



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 5Y4S / pdb_00005y4s
Title : Structure of a methyltransferase complex
Authors : Yan, X.; Xin, L.; Tan, Y.J.; Jin, S.; Liang, Z.X.; Gao, Y.G.
Deposited on : 2017-08-04
Resolution : 3.40 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:

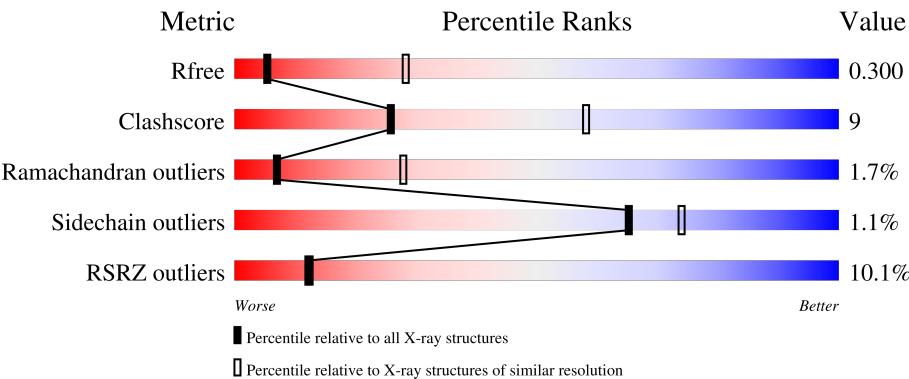
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	294	
1	B	294	
1	C	294	
1	D	294	
1	E	294	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	294	7% 74% 17% • 8%
1	G	294	9% 73% 16% • 8%
1	H	294	12% 77% 14% • 8%
1	I	294	10% 74% 16% • 8%
1	J	294	14% 74% 18% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19440 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 Chemotaxis protein methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2016	1285	351	368	12			
1	B	269	Total	C	N	O	S	0	0	0
			1831	1147	320	354	10			
1	C	270	Total	C	N	O	S	0	0	0
			1962	1249	334	369	10			
1	D	268	Total	C	N	O	S	0	0	0
			1888	1201	319	357	11			
1	E	270	Total	C	N	O	S	0	0	0
			1965	1247	338	368	12			
1	F	270	Total	C	N	O	S	0	0	0
			1952	1235	343	363	11			
1	G	270	Total	C	N	O	S	0	0	0
			1963	1239	346	366	12			
1	H	270	Total	C	N	O	S	0	0	0
			1974	1258	343	362	11			
1	I	270	Total	C	N	O	S	0	0	0
			1945	1233	342	360	10			
1	J	270	Total	C	N	O	S	0	0	0
			1944	1229	342	362	11			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O87131
A	-18	GLY	-	expression tag	UNP O87131
A	-17	SER	-	expression tag	UNP O87131
A	-16	SER	-	expression tag	UNP O87131
A	-15	HIS	-	expression tag	UNP O87131
A	-14	HIS	-	expression tag	UNP O87131
A	-13	HIS	-	expression tag	UNP O87131
A	-12	HIS	-	expression tag	UNP O87131
A	-11	HIS	-	expression tag	UNP O87131

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP O87131
A	-9	SER	-	expression tag	UNP O87131
A	-8	GLN	-	expression tag	UNP O87131
A	-7	ASP	-	expression tag	UNP O87131
A	-6	PRO	-	expression tag	UNP O87131
A	-5	GLU	-	expression tag	UNP O87131
A	-4	ASN	-	expression tag	UNP O87131
A	-3	LEU	-	expression tag	UNP O87131
A	-2	TYR	-	expression tag	UNP O87131
A	-1	PHE	-	expression tag	UNP O87131
A	0	GLN	-	expression tag	UNP O87131
A	1	GLY	-	expression tag	UNP O87131
B	-19	MET	-	expression tag	UNP O87131
B	-18	GLY	-	expression tag	UNP O87131
B	-17	SER	-	expression tag	UNP O87131
B	-16	SER	-	expression tag	UNP O87131
B	-15	HIS	-	expression tag	UNP O87131
B	-14	HIS	-	expression tag	UNP O87131
B	-13	HIS	-	expression tag	UNP O87131
B	-12	HIS	-	expression tag	UNP O87131
B	-11	HIS	-	expression tag	UNP O87131
B	-10	HIS	-	expression tag	UNP O87131
B	-9	SER	-	expression tag	UNP O87131
B	-8	GLN	-	expression tag	UNP O87131
B	-7	ASP	-	expression tag	UNP O87131
B	-6	PRO	-	expression tag	UNP O87131
B	-5	GLU	-	expression tag	UNP O87131
B	-4	ASN	-	expression tag	UNP O87131
B	-3	LEU	-	expression tag	UNP O87131
B	-2	TYR	-	expression tag	UNP O87131
B	-1	PHE	-	expression tag	UNP O87131
B	0	GLN	-	expression tag	UNP O87131
B	1	GLY	-	expression tag	UNP O87131
C	-19	MET	-	expression tag	UNP O87131
C	-18	GLY	-	expression tag	UNP O87131
C	-17	SER	-	expression tag	UNP O87131
C	-16	SER	-	expression tag	UNP O87131
C	-15	HIS	-	expression tag	UNP O87131
C	-14	HIS	-	expression tag	UNP O87131
C	-13	HIS	-	expression tag	UNP O87131
C	-12	HIS	-	expression tag	UNP O87131
C	-11	HIS	-	expression tag	UNP O87131

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP O87131
C	-9	SER	-	expression tag	UNP O87131
C	-8	GLN	-	expression tag	UNP O87131
C	-7	ASP	-	expression tag	UNP O87131
C	-6	PRO	-	expression tag	UNP O87131
C	-5	GLU	-	expression tag	UNP O87131
C	-4	ASN	-	expression tag	UNP O87131
C	-3	LEU	-	expression tag	UNP O87131
C	-2	TYR	-	expression tag	UNP O87131
C	-1	PHE	-	expression tag	UNP O87131
C	0	GLN	-	expression tag	UNP O87131
C	1	GLY	-	expression tag	UNP O87131
D	-19	MET	-	expression tag	UNP O87131
D	-18	GLY	-	expression tag	UNP O87131
D	-17	SER	-	expression tag	UNP O87131
D	-16	SER	-	expression tag	UNP O87131
D	-15	HIS	-	expression tag	UNP O87131
D	-14	HIS	-	expression tag	UNP O87131
D	-13	HIS	-	expression tag	UNP O87131
D	-12	HIS	-	expression tag	UNP O87131
D	-11	HIS	-	expression tag	UNP O87131
D	-10	HIS	-	expression tag	UNP O87131
D	-9	SER	-	expression tag	UNP O87131
D	-8	GLN	-	expression tag	UNP O87131
D	-7	ASP	-	expression tag	UNP O87131
D	-6	PRO	-	expression tag	UNP O87131
D	-5	GLU	-	expression tag	UNP O87131
D	-4	ASN	-	expression tag	UNP O87131
D	-3	LEU	-	expression tag	UNP O87131
D	-2	TYR	-	expression tag	UNP O87131
D	-1	PHE	-	expression tag	UNP O87131
D	0	GLN	-	expression tag	UNP O87131
D	1	GLY	-	expression tag	UNP O87131
E	-19	MET	-	expression tag	UNP O87131
E	-18	GLY	-	expression tag	UNP O87131
E	-17	SER	-	expression tag	UNP O87131
E	-16	SER	-	expression tag	UNP O87131
E	-15	HIS	-	expression tag	UNP O87131
E	-14	HIS	-	expression tag	UNP O87131
E	-13	HIS	-	expression tag	UNP O87131
E	-12	HIS	-	expression tag	UNP O87131
E	-11	HIS	-	expression tag	UNP O87131

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP O87131
E	-9	SER	-	expression tag	UNP O87131
E	-8	GLN	-	expression tag	UNP O87131
E	-7	ASP	-	expression tag	UNP O87131
E	-6	PRO	-	expression tag	UNP O87131
E	-5	GLU	-	expression tag	UNP O87131
E	-4	ASN	-	expression tag	UNP O87131
E	-3	LEU	-	expression tag	UNP O87131
E	-2	TYR	-	expression tag	UNP O87131
E	-1	PHE	-	expression tag	UNP O87131
E	0	GLN	-	expression tag	UNP O87131
E	1	GLY	-	expression tag	UNP O87131
F	-19	MET	-	expression tag	UNP O87131
F	-18	GLY	-	expression tag	UNP O87131
F	-17	SER	-	expression tag	UNP O87131
F	-16	SER	-	expression tag	UNP O87131
F	-15	HIS	-	expression tag	UNP O87131
F	-14	HIS	-	expression tag	UNP O87131
F	-13	HIS	-	expression tag	UNP O87131
F	-12	HIS	-	expression tag	UNP O87131
F	-11	HIS	-	expression tag	UNP O87131
F	-10	HIS	-	expression tag	UNP O87131
F	-9	SER	-	expression tag	UNP O87131
F	-8	GLN	-	expression tag	UNP O87131
F	-7	ASP	-	expression tag	UNP O87131
F	-6	PRO	-	expression tag	UNP O87131
F	-5	GLU	-	expression tag	UNP O87131
F	-4	ASN	-	expression tag	UNP O87131
F	-3	LEU	-	expression tag	UNP O87131
F	-2	TYR	-	expression tag	UNP O87131
F	-1	PHE	-	expression tag	UNP O87131
F	0	GLN	-	expression tag	UNP O87131
F	1	GLY	-	expression tag	UNP O87131
G	-19	MET	-	expression tag	UNP O87131
G	-18	GLY	-	expression tag	UNP O87131
G	-17	SER	-	expression tag	UNP O87131
G	-16	SER	-	expression tag	UNP O87131
G	-15	HIS	-	expression tag	UNP O87131
G	-14	HIS	-	expression tag	UNP O87131
G	-13	HIS	-	expression tag	UNP O87131
G	-12	HIS	-	expression tag	UNP O87131
G	-11	HIS	-	expression tag	UNP O87131

