



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:42 pm BST

PDB ID : 5Y4S  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

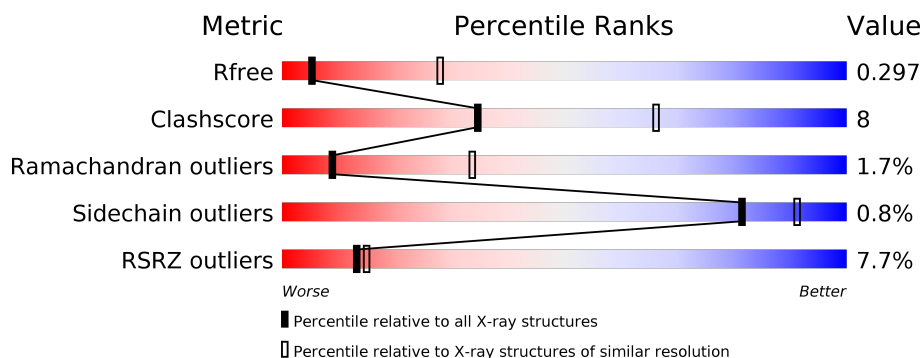
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	<div> <div>0%</div> <div> <div>70%</div> <div>21%</div> <div>8%</div> </div> </div>
1	B	294	<div> <div>5%</div> <div> <div>77%</div> <div>15%</div> <div>9%</div> </div> </div>
1	C	294	<div> <div>2%</div> <div> <div>73%</div> <div>18%</div> <div>8%</div> </div> </div>
1	D	294	<div> <div>4%</div> <div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
1	E	294	<div> <div>2%</div> <div> <div>70%</div> <div>21%</div> <div>8%</div> </div> </div>
1	F	294	<div> <div>8%</div> <div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	294	
1	H	294	
1	I	294	
1	J	294	

## 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

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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
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B	-9	SER	-	expression tag	UNP O87131
B	-8	GLN	-	expression tag	UNP O87131
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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
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Chain	Residue	Modelled	Actual	Comment	Reference
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C	-9	SER	-	expression tag	UNP O87131
C	-8	GLN	-	expression tag	UNP O87131
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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
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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
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F	-15	HIS	-	expression tag	UNP O87131
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F	-13	HIS	-	expression tag	UNP O87131
F	-12	HIS	-	expression tag	UNP O87131
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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
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I	-13	HIS	-	expression tag	UNP O87131
I	-12	HIS	-	expression tag	UNP O87131
I	-11	HIS	-	expression tag	UNP O87131

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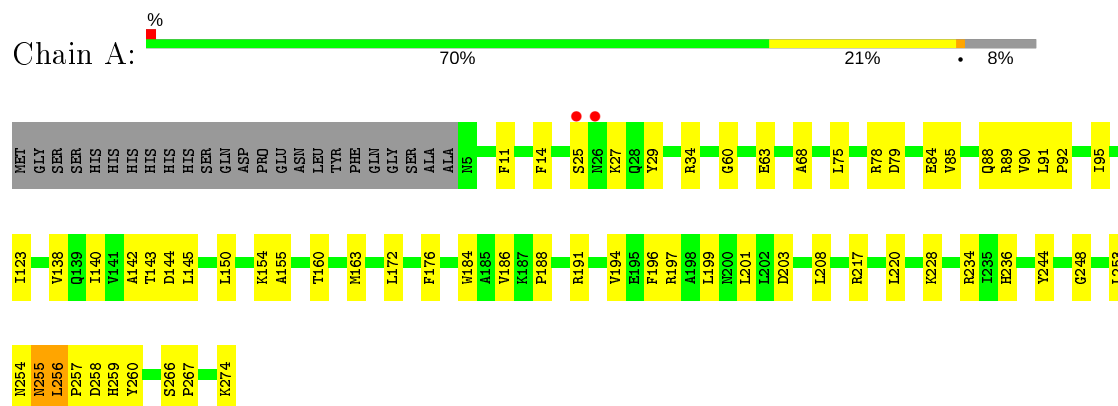
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J	-14	HIS	-	expression tag	UNP O87131
J	-13	HIS	-	expression tag	UNP O87131
J	-12	HIS	-	expression tag	UNP O87131
J	-11	HIS	-	expression tag	UNP O87131
J	-10	HIS	-	expression tag	UNP O87131
J	-9	SER	-	expression tag	UNP O87131
J	-8	GLN	-	expression tag	UNP O87131
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J	1	GLY	-	expression tag	UNP O87131

