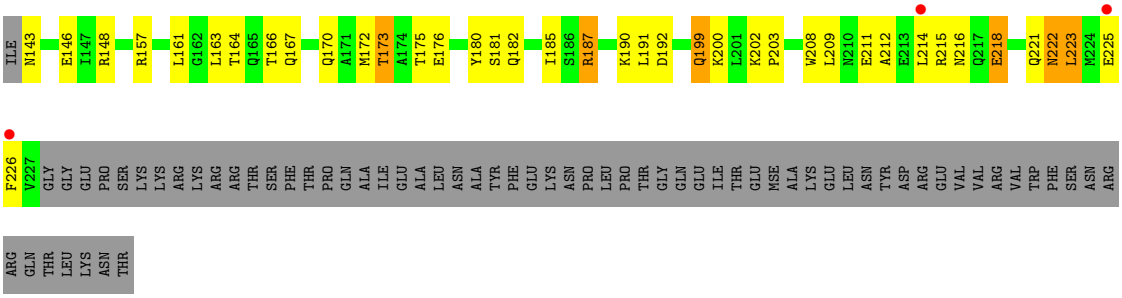


• Molecule 3: POU domain, class 6, transcription factor 1

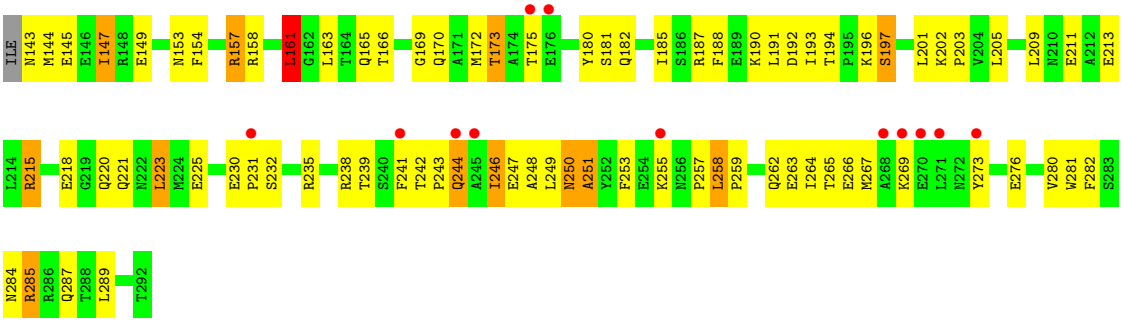


• Molecule 3: POU domain, class 6, transcription factor 1

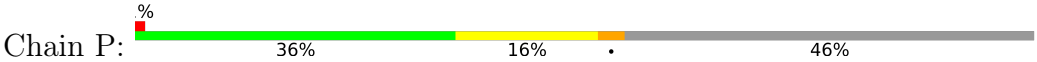


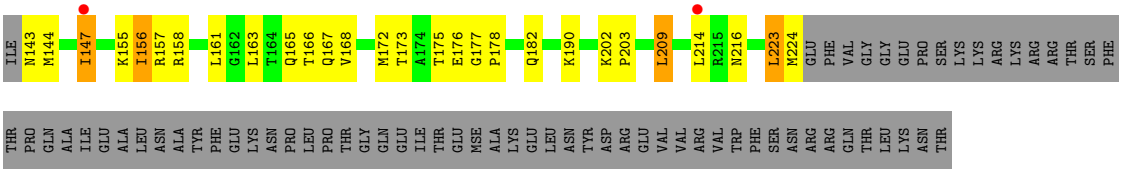


• Molecule 3: POU domain, class 6, transcription factor 1



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





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	2690 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 76.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.80	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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 28.

The worst 5 of 512 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: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 (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
3	I	148/151 (98%)	123 (83%)	17 (12%)	8 (5%)	2 2
3	J	84/151 (56%)	78 (93%)	6 (7%)	0	100 100
3	K	148/151 (98%)	119 (80%)	22 (15%)	7 (5%)	2 2
3	L	143/151 (95%)	122 (85%)	16 (11%)	5 (4%)	3 4
3	M	148/151 (98%)	136 (92%)	10 (7%)	2 (1%)	11 20
3	N	83/151 (55%)	79 (95%)	3 (4%)	1 (1%)	13 24
3	O	148/151 (98%)	127 (86%)	19 (13%)	2 (1%)	11 20
3	P	80/151 (53%)	70 (88%)	9 (11%)	1 (1%)	12 21
All	All	982/1208 (81%)	854 (87%)	102 (10%)	26 (3%)	5 8

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 (i)

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%)	2 3
3	J	69/129 (54%)	63 (91%)	6 (9%)	10 20
3	K	105/129 (81%)	89 (85%)	16 (15%)	3 5
3	L	115/129 (89%)	105 (91%)	10 (9%)	10 20
3	M	124/129 (96%)	96 (77%)	28 (23%)	1 1
3	N	68/129 (53%)	63 (93%)	5 (7%)	13 27
3	O	119/129 (92%)	98 (82%)	21 (18%)	2 3
3	P	62/129 (48%)	56 (90%)	6 (10%)	8 16
All	All	787/1032 (76%)	673 (86%)	114 (14%)	3 6

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

Mol	Chain	Res	Type
3	M	170	GLN
3	P	209	LEU
3	M	240	SER
3	P	155	LYS
3	O	232	SER

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

Mol	Chain	Res	Type
3	M	244	GLN
3	P	199	GLN
3	N	216	ASN
3	P	221	GLN
3	O	287	GLN

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 monosaccharides 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, 95^{th} 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%)	-0.18	0 100 100	42, 48, 57, 58	0
1	E	14/14 (100%)	-0.06	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%)	-0.10	0 100 100	34, 46, 58, 59	0
2	D	14/14 (100%)	-0.18	0 100 100	43, 50, 54, 55	0
2	F	14/14 (100%)	-0.03	0 100 100	33, 41, 45, 55	0
2	H	14/14 (100%)	-0.16	0 100 100	37, 44, 48, 52	0
3	I	146/151 (96%)	-0.07	0 100 100	34, 67, 102, 131	0
3	J	83/151 (54%)	0.12	3 (3%) 42 46	37, 60, 91, 103	0
3	K	146/151 (96%)	0.99	24 (16%) 1 1	51, 107, 136, 146	0
3	L	141/151 (93%)	0.42	11 (7%) 13 13	46, 67, 114, 142	0
3	M	146/151 (96%)	-0.04	1 (0%) 87 89	33, 57, 91, 123	0
3	N	82/151 (54%)	0.21	3 (3%) 41 45	38, 58, 88, 106	0
3	O	146/151 (96%)	0.37	12 (8%) 11 11	40, 79, 122, 136	0
3	P	79/151 (52%)	0.08	2 (2%) 57 61	43, 73, 107, 119	0
All	All	1081/1320 (81%)	0.24	56 (5%) 27 29	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	8.0
3	K	174	ALA	7.2
3	L	231	PRO	5.3
3	O	268	ALA	4.9

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 monosaccharides 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.