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	HIS	-	expression tag	UNP O87131
G	-9	SER	-	expression tag	UNP O87131
G	-8	GLN	-	expression tag	UNP O87131
G	-7	ASP	-	expression tag	UNP O87131
G	-6	PRO	-	expression tag	UNP O87131
G	-5	GLU	-	expression tag	UNP O87131
G	-4	ASN	-	expression tag	UNP O87131
G	-3	LEU	-	expression tag	UNP O87131
G	-2	TYR	-	expression tag	UNP O87131
G	-1	PHE	-	expression tag	UNP O87131
G	0	GLN	-	expression tag	UNP O87131
G	1	GLY	-	expression tag	UNP O87131
H	-19	MET	-	expression tag	UNP O87131
H	-18	GLY	-	expression tag	UNP O87131
H	-17	SER	-	expression tag	UNP O87131
H	-16	SER	-	expression tag	UNP O87131
H	-15	HIS	-	expression tag	UNP O87131
H	-14	HIS	-	expression tag	UNP O87131
H	-13	HIS	-	expression tag	UNP O87131
H	-12	HIS	-	expression tag	UNP O87131
H	-11	HIS	-	expression tag	UNP O87131
H	-10	HIS	-	expression tag	UNP O87131
H	-9	SER	-	expression tag	UNP O87131
H	-8	GLN	-	expression tag	UNP O87131
H	-7	ASP	-	expression tag	UNP O87131
H	-6	PRO	-	expression tag	UNP O87131
H	-5	GLU	-	expression tag	UNP O87131
H	-4	ASN	-	expression tag	UNP O87131
H	-3	LEU	-	expression tag	UNP O87131
H	-2	TYR	-	expression tag	UNP O87131
H	-1	PHE	-	expression tag	UNP O87131
H	0	GLN	-	expression tag	UNP O87131
H	1	GLY	-	expression tag	UNP O87131
I	-19	MET	-	expression tag	UNP O87131
I	-18	GLY	-	expression tag	UNP O87131
I	-17	SER	-	expression tag	UNP O87131
I	-16	SER	-	expression tag	UNP O87131
I	-15	HIS	-	expression tag	UNP O87131
I	-14	HIS	-	expression tag	UNP O87131
I	-13	HIS	-	expression tag	UNP O87131
I	-12	HIS	-	expression tag	UNP O87131
I	-11	HIS	-	expression tag	UNP O87131

Continued on next page...

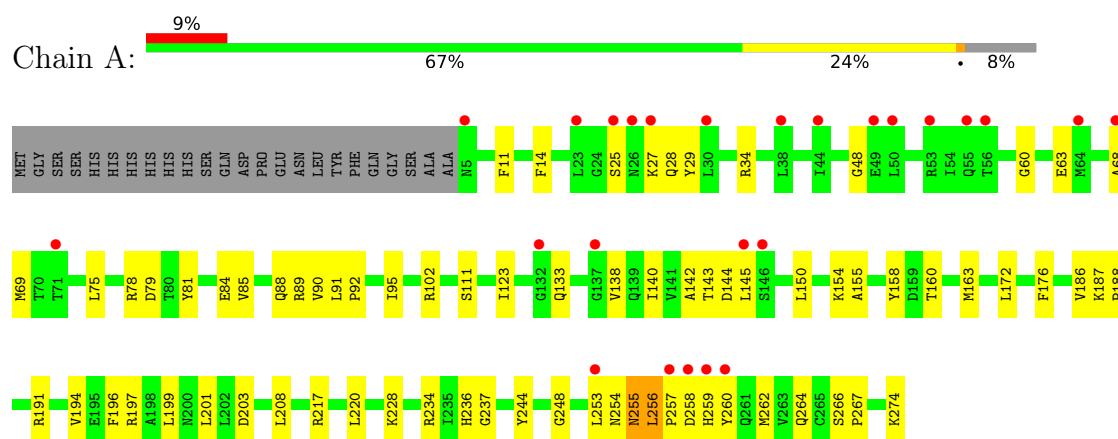
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP O87131
I	-9	SER	-	expression tag	UNP O87131
I	-8	GLN	-	expression tag	UNP O87131
I	-7	ASP	-	expression tag	UNP O87131
I	-6	PRO	-	expression tag	UNP O87131
I	-5	GLU	-	expression tag	UNP O87131
I	-4	ASN	-	expression tag	UNP O87131
I	-3	LEU	-	expression tag	UNP O87131
I	-2	TYR	-	expression tag	UNP O87131
I	-1	PHE	-	expression tag	UNP O87131
I	0	GLN	-	expression tag	UNP O87131
I	1	GLY	-	expression tag	UNP O87131
J	-19	MET	-	expression tag	UNP O87131
J	-18	GLY	-	expression tag	UNP O87131
J	-17	SER	-	expression tag	UNP O87131
J	-16	SER	-	expression tag	UNP O87131
J	-15	HIS	-	expression tag	UNP O87131
J	-14	HIS	-	expression tag	UNP O87131
J	-13	HIS	-	expression tag	UNP O87131
J	-12	HIS	-	expression tag	UNP O87131
J	-11	HIS	-	expression tag	UNP O87131
J	-10	HIS	-	expression tag	UNP O87131
J	-9	SER	-	expression tag	UNP O87131
J	-8	GLN	-	expression tag	UNP O87131
J	-7	ASP	-	expression tag	UNP O87131
J	-6	PRO	-	expression tag	UNP O87131
J	-5	GLU	-	expression tag	UNP O87131
J	-4	ASN	-	expression tag	UNP O87131
J	-3	LEU	-	expression tag	UNP O87131
J	-2	TYR	-	expression tag	UNP O87131
J	-1	PHE	-	expression tag	UNP O87131
J	0	GLN	-	expression tag	UNP O87131
J	1	GLY	-	expression tag	UNP O87131

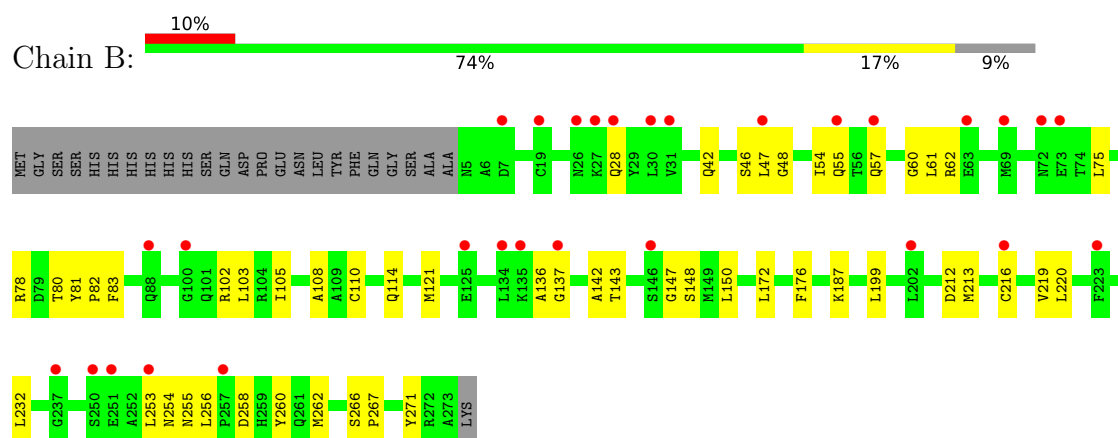
3 Residue-property plots [i](#)

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.

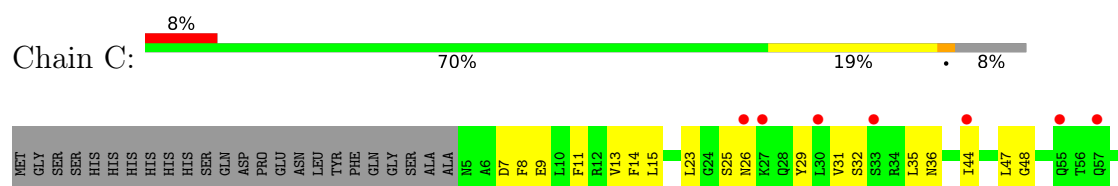
• Molecule 1: Chemotaxis protein methyltransferase 1

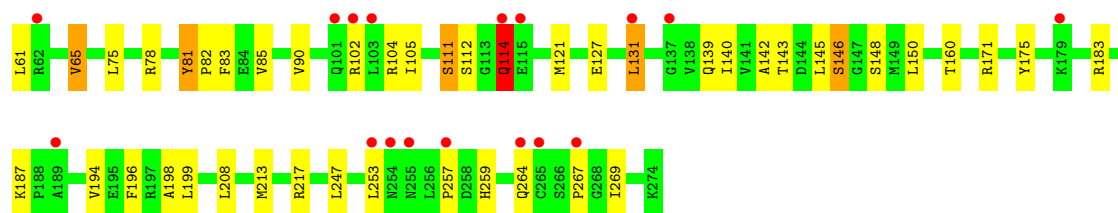


• Molecule 1: Chemotaxis protein methyltransferase 1

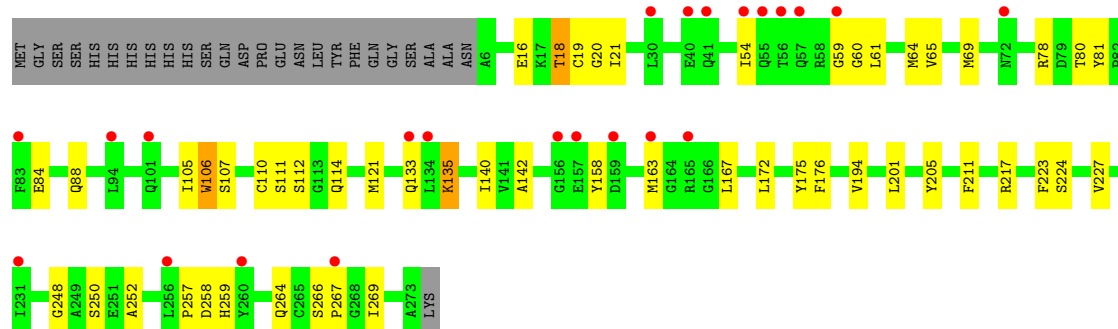
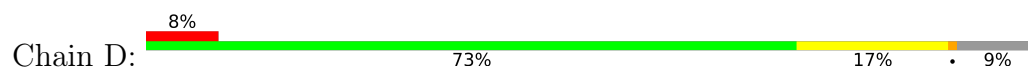