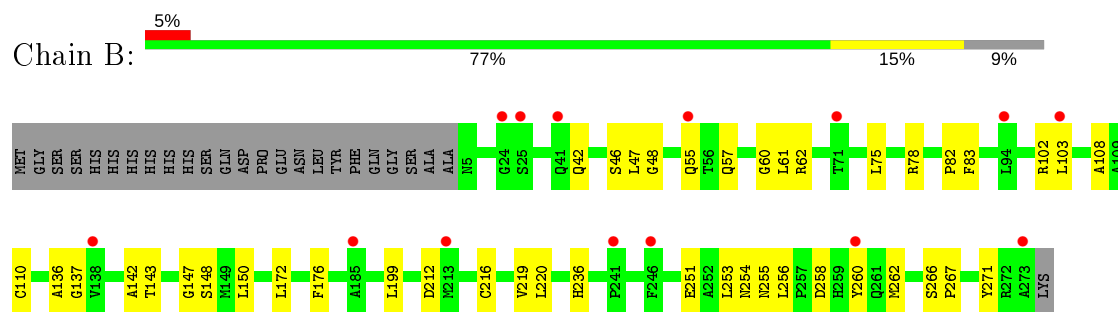
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

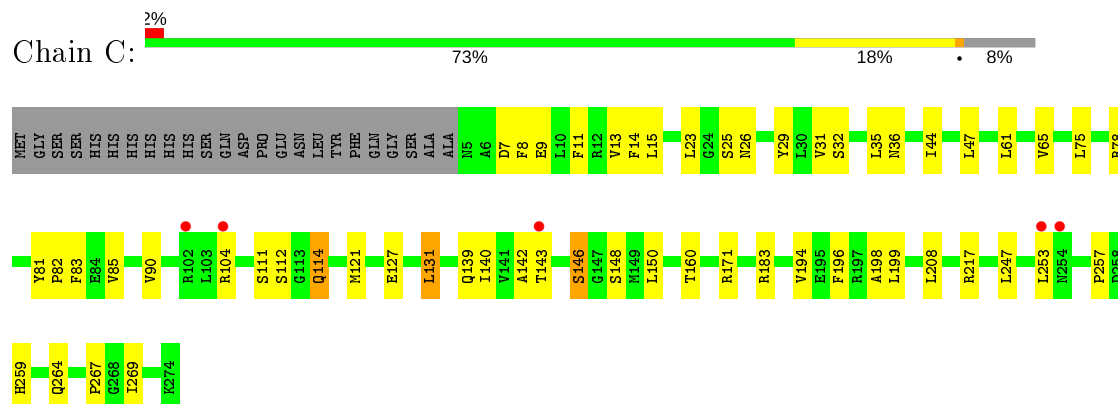
#### • Molecule 1: Chemotaxis protein methyltransferase 1



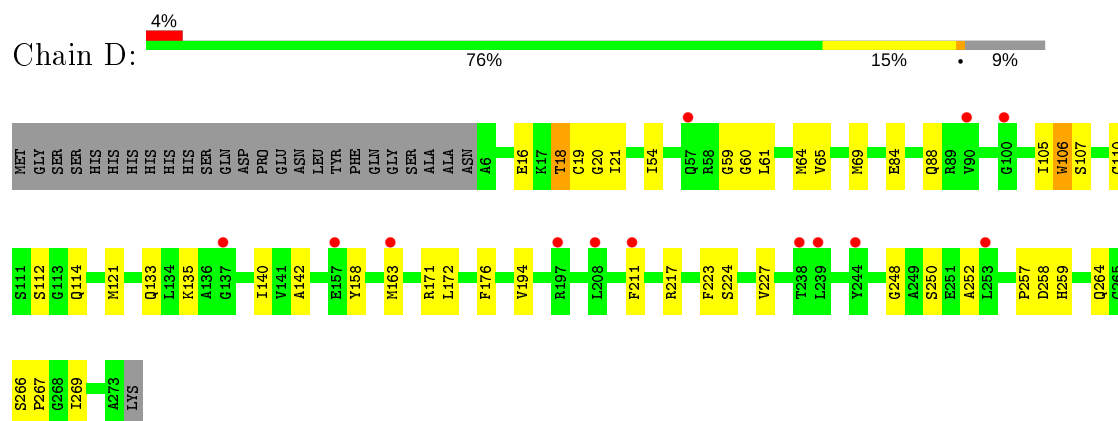
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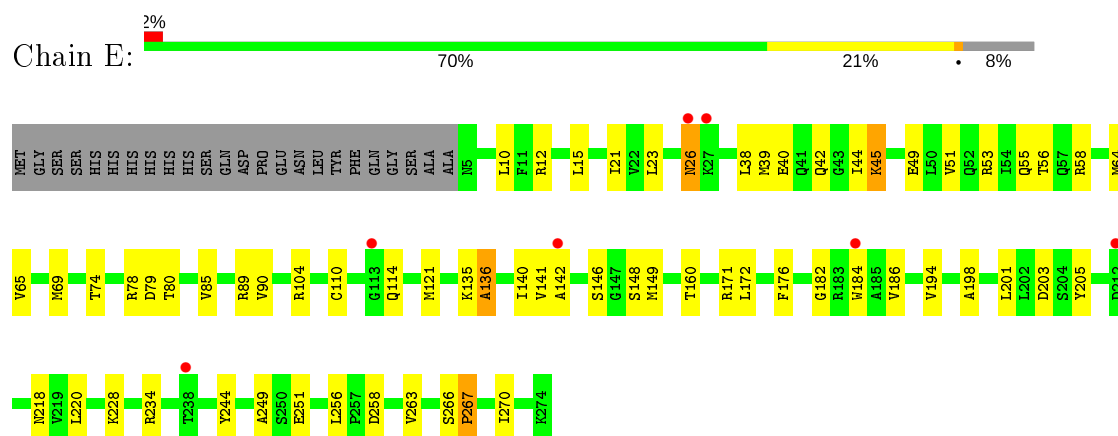
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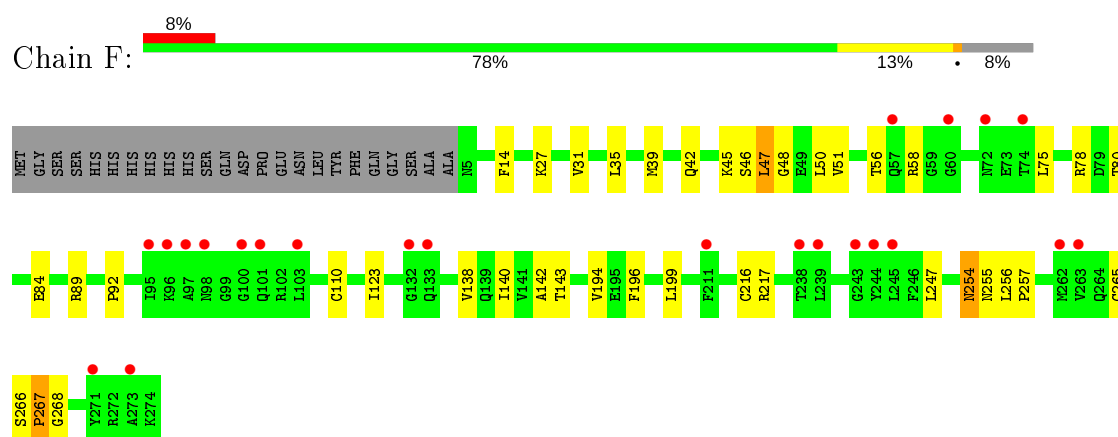
- Molecule 1: Chemotaxis protein methyltransferase 1



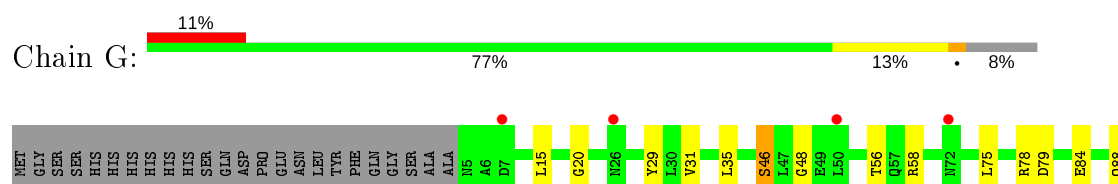
- Molecule 1: Chemotaxis protein methyltransferase 1