• Molecule 1: Chemotaxis protein methyltransferase 1

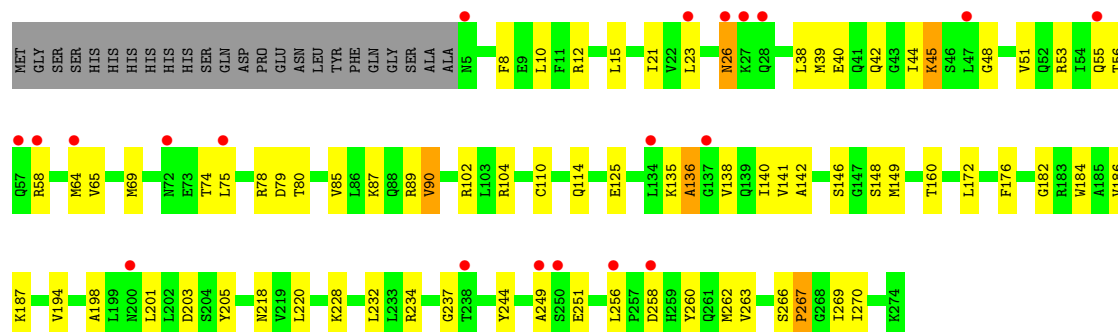




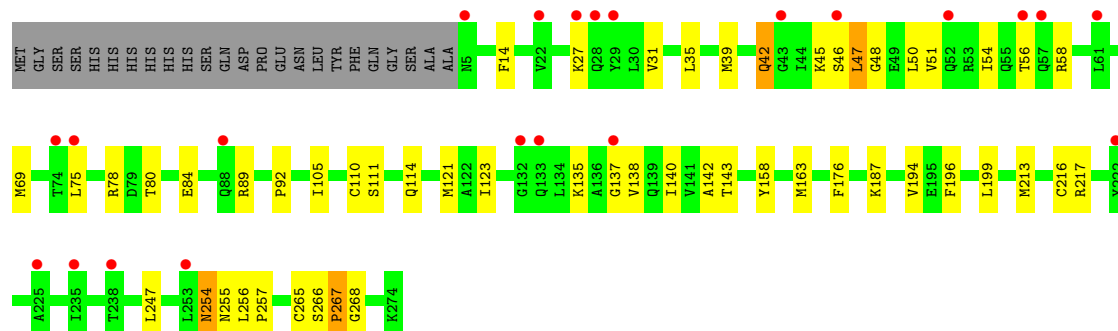
• Molecule 1: Chemotaxis protein methyltransferase 1



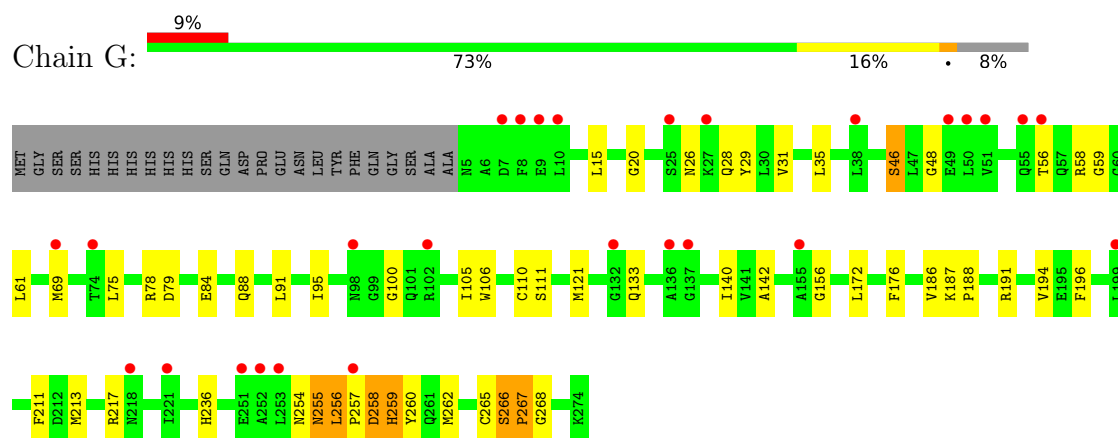
• Molecule 1: Chemotaxis protein methyltransferase 1



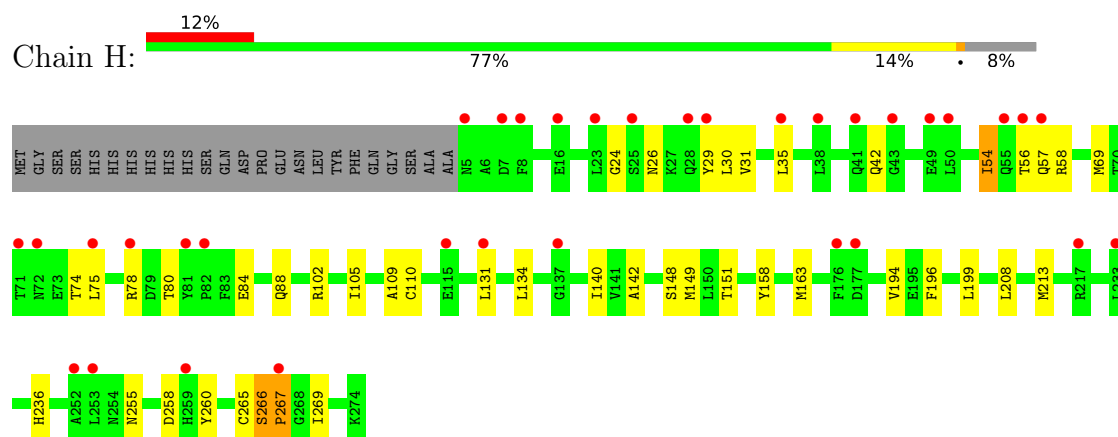
• Molecule 1: Chemotaxis protein methyltransferase 1



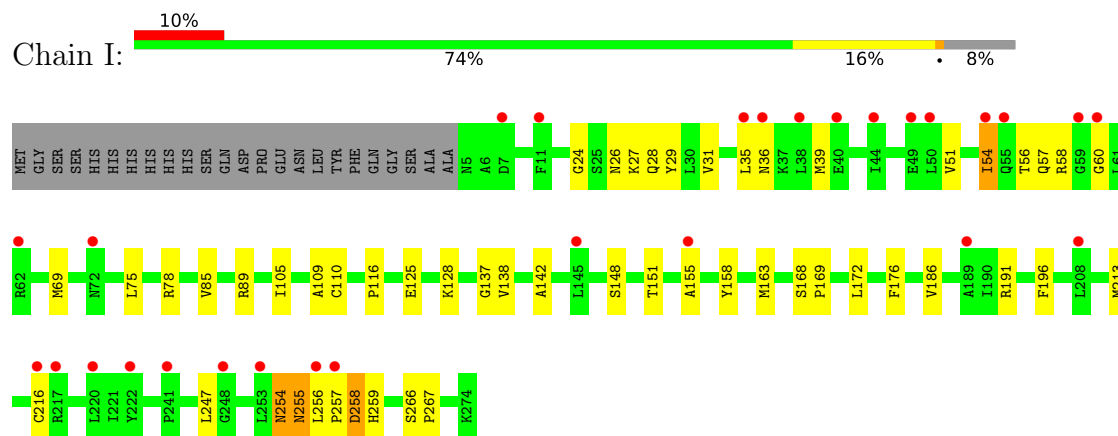
- Molecule 1: Chemotaxis protein methyltransferase 1



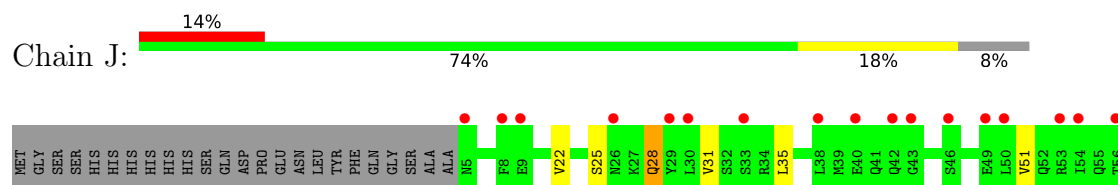
- Molecule 1: Chemotaxis protein methyltransferase 1

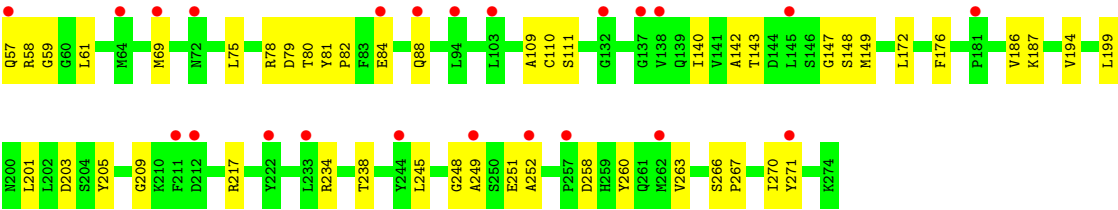


- Molecule 1: Chemotaxis protein methyltransferase 1



- Molecule 1: Chemotaxis protein methyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	279.55Å 279.55Å 138.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.40 49.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-3.40) 100.0 (49.42-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.260 , 0.293 0.267 , 0.300	Depositor DCC
R_{free} test set	7079 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å ²)	116.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 135.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19440	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 ⓘ