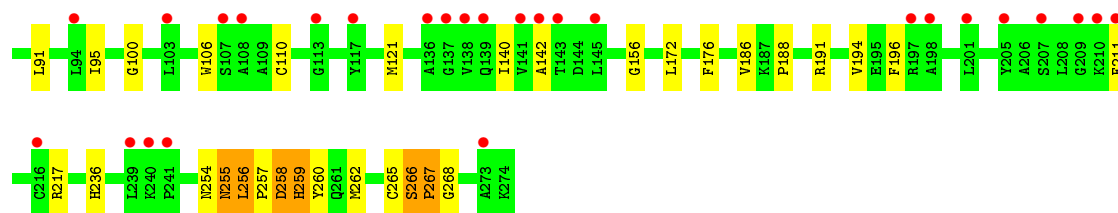


- Molecule 1: Chemotaxis protein methyltransferase 1

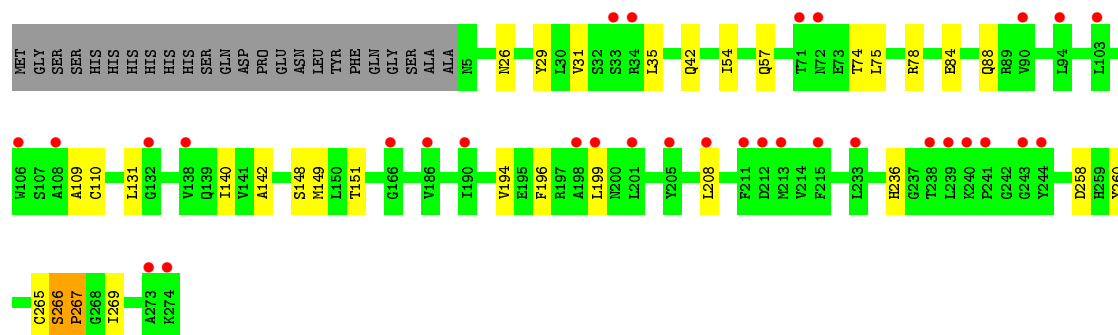
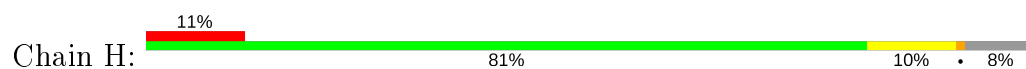


- Molecule 1: Chemotaxis protein methyltransferase 1

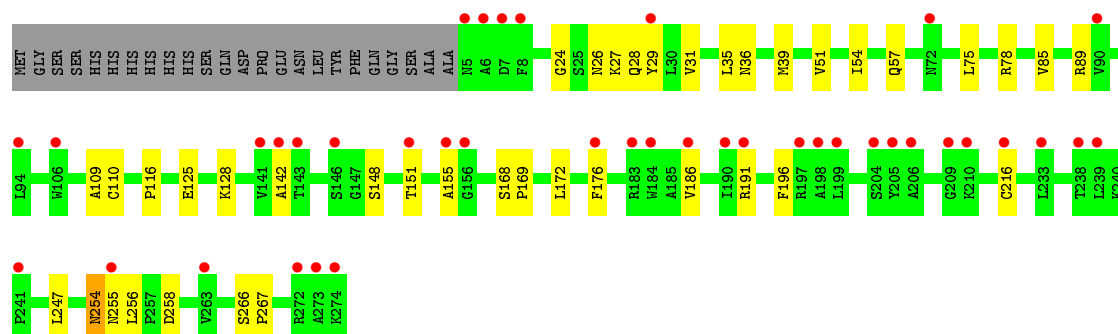
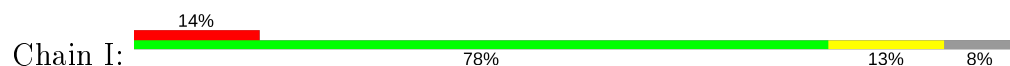




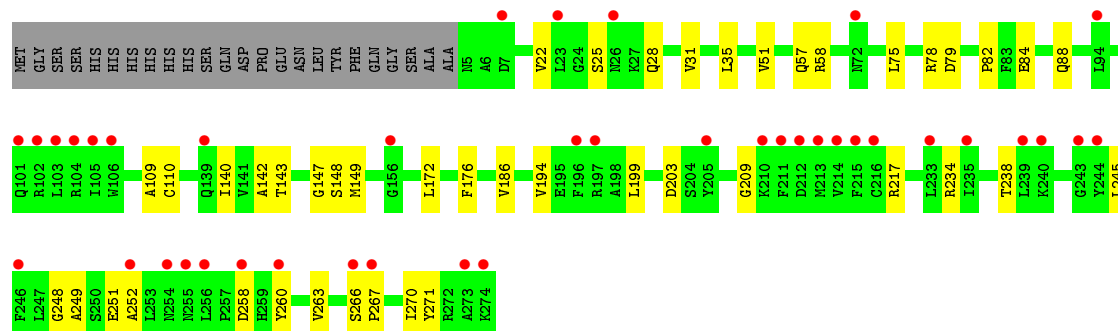
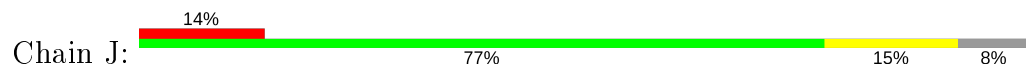
• Molecule 1: Chemotaxis protein methyltransferase 1



• 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, $\alpha$ , $\beta$ , $\gamma$	279.55Å 279.55Å 138.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.40 49.42 – 3.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-3.40) 100.0 (49.42-3.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.260 , 0.293 0.263 , 0.297	Depositor DCC
$R_{free}$ test set	7079 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 119.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/2054	0.57	0/2780
1	B	0.26	0/1867	0.54	0/2548
1	C	0.27	0/2000	0.52	0/2723
1	D	0.26	0/1924	0.51	0/2620
1	E	0.28	0/2002	0.57	0/2720
1	F	0.26	0/1984	0.50	0/2691
1	G	0.26	0/1997	0.49	0/2710
1	H	0.27	0/2009	0.52	0/2728
1	I	0.25	0/1980	0.51	0/2689
1	J	0.24	0/1977	0.50	0/2684
All	All	0.27	0/19794	0.52	0/26893

There are no bond length outliers.

There are no bond angle outliers.

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	2016	0	1938	51	0
1	B	1831	0	1526	24	0
1	C	1962	0	1818	38	0
1	D	1888	0	1699	39	0
1	E	1965	0	1823	39	0
1	F	1952	0	1845	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1963	0	1842	39	0
1	H	1974	0	1888	21	0
1	I	1945	0	1812	27	0
1	J	1944	0	1817	27	0
All	All	19440	0	18008	309	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 8.