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	0.39	0/2054	0.95	11/2780 (0.4%)
1	B	0.36	0/1867	0.93	7/2548 (0.3%)
1	C	0.35	0/2000	0.90	9/2723 (0.3%)
1	D	0.35	0/1924	0.89	4/2620 (0.2%)
1	E	0.38	0/2002	0.94	9/2720 (0.3%)
1	F	0.35	0/1984	0.87	7/2691 (0.3%)
1	G	0.34	0/1997	0.83	5/2710 (0.2%)
1	H	0.35	0/2009	0.87	3/2728 (0.1%)
1	I	0.35	0/1980	0.86	3/2689 (0.1%)
1	J	0.34	0/1977	0.88	7/2684 (0.3%)
All	All	0.36	0/19794	0.89	65/26893 (0.2%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	28	GLN	N-CA-C	-9.66	100.69	114.12
1	B	28	GLN	N-CA-C	-9.06	101.20	112.88
1	C	48	GLY	N-CA-C	-7.98	104.86	115.32
1	A	28	GLN	N-CA-C	-7.72	102.91	114.64
1	H	69	MET	N-CA-C	-7.69	103.90	113.28
1	J	69	MET	N-CA-C	-7.48	104.15	113.28
1	E	75	LEU	N-CA-C	7.31	121.19	110.59
1	A	102	ARG	N-CA-C	7.26	120.10	111.02
1	I	255	ASN	N-CA-C	6.99	120.92	109.94
1	A	69	MET	N-CA-C	-6.92	104.84	113.28
1	H	102	ARG	N-CA-C	6.48	119.12	111.02
1	G	133	GLN	N-CA-C	-6.40	105.62	113.50
1	B	81	TYR	CA-C-N	-6.15	113.35	119.56
1	B	81	TYR	C-N-CA	-6.15	113.35	119.56
1	E	8	PHE	N-CA-C	-6.11	105.73	113.43
1	A	133	GLN	N-CA-C	-6.05	106.06	113.50
1	A	111	SER	CB-CA-C	-6.03	109.64	116.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	ARG	N-CA-C	5.97	119.35	111.28
1	A	48	GLY	N-CA-C	-5.97	107.25	114.66
1	C	111	SER	CB-CA-C	-5.89	109.22	117.23
1	E	237	GLY	N-CA-C	-5.88	102.41	112.30
1	J	111	SER	CB-CA-C	-5.79	109.91	116.63
1	E	138	VAL	N-CA-C	-5.71	99.00	107.51
1	G	69	MET	N-CA-C	-5.70	106.33	113.28
1	E	90	VAL	N-CA-C	5.69	115.77	110.42
1	D	135	LYS	CB-CA-C	-5.67	109.52	117.23
1	H	30	LEU	N-CA-C	-5.59	106.41	113.18
1	F	42	GLN	N-CA-C	-5.58	100.99	108.86
1	G	111	SER	CB-CA-C	-5.53	110.22	116.63
1	D	111	SER	CB-CA-C	-5.49	110.26	116.63
1	E	48	GLY	N-CA-C	-5.37	108.00	114.66
1	I	60	GLY	N-CA-C	5.35	122.58	114.61
1	E	187	LYS	CA-C-N	5.33	125.65	119.47
1	E	187	LYS	C-N-CA	5.33	125.65	119.47
1	A	237	GLY	N-CA-C	-5.30	103.40	112.30
1	A	187	LYS	CA-C-N	5.28	125.59	119.47
1	A	187	LYS	C-N-CA	5.28	125.59	119.47
1	B	54	ILE	N-CA-C	5.26	116.03	110.72
1	F	137	GLY	N-CA-C	-5.26	102.86	110.90
1	A	81	TYR	CA-C-N	-5.24	114.27	119.56
1	A	81	TYR	C-N-CA	-5.24	114.27	119.56
1	C	81	TYR	CA-C-N	-5.24	114.27	119.56
1	C	81	TYR	C-N-CA	-5.24	114.27	119.56
1	C	114	GLN	N-CA-C	5.19	117.34	111.11
1	C	102	ARG	N-CA-C	5.16	118.32	111.30
1	C	187	LYS	CA-C-N	5.15	125.45	119.47
1	C	187	LYS	C-N-CA	5.15	125.45	119.47
1	J	187	LYS	CA-C-N	5.09	125.38	119.47
1	J	187	LYS	C-N-CA	5.09	125.38	119.47
1	D	81	TYR	CA-C-N	-5.08	114.43	119.56
1	D	81	TYR	C-N-CA	-5.08	114.43	119.56
1	J	81	TYR	CA-C-N	-5.07	114.44	119.56
1	J	81	TYR	C-N-CA	-5.07	114.44	119.56
1	B	114	GLN	N-CA-C	5.06	117.18	111.11
1	F	111	SER	CB-CA-C	-5.05	110.36	117.23
1	I	69	MET	N-CA-C	-5.04	107.13	113.28
1	F	114	GLN	N-CA-C	5.04	117.16	111.02
1	F	187	LYS	CA-C-N	5.03	125.31	119.47
1	F	187	LYS	C-N-CA	5.03	125.31	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	N-CA-C	5.03	117.84	110.30
1	B	187	LYS	CA-C-N	5.03	125.30	119.47
1	B	187	LYS	C-N-CA	5.03	125.30	119.47
1	F	135	LYS	N-CA-C	-5.03	101.11	109.46
1	G	187	LYS	CA-C-N	5.00	125.27	119.47
1	G	187	LYS	C-N-CA	5.00	125.27	119.47

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	2016	0	1938	53	0
1	B	1831	0	1526	29	0
1	C	1962	0	1818	40	0
1	D	1888	0	1699	43	0
1	E	1965	0	1823	42	0
1	F	1952	0	1845	34	0
1	G	1963	0	1842	45	0
1	H	1974	0	1888	26	0
1	I	1945	0	1812	34	0
1	J	1944	0	1817	31	0
All	All	19440	0	18008	355	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 9.