All (309) 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
1:F:45:LYS:O	1:F:47:LEU:N	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG3	1:E:45:LYS:O	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: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:I:26:ASN:C	1:I:28:GLN:H	2.07	0.58
1:G:140:ILE:HB	1:G:194:VAL:HG12	1.85	0.58
1:A:253:LEU:O	1:A:255:ASN:N	2.36	0.58
1:G:121:MET:HE1	1:G:176:PHE:HZ	1.68	0.58
1:D:158:TYR:HB3	1:D:163:MET:HE3	1.85	0.58
1:G:46:SER:O	1:G:48:GLY:N	2.34	0.58
1:B:143:THR:HB	1:B:199:LEU:HB3	1.86	0.57
1:B:60:GLY:O	1:B:62:ARG:N	2.30	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:B:236:HIS:HD1	1:B:260:TYR:HE1	1.50	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: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:E:56:THR:C	1:E:58:ARG:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:39:MET:HE3	1:E:45:LYS:H	1.72	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: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
1:C:121:MET:HE3	1:C:171:ARG:HB3	1.90	0.54
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: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:236:HIS:HD1	1:H:260:TYR:HE1	1.58	0.52
1:H:31:VAL:O	1:H:35:LEU:HG	2.09	0.52
1:I:176:PHE:HE1	1:I:186:VAL:HG22	1.74	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:G:121:MET:HE1	1:G:176:PHE:CZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:121:MET:CE	1:G:176:PHE:CZ	2.94	0.51
1:G:78:ARG:HB2	1:G:217:ARG:NH1	2.25	0.51
1:I:31:VAL:O	1:I:35:LEU:HG	2.11	0.51
1:F:56:THR:C	1:F:58:ARG:H	2.14	0.50
1:E:23:LEU:HD11	1:E:69:MET:CE	2.41	0.50
1:A:188:PRO:HA	1:A:191:ARG:HB3	1.92	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: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: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:E:121:MET:HE1	1:E:171:ARG:HB3	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:142:ALA:HB3	1:G:196:PHE:CD1	2.49	0.47
1:D:158:TYR:HB3	1:D:163:MET:CE	2.44	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: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: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: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: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: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:I:148:SER:HB3	1:J:51:VAL:HB	1.97	0.46
1:A:123:ILE:HG13	1:A:138:VAL:HG21	1.97	0.46
1:D:61:LEU:HD12	1:D:64:MET:HE3	1.98	0.46
1:A:258:ASP:O	1:A:260:TYR:N	2.41	0.46
1:A:84:GLU:O	1:A:88:GLN:HG2	2.16	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:B:57:GLN:O	1:H:109:ALA:CB	2.64	0.46
1:C:35:LEU:HD21	1:C:65:VAL:HG23	1.98	0.46
1:D:106:TRP:HA	1:D:106:TRP:HE3	1.81	0.46
1:E:53:ARG:C	1:E:55:GLN:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:56:THR:C	1:E:58:ARG:N	2.69	0.45
1:D:133:GLN:C	1:D:135:LYS:H	2.19	0.45
1:G:257:PRO:O	1:G:258:ASP:C	2.55	0.45
1:J:143:THR:HB	1:J:199:LEU:HB3	1.99	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:A:199:LEU:HD22	1:A:208:LEU:HD11	1.99	0.44
1:E:90:VAL:HG13	1:E:244:TYR:HD2	1.82	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:160:THR:HG22	1:E:184:TRP:HE1	1.82	0.44
1:E:38:LEU:HD11	1:E:64:MET:HB3	1.99	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:F:56:THR:C	1:F:58:ARG:N	2.70	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: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:E:12:ARG:HH12	1:E:26:ASN:H	1.66	0.44
1:C:85:VAL:HG12	1:C:90:VAL:HG23	2.00	0.44
1:J:31:VAL:O	1:J:35:LEU:HG	2.18	0.44
1:A:163:MET:HE2	1:A:184:TRP:HB2	2.00	0.43
1:D:106:TRP:HA	1:D:106:TRP:CE3	2.53	0.43
1:D:112:SER:OG	1:D:114:GLN:OE1	2.35	0.43
1:D:84:GLU:O	1:D:88:GLN:HG2	2.18	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:B:46:SER:C	1:B:48:GLY:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:267:PRO:HG2	1:F:268:GLY:H	1.84	0.43
1:F:80:THR:O	1:F:84:GLU:HG3	2.18	0.43
1:G:121:MET:CE	1:G:176:PHE:HZ	2.29	0.43
1:C:148:SER:O	1:C:150:LEU:N	2.44	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: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:D:121:MET:HE3	1:D:171:ARG:HB3	2.01	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:D:106:TRP:C	1:D:106:TRP:CE3	2.93	0.42
1:E:40:GLU:C	1:E:42:GLN:H	2.23	0.42
1:I:168:SER:HA	1:I:169:PRO:HD3	1.94	0.42
1:E:15:LEU:HD13	1:E:21:ILE:HD11	2.01	0.42
1:C:11:PHE:O	1:C:14:PHE:HB3	2.20	0.42
1:C:26:ASN:N	1:C:26:ASN:OD1	2.45	0.42
1:G:255:ASN:O	1:G:256:LEU:HB2	2.19	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:E:160:THR:HG23	1:E:182:GLY:C	2.40	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:H:269:ILE:HG13	1:H:269:ILE:O	2.20	0.42
1:F:266:SER:HB3	1:I:29:TYR:CE1	2.55	0.42
1:B:253:LEU:O	1:B:255:ASN:N	2.53	0.42
1:C:121:MET:CE	1:C:171:ARG:HB3	2.50	0.42
1:C:81:TYR:CD2	1:C:82:PRO:HD3	2.54	0.42
1:D:18:THR:C	1:D:20:GLY:N	2.73	0.42
1:G:267:PRO:HB3	1:H:26:ASN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:56:THR:C	1:G:58:ARG:N	2.73	0.41
1:A:60:GLY:HA2	1:A:63:GLU:OE1	2.20	0.41
1:B:219:VAL:HG13	1:H:57:GLN:O	2.20	0.41
1:B:55:GLN:CB	1:H:149:MET:HB2	2.50	0.41
1:E:78:ARG:C	1:E:80:THR:H	2.23	0.41
1:A:217:ARG:NH2	1:A:248:GLY:HA2	2.36	0.41
1:I:142:ALA:HB3	1:I:196:PHE:CD1	2.55	0.41
1:I:51:VAL:O	1:J:149:MET:HG2	2.20	0.41
1:G:15:LEU:O	1:G:20:GLY:N	2.53	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:I:26:ASN:C	1:I:28:GLN:N	2.73	0.41
1:A:236:HIS:HB2	1:A:260:TYR:CE1	2.55	0.41
1:E:263:VAL:HB	1:E:270:ILE:HG13	2.02	0.41
1:I:24:GLY:C	1:I:26:ASN:H	2.23	0.41
1:B:172:LEU:O	1:B:176:PHE:HB2	2.21	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: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:J:245:LEU:N	1:J:271:TYR:O	2.48	0.41
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:F:89:ARG:C	1:F:92:PRO:HD2	2.42	0.40
1:I:36:ASN:HA	1:I:39:MET:HB2	2.03	0.40
1:E:201:LEU:O	1:E:205:TYR:OH	2.32	0.40
1:F:142:ALA:HB3	1:F:196:PHE:CD1	2.56	0.40
1:G:121:MET:HE2	1:G:176:PHE:CZ	2.55	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	268/294 (91%)	227 (85%)	35 (13%)	6 (2%)	6	29
1	B	267/294 (91%)	227 (85%)	33 (12%)	7 (3%)	5	26
1	C	268/294 (91%)	230 (86%)	34 (13%)	4 (2%)	10	36
1	D	266/294 (90%)	231 (87%)	32 (12%)	3 (1%)	14	44
1	E	268/294 (91%)	231 (86%)	31 (12%)	6 (2%)	6	29
1	F	268/294 (91%)	225 (84%)	38 (14%)	5 (2%)	8	31
1	G	268/294 (91%)	222 (83%)	40 (15%)	6 (2%)	6	29
1	H	268/294 (91%)	217 (81%)	47 (18%)	4 (2%)	10	36
1	I	268/294 (91%)	224 (84%)	40 (15%)	4 (2%)	10	36
1	J	268/294 (91%)	230 (86%)	37 (14%)	1 (0%)	34	67
All	All	2677/2940 (91%)	2264 (85%)	367 (14%)	46 (2%)	9	34