All (355) 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:F:78:ARG:HB2	1:F:217:ARG:HH12	1.40	0.85
1:G:29:TYR:CB	1:H:267:PRO:HG3	2.14	0.78
1:C:257:PRO:HG2	1:C:259:HIS:CE1	2.20	0.77
1:D:20:GLY:O	1:D:252:ALA:CB	2.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LYS:O	1:F:47:LEU:N	2.16	0.76
1:D:158:TYR:HB3	1:D:163:MET:HE3	1.66	0.76
1:F:75:LEU:HB2	1:F:78:ARG:HG2	1.69	0.73
1:G:75:LEU:HB2	1:G:78:ARG:HG2	1.71	0.73
1:J:78:ARG:HB2	1:J:217:ARG:HH12	1.52	0.73
1:B:102:ARG:HB2	1:B:136:ALA:CB	2.19	0.73
1:D:106:TRP:CE3	1:D:107:SER:N	2.57	0.72
1:F:14:PHE:CB	1:F:50:LEU:HD11	2.19	0.72
1:G:78:ARG:HB2	1:G:217:ARG:HH12	1.53	0.72
1:G:29:TYR:CB	1:H:267:PRO:CG	2.68	0.72
1:A:236:HIS:HB2	1:A:260:TYR:OH	1.88	0.71
1:A:203:ASP:O	1:A:234:ARG:NH2	2.23	0.70
1:D:106:TRP:HB2	1:D:211:PHE:CD2	2.26	0.70
1:C:75:LEU:HB2	1:C:78:ARG:HG3	1.73	0.70
1:J:176:PHE:HE1	1:J:186:VAL:HG22	1.56	0.69
1:D:59:GLY:O	1:D:61:LEU:N	2.26	0.69
1:C:146:SER:HB3	1:C:198:ALA:HB1	1.74	0.68
1:C:199:LEU:HD22	1:C:208:LEU:HD11	1.75	0.67
1:C:112:SER:OG	1:C:114:GLN:NE2	2.28	0.66
1:I:26:ASN:O	1:I:28:GLN:N	2.27	0.66
1:C:257:PRO:HG2	1:C:259:HIS:HE1	1.58	0.66
1:J:25:SER:O	1:J:28:GLN:HB2	1.96	0.66
1:D:16:GLU:O	1:D:20:GLY:HA2	1.95	0.66
1:H:75:LEU:HB2	1:H:78:ARG:HG2	1.79	0.65
1:B:102:ARG:HB2	1:B:136:ALA:HB1	1.77	0.64
1:A:78:ARG:HB2	1:A:217:ARG:HH12	1.63	0.63
1:D:20:GLY:O	1:D:252:ALA:HB3	1.96	0.63
1:D:20:GLY:O	1:D:252:ALA:HB2	1.99	0.63
1:I:26:ASN:C	1:I:28:GLN:H	2.07	0.63
1:G:254:ASN:O	1:G:255:ASN:HB2	1.98	0.62
1:E:74:THR:HB	1:E:114:GLN:OE1	2.00	0.62
1:G:265:CYS:HB2	1:G:268:GLY:O	2.00	0.61
1:E:45:LYS:O	1:E:45:LYS:HG3	2.00	0.61
1:D:264:GLN:HA	1:D:269:ILE:HG22	1.82	0.60
1:I:110:CYS:HB3	1:I:142:ALA:HB1	1.82	0.60
1:B:46:SER:O	1:B:48:GLY:N	2.32	0.60
1:E:56:THR:C	1:E:58:ARG:H	2.08	0.60
1:H:140:ILE:HB	1:H:194:VAL:HG12	1.84	0.60
1:A:236:HIS:CA	1:A:260:TYR:OH	2.50	0.58
1:E:39:MET:HE3	1:E:45:LYS:H	1.68	0.58
1:G:140:ILE:HB	1:G:194:VAL:HG12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:O	1:A:255:ASN:N	2.36	0.58
1:G:46:SER:O	1:G:48:GLY:N	2.34	0.58
1:B:60:GLY:O	1:B:62:ARG:N	2.30	0.57
1:B:143:THR:HB	1:B:199:LEU:HB3	1.86	0.57
1:H:105:ILE:HG12	1:H:213:MET:HE3	1.86	0.57
1:E:220:LEU:HB3	1:E:228:LYS:HG2	1.86	0.57
1:A:140:ILE:HB	1:A:194:VAL:HG12	1.87	0.57
1:D:21:ILE:HG23	1:D:250:SER:O	2.04	0.57
1:C:140:ILE:HB	1:C:194:VAL:HG12	1.86	0.57
1:F:14:PHE:CB	1:F:50:LEU:CD1	2.83	0.57
1:A:256:LEU:O	1:A:258:ASP:N	2.38	0.56
1:G:105:ILE:HG12	1:G:213:MET:HE3	1.87	0.56
1:A:259:HIS:O	1:A:274:LYS:N	2.26	0.56
1:D:257:PRO:O	1:D:259:HIS:ND1	2.39	0.56
1:A:236:HIS:CB	1:A:260:TYR:OH	2.54	0.56
1:C:148:SER:HB3	1:D:54:ILE:HD12	1.85	0.56
1:A:220:LEU:HB3	1:A:228:LYS:HG3	1.87	0.56
1:E:160:THR:HG23	1:E:182:GLY:O	2.05	0.56
1:J:203:ASP:O	1:J:234:ARG:NH2	2.38	0.56
1:A:79:ASP:OD2	1:A:217:ARG:NH2	2.34	0.56
1:F:110:CYS:HB3	1:F:142:ALA:HB1	1.87	0.56
1:G:267:PRO:HD2	1:G:268:GLY:H	1.70	0.56
1:A:142:ALA:HB3	1:A:196:PHE:CD1	2.41	0.55
1:G:106:TRP:HB2	1:G:211:PHE:CD2	2.41	0.55
1:F:56:THR:C	1:F:58:ARG:H	2.14	0.55
1:J:140:ILE:HB	1:J:194:VAL:HG12	1.88	0.55
1:B:102:ARG:HB2	1:B:136:ALA:HB3	1.89	0.55
1:E:203:ASP:O	1:E:234:ARG:NH2	2.40	0.55
1:G:29:TYR:CB	1:H:267:PRO:HG2	2.37	0.55
1:E:176:PHE:HD1	1:E:186:VAL:HA	1.71	0.55
1:G:121:MET:HE1	1:G:176:PHE:HZ	1.71	0.55
1:I:75:LEU:HB2	1:I:78:ARG:HG2	1.88	0.55
1:C:143:THR:HB	1:C:199:LEU:HB3	1.89	0.55
1:D:65:VAL:O	1:D:69:MET:HG2	2.07	0.55
1:G:84:GLU:O	1:G:88:GLN:HG2	2.07	0.55
1:D:106:TRP:CZ3	1:D:107:SER:O	2.60	0.55
1:H:84:GLU:O	1:H:88:GLN:HG2	2.07	0.55
1:E:218:ASN:N	1:E:251:GLU:OE2	2.41	0.54
1:B:105:ILE:HG12	1:B:213:MET:HE3	1.89	0.54
1:I:266:SER:HB2	1:I:267:PRO:HD3	1.90	0.54
1:A:201:LEU:O	1:A:234:ARG:NH2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:HIS:N	1:A:260:TYR:OH	2.41	0.54
1:E:44:ILE:O	1:E:45:LYS:HB3	2.08	0.54
1:J:84:GLU:O	1:J:88:GLN:HG2	2.08	0.54
1:I:105:ILE:HG12	1:I:213:MET:HE3	1.90	0.54
1:E:176:PHE:CD1	1:E:186:VAL:HA	2.43	0.53
1:D:140:ILE:HB	1:D:194:VAL:HG12	1.91	0.53
1:E:39:MET:O	1:E:42:GLN:O	2.26	0.53
1:I:57:GLN:O	1:J:109:ALA:CB	2.56	0.53
1:D:106:TRP:HE3	1:D:107:SER:N	2.04	0.53
1:C:217:ARG:NH1	1:C:247:LEU:O	2.42	0.52
1:G:266:SER:CB	1:G:267:PRO:HD3	2.39	0.52
1:A:155:ALA:O	1:A:191:ARG:NH2	2.41	0.52
1:H:31:VAL:O	1:H:35:LEU:HG	2.09	0.52
1:H:236:HIS:HD1	1:H:260:TYR:HE1	1.58	0.52
1:D:201:LEU:O	1:D:205:TYR:OH	2.22	0.52
1:H:158:TYR:HB2	1:H:163:MET:HE2	1.92	0.52
1:I:176:PHE:HE1	1:I:186:VAL:HG22	1.74	0.52
1:F:121:MET:HE1	1:F:176:PHE:CZ	2.45	0.52
1:B:262:MET:HA	1:B:271:TYR:HD1	1.74	0.52
1:E:104:ARG:HH21	1:E:141:VAL:HG21	1.74	0.52
1:H:199:LEU:HD22	1:H:208:LEU:HD11	1.92	0.52
1:I:54:ILE:HG21	1:J:147:GLY:HA3	1.92	0.52
1:A:217:ARG:NE	1:A:248:GLY:HA2	2.25	0.51
1:F:31:VAL:O	1:F:35:LEU:HG	2.10	0.51
1:E:146:SER:HB2	1:E:198:ALA:HB1	1.91	0.51
1:A:144:ASP:OD1	1:A:145:LEU:N	2.42	0.51
1:C:142:ALA:HB3	1:C:196:PHE:CD1	2.46	0.51
1:B:110:CYS:HB3	1:B:142:ALA:HB1	1.92	0.51
1:F:48:GLY:O	1:F:51:VAL:HG22	2.11	0.51
1:J:75:LEU:HB2	1:J:78:ARG:HG2	1.93	0.51
1:A:236:HIS:HD2	1:A:260:TYR:CE1	2.29	0.51
1:B:75:LEU:HB2	1:B:78:ARG:HG2	1.93	0.51
1:G:75:LEU:H	1:G:78:ARG:HH11	1.59	0.51
1:H:266:SER:HB3	1:H:267:PRO:HD3	1.91	0.51
1:B:46:SER:C	1:B:48:GLY:H	2.18	0.51
1:G:78:ARG:HB2	1:G:217:ARG:NH1	2.25	0.51
1:G:121:MET:CE	1:G:176:PHE:CZ	2.94	0.51
1:I:31:VAL:O	1:I:35:LEU:HG	2.11	0.51
1:E:23:LEU:HD11	1:E:69:MET:CE	2.41	0.50
1:E:53:ARG:C	1:E:55:GLN:H	2.19	0.50
1:A:188:PRO:HA	1:A:191:ARG:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:THR:C	1:E:58:ARG:N	2.69	0.50
1:I:54:ILE:HD12	1:J:148:SER:H	1.77	0.50
1:C:264:GLN:HA	1:C:269:ILE:HG22	1.94	0.50
1:F:105:ILE:HG12	1:F:213:MET:HE3	1.93	0.50
1:D:223:PHE:HB3	1:D:227:VAL:HG23	1.93	0.50
1:E:85:VAL:O	1:E:89:ARG:HB3	2.11	0.49
1:G:257:PRO:O	1:G:258:ASP:C	2.55	0.49
1:D:133:GLN:C	1:D:135:LYS:H	2.19	0.49
1:A:158:TYR:HB2	1:A:163:MET:HE2	1.94	0.49
1:A:160:THR:HG23	1:C:160:THR:HG21	1.94	0.49
1:D:217:ARG:HE	1:D:248:GLY:HA2	1.77	0.49
1:F:254:ASN:O	1:F:255:ASN:HB2	2.12	0.49
1:A:262:MET:HE2	1:A:264:GLN:HG3	1.94	0.49
1:H:74:THR:HG22	1:H:78:ARG:NH2	2.28	0.49
1:J:79:ASP:OD2	1:J:249:ALA:HB2	2.13	0.49
1:D:16:GLU:HA	1:D:21:ILE:O	2.13	0.49
1:F:265:CYS:HB2	1:F:267:PRO:HD2	1.94	0.49
1:I:172:LEU:O	1:I:176:PHE:HB2	2.12	0.49
1:C:8:PHE:HE1	1:C:31:VAL:HG21	1.78	0.49
1:D:121:MET:HE1	1:D:167:LEU:HD11	1.95	0.49
1:A:267:PRO:HG3	1:C:29:TYR:CE2	2.48	0.49
1:E:65:VAL:O	1:E:69:MET:HG2	2.12	0.49
1:F:39:MET:O	1:F:42:GLN:O	2.31	0.49
1:A:75:LEU:HB2	1:A:78:ARG:HG2	1.95	0.48
1:C:15:LEU:HD12	1:C:23:LEU:HD11	1.95	0.48
1:C:105:ILE:HG12	1:C:213:MET:HE3	1.95	0.48
1:E:140:ILE:HB	1:E:194:VAL:HG12	1.95	0.48
1:H:110:CYS:HB3	1:H:142:ALA:HB1	1.95	0.48
1:I:110:CYS:HB2	1:I:116:PRO:HG3	1.94	0.48
1:J:78:ARG:HB2	1:J:217:ARG:NH1	2.22	0.48
1:A:75:LEU:H	1:A:78:ARG:HH11	1.60	0.48
1:F:123:ILE:HG13	1:F:138:VAL:HG21	1.96	0.48
1:F:56:THR:C	1:F:58:ARG:N	2.70	0.48
1:G:110:CYS:HB3	1:G:142:ALA:HB1	1.96	0.48
1:J:263:VAL:HB	1:J:270:ILE:HG13	1.94	0.48
1:G:31:VAL:O	1:G:35:LEU:HG	2.14	0.48
1:C:247:LEU:HD11	1:C:253:LEU:HD23	1.96	0.48
1:F:143:THR:HB	1:F:199:LEU:HB3	1.95	0.48
1:A:91:LEU:O	1:A:95:ILE:HG12	2.14	0.47
1:F:140:ILE:HB	1:F:194:VAL:HG12	1.95	0.47
1:A:78:ARG:HB2	1:A:217:ARG:NH1	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ALA:HB3	1:G:196:PHE:CD1	2.49	0.47
1:D:121:MET:HE3	1:D:175:TYR:CD2	2.48	0.47
1:A:154:LYS:HG2	1:A:196:PHE:HD2	1.79	0.47
1:D:110:CYS:HB3	1:D:142:ALA:HB1	1.96	0.47
1:G:121:MET:HE1	1:G:176:PHE:CZ	2.49	0.47
1:G:267:PRO:CD	1:G:268:GLY:H	2.27	0.47
1:A:217:ARG:HE	1:A:248:GLY:HA2	1.80	0.47
1:C:127:GLU:O	1:C:131:LEU:HA	2.15	0.47
1:D:106:TRP:CE3	1:D:106:TRP:C	2.93	0.47
1:H:148:SER:O	1:H:151:THR:N	2.47	0.47
1:C:32:SER:O	1:C:36:ASN:HB2	2.15	0.47
1:G:266:SER:HB3	1:G:267:PRO:HD3	1.96	0.47
1:B:148:SER:O	1:B:150:LEU:N	2.42	0.47
1:C:127:GLU:O	1:C:131:LEU:N	2.46	0.47
1:E:262:MET:HE3	1:E:269:ILE:HD13	1.96	0.47
1:E:160:THR:HG23	1:E:182:GLY:C	2.40	0.47
1:G:236:HIS:HD1	1:G:260:TYR:HE1	1.63	0.47
1:G:186:VAL:HG12	1:G:191:ARG:HG3	1.96	0.47
1:A:142:ALA:HB3	1:A:196:PHE:HD1	1.79	0.46
1:E:40:GLU:C	1:E:42:GLN:H	2.23	0.46
1:F:45:LYS:C	1:F:47:LEU:N	2.73	0.46
1:J:266:SER:HB2	1:J:267:PRO:HD3	1.98	0.46
1:E:172:LEU:O	1:E:176:PHE:HB2	2.15	0.46
1:A:266:SER:HB3	1:A:267:PRO:HD3	1.97	0.46
1:E:266:SER:HB3	1:E:267:PRO:HD3	1.98	0.46
1:I:148:SER:HB3	1:J:51:VAL:HB	1.97	0.46
1:J:110:CYS:HB3	1:J:142:ALA:HB1	1.97	0.46
1:J:217:ARG:NH2	1:J:248:GLY:HA2	2.31	0.46
1:A:123:ILE:HG13	1:A:138:VAL:HG21	1.97	0.46
1:F:121:MET:HE1	1:F:176:PHE:HZ	1.81	0.46
1:A:84:GLU:O	1:A:88:GLN:HG2	2.16	0.46
1:A:258:ASP:O	1:A:260:TYR:N	2.41	0.46
1:B:108:ALA:HB3	1:B:216:CYS:HB3	1.98	0.46
1:C:13:VAL:HA	1:E:10:LEU:HD11	1.98	0.46
1:G:256:LEU:HB3	1:G:259:HIS:HB2	1.98	0.46
1:I:148:SER:O	1:I:151:THR:N	2.48	0.46
1:A:236:HIS:HB2	1:A:260:TYR:CZ	2.50	0.46
1:A:172:LEU:O	1:A:176:PHE:HB2	2.16	0.46
1:D:105:ILE:HD12	1:D:140:ILE:HG12	1.98	0.46
1:E:201:LEU:O	1:E:205:TYR:OH	2.32	0.46
1:B:57:GLN:O	1:H:109:ALA:CB	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD21	1:C:65:VAL:HG23	1.98	0.46
1:D:106:TRP:HE3	1:D:106:TRP:HA	1.81	0.46
1:I:24:GLY:C	1:I:26:ASN:H	2.23	0.46
1:A:90:VAL:HG13	1:A:244:TYR:CD2	2.51	0.46
1:C:61:LEU:O	1:C:65:VAL:HG12	2.16	0.46
1:D:106:TRP:HE3	1:D:107:SER:H	1.63	0.46
1:E:110:CYS:HB3	1:E:142:ALA:HB1	1.97	0.46
1:D:266:SER:HB2	1:D:267:PRO:HD3	1.96	0.45
1:F:267:PRO:CG	1:F:268:GLY:H	2.29	0.45
1:A:150:LEU:HD11	1:A:196:PHE:HB3	1.99	0.45
1:G:56:THR:C	1:G:58:ARG:N	2.73	0.45
1:B:121:MET:HE1	1:B:176:PHE:CE2	2.51	0.45
1:B:220:LEU:HD12	1:B:220:LEU:H	1.81	0.45
1:E:135:LYS:O	1:E:136:ALA:HB3	2.17	0.45
1:F:89:ARG:C	1:F:92:PRO:HD2	2.42	0.45
1:A:163:MET:HE1	1:A:176:PHE:CE1	2.52	0.45
1:E:78:ARG:C	1:E:80:THR:H	2.23	0.45
1:J:143:THR:HB	1:J:199:LEU:HB3	1.99	0.45
1:D:78:ARG:C	1:D:80:THR:H	2.25	0.45
1:F:75:LEU:H	1:F:78:ARG:HH11	1.62	0.45
1:A:85:VAL:O	1:A:89:ARG:HB2	2.17	0.45
1:B:262:MET:HA	1:B:271:TYR:CD1	2.51	0.45
1:G:121:MET:HE2	1:G:176:PHE:CZ	2.52	0.44
1:A:199:LEU:HD22	1:A:208:LEU:HD11	1.99	0.44
1:C:121:MET:HE3	1:C:175:TYR:CD2	2.52	0.44
1:E:90:VAL:HG13	1:E:244:TYR:HD2	1.82	0.44
1:G:121:MET:CE	1:G:176:PHE:HZ	2.29	0.44
1:B:266:SER:HB3	1:B:267:PRO:HD3	2.00	0.44
1:C:82:PRO:HG2	1:C:83:PHE:CD1	2.53	0.44
1:E:38:LEU:HD11	1:E:64:MET:HB3	1.99	0.44
1:E:160:THR:HG22	1:E:184:TRP:HE1	1.82	0.44
1:G:91:LEU:O	1:G:95:ILE:HG12	2.17	0.44
1:I:125:GLU:O	1:I:128:LYS:HG2	2.16	0.44
1:I:216:CYS:O	1:I:247:LEU:HA	2.18	0.44
1:D:106:TRP:HB2	1:D:211:PHE:CG	2.51	0.44
1:C:104:ARG:HA	1:C:139:GLN:O	2.17	0.44
1:F:256:LEU:HA	1:F:257:PRO:HD3	1.88	0.44
1:H:78:ARG:C	1:H:80:THR:H	2.24	0.44
1:A:143:THR:HB	1:A:199:LEU:HB3	1.99	0.44
1:A:236:HIS:CD2	1:A:260:TYR:CE1	3.06	0.44
1:D:61:LEU:HD12	1:D:64:MET:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ARG:HH12	1:E:26:ASN:H	1.66	0.44
1:F:31:VAL:HG22	1:F:69:MET:HE1	2.00	0.44
1:F:158:TYR:HB2	1:F:163:MET:HE2	1.99	0.44
1:C:85:VAL:HG12	1:C:90:VAL:HG23	2.00	0.44
1:E:232:LEU:O	1:E:260:TYR:OH	2.34	0.44
1:J:31:VAL:O	1:J:35:LEU:HG	2.18	0.44
1:D:84:GLU:O	1:D:88:GLN:HG2	2.18	0.43
1:D:106:TRP:CE3	1:D:106:TRP:HA	2.53	0.43
1:D:112:SER:OG	1:D:114:GLN:OE1	2.35	0.43
1:G:59:GLY:C	1:G:61:LEU:H	2.25	0.43
1:J:59:GLY:C	1:J:61:LEU:H	2.25	0.43
1:C:9:GLU:O	1:C:13:VAL:HG23	2.18	0.43
1:E:79:ASP:OD2	1:E:249:ALA:HB2	2.17	0.43
1:F:216:CYS:O	1:F:247:LEU:HA	2.18	0.43
1:J:172:LEU:O	1:J:176:PHE:HB2	2.18	0.43
1:D:18:THR:C	1:D:20:GLY:N	2.73	0.43
1:I:109:ALA:CB	1:J:57:GLN:O	2.67	0.43
1:I:155:ALA:O	1:I:191:ARG:NH2	2.39	0.43
1:J:78:ARG:C	1:J:80:THR:H	2.26	0.43
1:A:91:LEU:HB2	1:A:92:PRO:HD3	2.00	0.43
1:F:265:CYS:HB2	1:F:268:GLY:O	2.19	0.43
1:B:82:PRO:HG2	1:B:83:PHE:CD2	2.54	0.43
1:C:7:ASP:O	1:C:47:LEU:HD23	2.19	0.43
1:D:158:TYR:HB3	1:D:163:MET:CE	2.44	0.43
1:F:80:THR:O	1:F:84:GLU:HG3	2.18	0.43
1:F:267:PRO:HG2	1:F:268:GLY:H	1.84	0.43
1:C:148:SER:O	1:C:150:LEU:N	2.44	0.43
1:I:56:THR:O	1:I:57:GLN:C	2.61	0.43
1:B:103:LEU:HA	1:B:212:ASP:OD1	2.19	0.43
1:D:106:TRP:CE3	1:D:106:TRP:CA	3.02	0.43
1:F:163:MET:HE1	1:F:176:PHE:CE1	2.54	0.43
1:I:26:ASN:C	1:I:28:GLN:N	2.73	0.42
1:J:22:VAL:HG13	1:J:252:ALA:HB2	2.01	0.42
1:J:258:ASP:O	1:J:260:TYR:N	2.50	0.42
1:A:29:TYR:HE2	1:C:85:VAL:CG2	2.32	0.42
1:G:188:PRO:HA	1:G:191:ARG:HB2	2.01	0.42
1:G:188:PRO:HA	1:G:191:ARG:HD3	2.01	0.42
1:A:176:PHE:CE1	1:A:186:VAL:HG22	2.54	0.42
1:B:78:ARG:C	1:B:80:THR:H	2.26	0.42
1:G:56:THR:C	1:G:58:ARG:H	2.27	0.42
1:I:168:SER:HA	1:I:169:PRO:HD3	1.94	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:HD13	1:E:21:ILE:HD11	2.01	0.42
1:I:257:PRO:O	1:I:258:ASP:C	2.62	0.42
1:J:201:LEU:O	1:J:205:TYR:OH	2.23	0.42
1:C:11:PHE:O	1:C:14:PHE:HB3	2.20	0.42
1:C:26:ASN:OD1	1:C:26:ASN:N	2.45	0.42
1:G:255:ASN:O	1:G:256:LEU:HB2	2.19	0.42
1:I:24:GLY:C	1:I:26:ASN:N	2.77	0.42
1:A:29:TYR:HE2	1:C:85:VAL:HG23	1.83	0.42
1:E:148:SER:O	1:E:149:MET:HB2	2.20	0.42
1:A:34:ARG:HB3	1:A:68:ALA:HB1	1.99	0.42
1:B:147:GLY:HA3	1:H:54:ILE:HG21	2.02	0.42
1:A:11:PHE:O	1:A:14:PHE:HB3	2.20	0.42
1:D:224:SER:OG	1:D:227:VAL:HG22	2.20	0.42
1:A:143:THR:HA	1:A:197:ARG:O	2.20	0.42
1:F:266:SER:HB3	1:I:29:TYR:CE1	2.55	0.42
1:H:269:ILE:O	1:H:269:ILE:HG13	2.20	0.42
1:B:253:LEU:O	1:B:255:ASN:N	2.53	0.42
1:C:81:TYR:CD2	1:C:82:PRO:HD3	2.54	0.42
1:C:121:MET:CE	1:C:171:ARG:HB3	2.50	0.42
1:G:267:PRO:HB3	1:H:26:ASN:O	2.20	0.42
1:I:110:CYS:CB	1:I:142:ALA:HB1	2.49	0.42
1:D:18:THR:O	1:D:20:GLY:N	2.53	0.41
1:H:56:THR:C	1:H:58:ARG:H	2.28	0.41
1:I:158:TYR:HB2	1:I:163:MET:HE2	2.01	0.41
1:A:60:GLY:HA2	1:A:63:GLU:OE1	2.20	0.41
1:B:55:GLN:CB	1:H:149:MET:HB2	2.50	0.41
1:B:219:VAL:HG13	1:H:57:GLN:O	2.20	0.41
1:A:217:ARG:NH2	1:A:248:GLY:HA2	2.36	0.41
1:C:104:ARG:C	1:C:105:ILE:HG13	2.45	0.41
1:I:51:VAL:O	1:J:149:MET:HG2	2.20	0.41
1:I:142:ALA:HB3	1:I:196:PHE:CD1	2.55	0.41
1:G:15:LEU:O	1:G:20:GLY:N	2.53	0.41
1:H:24:GLY:C	1:H:26:ASN:N	2.76	0.41
1:I:137:GLY:O	1:I:138:VAL:C	2.63	0.41
1:C:111:SER:HB3	1:C:112:SER:H	1.52	0.41
1:D:172:LEU:O	1:D:176:PHE:HB2	2.21	0.41
1:G:79:ASP:OD2	1:G:217:ARG:NH2	2.49	0.41
1:A:236:HIS:HB2	1:A:260:TYR:CE1	2.55	0.41
1:B:60:GLY:C	1:B:62:ARG:N	2.79	0.41
1:E:263:VAL:HB	1:E:270:ILE:HG13	2.02	0.41
1:B:172:LEU:O	1:B:176:PHE:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:O	1:B:260:TYR:OH	2.36	0.41
1:I:85:VAL:O	1:I:89:ARG:HB2	2.21	0.41
1:J:82:PRO:HG3	1:J:217:ARG:NH2	2.35	0.41
1:D:133:GLN:C	1:D:135:LYS:N	2.79	0.41
1:F:48:GLY:C	1:F:50:LEU:N	2.77	0.41
1:G:26:ASN:C	1:G:28:GLN:H	2.29	0.41
1:G:59:GLY:C	1:G:61:LEU:N	2.79	0.41
1:G:172:LEU:HA	1:G:176:PHE:HD2	1.86	0.41
1:H:142:ALA:HB3	1:H:196:PHE:CE1	2.56	0.41
1:I:56:THR:C	1:I:58:ARG:N	2.77	0.41
1:J:245:LEU:N	1:J:271:TYR:O	2.48	0.41
1:B:121:MET:HE1	1:B:176:PHE:CZ	2.55	0.41
1:E:87:LYS:NZ	1:E:125:GLU:OE1	2.42	0.41
1:G:46:SER:C	1:G:48:GLY:N	2.80	0.40
1:G:156:GLY:O	1:G:186:VAL:HG23	2.21	0.40
1:D:110:CYS:CB	1:D:142:ALA:HB1	2.51	0.40
1:H:142:ALA:HB3	1:H:196:PHE:CD1	2.56	0.40
1:J:209:GLY:O	1:J:238:THR:HB	2.21	0.40
1:C:25:SER:HB2	1:E:51:VAL:HG22	2.03	0.40
1:E:40:GLU:C	1:E:42:GLN:N	2.80	0.40
1:I:36:ASN:HA	1:I:39:MET:HB2	2.03	0.40
1:F:142:ALA:HB3	1:F:196:PHE:CD1	2.56	0.40
1:J:79:ASP:CG	1:J:249:ALA:HB2	2.47	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	268/294 (91%)	227 (85%)	35 (13%)	6 (2%)	5	24
1	B	267/294 (91%)	227 (85%)	33 (12%)	7 (3%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	268/294 (91%)	230 (86%)	34 (13%)	4 (2%)	8	30
1	D	266/294 (90%)	231 (87%)	32 (12%)	3 (1%)	11	38
1	E	268/294 (91%)	231 (86%)	31 (12%)	6 (2%)	5	24
1	F	268/294 (91%)	225 (84%)	38 (14%)	5 (2%)	6	26
1	G	268/294 (91%)	222 (83%)	40 (15%)	6 (2%)	5	24
1	H	268/294 (91%)	217 (81%)	47 (18%)	4 (2%)	8	30
1	I	268/294 (91%)	224 (84%)	40 (15%)	4 (2%)	8	30
1	J	268/294 (91%)	230 (86%)	37 (14%)	1 (0%)	30	59
All	All	2677/2940 (91%)	2264 (85%)	367 (14%)	46 (2%)	7	28

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	B	47	LEU
1	B	254	ASN
1	B	258	ASP
1	C	267	PRO
1	D	60	GLY
1	E	258	ASP
1	F	47	LEU
1	F	267	PRO
1	H	29	TYR
1	H	258	ASP
1	I	27	LYS
1	B	42	GLN
1	D	258	ASP
1	E	45	LYS
1	G	255	ASN
1	I	254	ASN
1	J	58	ARG
1	A	255	ASN
1	A	256	LEU
1	C	146	SER
1	E	267	PRO
1	F	46	SER
1	G	100	GLY
1	H	267	PRO
1	A	25	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	61	LEU
1	C	131	LEU
1	D	19	CYS
1	E	26	ASN
1	E	136	ALA
1	G	258	ASP
1	A	27	LYS
1	A	257	PRO
1	F	27	LYS
1	F	254	ASN
1	G	46	SER
1	H	42	GLN
1	I	258	ASP
1	G	267	PRO
1	B	137	GLY
1	B	256	LEU
1	C	44	ILE
1	G	256	LEU
1	I	256	LEU
1	E	256	LEU

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	195/246 (79%)	195 (100%)	0	100	100
1	B	147/246 (60%)	147 (100%)	0	100	100
1	C	185/246 (75%)	182 (98%)	3 (2%)	55	68
1	D	168/246 (68%)	166 (99%)	2 (1%)	63	72
1	E	185/246 (75%)	185 (100%)	0	100	100
1	F	184/246 (75%)	183 (100%)	1 (0%)	81	81
1	G	185/246 (75%)	182 (98%)	3 (2%)	55	68
1	H	189/246 (77%)	183 (97%)	6 (3%)	34	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	179/246 (73%)	175 (98%)	4 (2%)	45	63
1	J	180/246 (73%)	179 (99%)	1 (1%)	78	80
All	All	1797/2460 (73%)	1777 (99%)	20 (1%)	65	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	VAL
1	C	114	GLN
1	C	183	ARG
1	D	18	THR
1	D	106	TRP
1	F	54	ILE
1	G	259	HIS
1	G	262	MET
1	G	266	SER
1	H	54	ILE
1	H	131	LEU
1	H	134	LEU
1	H	255	ASN
1	H	265	CYS
1	H	266	SER
1	I	54	ILE
1	I	254	ASN
1	I	255	ASN
1	I	259	HIS
1	J	251	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	236	HIS
1	B	259	HIS
1	C	42	GLN
1	C	114	GLN
1	C	218	ASN
1	C	259	HIS
1	D	36	ASN
1	D	57	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	200	ASN
1	F	139	GLN
1	J	255	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	270/294 (91%)	0.54	25 (9%)	14 14	60, 106, 166, 212	0
1	B	269/294 (91%)	0.75	29 (10%)	11 11	83, 147, 196, 228	0
1	C	270/294 (91%)	0.60	24 (8%)	15 14	69, 120, 168, 219	0
1	D	268/294 (91%)	0.65	23 (8%)	16 15	88, 149, 201, 245	0
1	E	270/294 (91%)	0.65	20 (7%)	20 17	86, 129, 183, 275	0
1	F	270/294 (91%)	0.75	22 (8%)	18 16	129, 179, 218, 267	0
1	G	270/294 (91%)	0.79	27 (10%)	12 12	124, 175, 217, 255	0
1	H	270/294 (91%)	0.79	34 (12%)	8 9	118, 165, 218, 235	0
1	I	270/294 (91%)	0.88	28 (10%)	11 12	144, 199, 247, 268	0
1	J	270/294 (91%)	0.90	40 (14%)	5 7	111, 197, 251, 297	0
All	All	2697/2940 (91%)	0.73	272 (10%)	12 12	60, 159, 226, 297	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	GLU	5.2
1	G	7	ASP	4.9
1	H	57	GLN	4.9
1	D	59	GLY	4.8
1	C	30	LEU	4.5
1	J	49	GLU	4.5
1	J	212	ASP	4.3
1	C	102	ARG	4.3
1	F	74	THR	4.3
1	B	216	CYS	4.0
1	A	26	ASN	4.0
1	B	88	GLN	4.0
1	G	251	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	82	PRO	3.8
1	B	72	ASN	3.8
1	I	38	LEU	3.8
1	C	264	GLN	3.8
1	E	238	THR	3.8
1	A	253	LEU	3.7
1	I	72	ASN	3.7
1	J	30	LEU	3.6
1	J	233	LEU	3.6
1	G	49	GLU	3.6
1	E	27	LYS	3.6
1	E	57	GLN	3.6
1	G	10	LEU	3.6
1	B	28	GLN	3.5
1	E	26	ASN	3.5
1	A	25	SER	3.5
1	F	28	GLN	3.5
1	A	38	LEU	3.5
1	B	27	LYS	3.5
1	J	57	GLN	3.5
1	H	55	GLN	3.4
1	C	254	ASN	3.3
1	E	58	ARG	3.3
1	J	69	MET	3.3
1	I	59	GLY	3.3
1	E	256	LEU	3.3
1	A	5	ASN	3.3
1	A	27	LYS	3.3
1	G	221	ILE	3.3
1	H	23	LEU	3.3
1	H	253	LEU	3.3
1	B	223	PHE	3.2
1	B	69	MET	3.2
1	D	56	THR	3.2
1	G	137	GLY	3.2
1	J	72	ASN	3.2
1	H	177	ASP	3.2
1	C	55	GLN	3.2
1	B	63	GLU	3.2
1	G	56	THR	3.2
1	G	50	LEU	3.1
1	J	84	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	3.1
1	C	131	LEU	3.1
1	A	259	HIS	3.1
1	H	28	GLN	3.1
1	J	33	SER	3.1
1	G	27	LYS	3.1
1	J	5	ASN	3.1
1	D	133	GLN	3.1
1	A	137	GLY	3.1
1	C	267	PRO	3.1
1	E	55	GLN	3.0
1	I	55	GLN	3.0
1	C	137	GLY	3.0
1	D	156	GLY	3.0
1	B	73	GLU	3.0
1	H	267	PRO	3.0
1	C	26	ASN	3.0
1	A	56	THR	3.0
1	A	146	SER	3.0
1	B	26	ASN	3.0
1	D	41	GLN	3.0
1	D	57	GLN	3.0
1	B	257	PRO	3.0
1	J	29	TYR	3.0
1	D	55	GLN	3.0
1	F	88	GLN	3.0
1	I	40	GLU	3.0
1	B	7	ASP	3.0
1	I	216	CYS	3.0
1	C	103	LEU	2.9
1	I	50	LEU	2.9
1	G	102	ARG	2.9
1	J	271	TYR	2.9
1	F	52	GLN	2.9
1	H	41	GLN	2.9
1	C	253	LEU	2.9
1	H	72	ASN	2.9
1	C	27	LYS	2.9
1	D	159	ASP	2.9
1	J	42	GLN	2.9
1	G	38	LEU	2.9
1	A	55	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	55	GLN	2.9
1	F	238	THR	2.9
1	A	30	LEU	2.9
1	H	7	ASP	2.8
1	D	267	PRO	2.8
1	J	94	LEU	2.8
1	A	49	GLU	2.8
1	I	49	GLU	2.8
1	E	137	GLY	2.8
1	B	237	GLY	2.8
1	C	255	ASN	2.8
1	I	241	PRO	2.8
1	J	257	PRO	2.8
1	E	5	ASN	2.7
1	H	5	ASN	2.7
1	F	57	GLN	2.7
1	I	253	LEU	2.7
1	H	35	LEU	2.7
1	H	233	LEU	2.7
1	J	249	ALA	2.7
1	B	202	LEU	2.7
1	F	253	LEU	2.7
1	J	181	PRO	2.7
1	J	137	GLY	2.7
1	D	260	TYR	2.7
1	F	22	VAL	2.7
1	H	49	GLU	2.7
1	D	101	GLN	2.6
1	J	211	PHE	2.6
1	F	29	TYR	2.6
1	I	11	PHE	2.6
1	H	43	GLY	2.6
1	A	145	LEU	2.6
1	I	145	LEU	2.6
1	B	55	GLN	2.6
1	B	100	GLY	2.6
1	B	251	GLU	2.6
1	J	53	ARG	2.6
1	C	57	GLN	2.6
1	C	257	PRO	2.6
1	C	101	GLN	2.6
1	H	137	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	131	LEU	2.6
1	E	200	ASN	2.5
1	D	231	ILE	2.5
1	I	54	ILE	2.5
1	I	220	LEU	2.5
1	H	78	ARG	2.5
1	G	51	VAL	2.5
1	G	9	GLU	2.5
1	A	257	PRO	2.5
1	J	244	TYR	2.5
1	H	25	SER	2.5
1	J	43	GLY	2.5
1	B	57	GLN	2.5
1	G	136	ALA	2.4
1	B	30	LEU	2.4
1	H	56	THR	2.4
1	H	71	THR	2.4
1	J	56	THR	2.4
1	H	81	TYR	2.4
1	A	132	GLY	2.4
1	J	88	GLN	2.4
1	E	47	LEU	2.4
1	B	31	VAL	2.4
1	F	43	GLY	2.4
1	A	68	ALA	2.4
1	E	23	LEU	2.4
1	G	253	LEU	2.4
1	H	50	LEU	2.4
1	A	260	TYR	2.4
1	H	259	HIS	2.4
1	I	155	ALA	2.4
1	J	8	PHE	2.4
1	D	256	LEU	2.4
1	F	75	LEU	2.4
1	F	137	GLY	2.4
1	I	7	ASP	2.4
1	F	222	TYR	2.3
1	G	252	ALA	2.3
1	D	30	LEU	2.3
1	E	28	GLN	2.3
1	H	38	LEU	2.3
1	G	155	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	5	ASN	2.3
1	A	50	LEU	2.3
1	I	256	LEU	2.3
1	H	115	GLU	2.3
1	H	252	ALA	2.3
1	J	138	VAL	2.3
1	G	8	PHE	2.3
1	A	258	ASP	2.3
1	F	132	GLY	2.3
1	E	134	LEU	2.3
1	J	50	LEU	2.3
1	A	44	ILE	2.2
1	D	54	ILE	2.2
1	A	64	MET	2.2
1	H	176	PHE	2.2
1	I	36	ASN	2.2
1	I	44	ILE	2.2
1	G	257	PRO	2.2
1	J	38	LEU	2.2
1	B	135	LYS	2.2
1	C	179	LYS	2.2
1	C	62	ARG	2.2
1	H	16	GLU	2.2
1	J	262	MET	2.2
1	J	222	TYR	2.2
1	F	235	ILE	2.2
1	G	218	ASN	2.2
1	E	75	LEU	2.2
1	E	249	ALA	2.2
1	I	35	LEU	2.2
1	C	115	GLU	2.2
1	J	64	MET	2.2
1	B	137	GLY	2.2
1	E	258	ASP	2.2
1	F	133	GLN	2.1
1	G	199	LEU	2.1
1	F	46	SER	2.1
1	J	252	ALA	2.1
1	J	54	ILE	2.1
1	A	23	LEU	2.1
1	F	27	LYS	2.1
1	C	114	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	125	GLU	2.1
1	B	146	SER	2.1
1	J	132	GLY	2.1
1	G	98	ASN	2.1
1	D	163	MET	2.1
1	G	69	MET	2.1
1	I	62	ARG	2.1
1	I	217	ARG	2.1
1	C	33	SER	2.1
1	D	83	PHE	2.1
1	B	19	CYS	2.1
1	J	145	LEU	2.1
1	F	56	THR	2.1
1	E	64	MET	2.1
1	I	189	ALA	2.1
1	J	46	SER	2.1
1	B	47	LEU	2.1
1	C	44	ILE	2.1
1	D	165	ARG	2.1
1	J	103	LEU	2.1
1	A	71	THR	2.1
1	C	265	CYS	2.1
1	F	225	ALA	2.1
1	J	40	GLU	2.1
1	E	250	SER	2.0
1	B	134	LEU	2.0
1	D	94	LEU	2.0
1	H	75	LEU	2.0
1	C	189	ALA	2.0
1	G	74	THR	2.0
1	G	132	GLY	2.0
1	I	60	GLY	2.0
1	J	9	GLU	2.0
1	A	53	ARG	2.0
1	F	61	LEU	2.0
1	I	208	LEU	2.0
1	B	250	SER	2.0
1	G	25	SER	2.0
1	D	72	ASN	2.0
1	E	72	ASN	2.0
1	J	26	ASN	2.0
1	H	29	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	222	TYR	2.0
1	H	8	PHE	2.0
1	I	248	GLY	2.0
1	I	257	PRO	2.0
1	D	40	GLU	2.0
1	H	217	ARG	2.0
1	D	134	LEU	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.