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

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Mol	Chain	Res	Type
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
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%)	146 (99%)	1 (1%)	84	92
1	C	185/246 (75%)	183 (99%)	2 (1%)	73	86
1	D	168/246 (68%)	166 (99%)	2 (1%)	71	85
1	E	185/246 (75%)	184 (100%)	1 (0%)	88	94
1	F	184/246 (75%)	184 (100%)	0	100	100
1	G	185/246 (75%)	182 (98%)	3 (2%)	62	81
1	H	189/246 (77%)	186 (98%)	3 (2%)	62	81
1	I	179/246 (73%)	177 (99%)	2 (1%)	73	86
1	J	180/246 (73%)	179 (99%)	1 (1%)	86	94
All	All	1797/2460 (73%)	1782 (99%)	15 (1%)	81	91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251	GLU
1	C	114	GLN
1	C	183	ARG
1	D	18	THR
1	D	106	TRP
1	E	49	GLU
1	G	259	HIS
1	G	262	MET
1	G	266	SER
1	H	131	LEU
1	H	265	CYS
1	H	266	SER
1	I	254	ASN
1	I	255	ASN
1	J	251	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	236	HIS
1	C	114	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	270/294 (91%)	0.07	2 (0%) 87 87	60, 106, 166, 212	0
1	B	269/294 (91%)	0.30	14 (5%) 27 27	83, 147, 196, 228	0
1	C	270/294 (91%)	0.23	5 (1%) 66 65	69, 120, 168, 219	0
1	D	268/294 (91%)	0.35	13 (4%) 29 29	88, 149, 201, 245	0
1	E	270/294 (91%)	0.30	7 (2%) 56 54	86, 129, 183, 275	0
1	F	270/294 (91%)	0.48	23 (8%) 10 12	129, 179, 218, 267	0
1	G	270/294 (91%)	0.63	31 (11%) 4 5	124, 175, 217, 255	0
1	H	270/294 (91%)	0.83	32 (11%) 4 5	118, 165, 218, 235	0
1	I	270/294 (91%)	0.86	40 (14%) 2 3	144, 199, 247, 268	0
1	J	270/294 (91%)	0.78	40 (14%) 2 3	111, 197, 251, 297	0
All	All	2697/2940 (91%)	0.48	207 (7%) 13 15	60, 159, 226, 297	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	212	ASP	7.6
1	J	254	ASN	6.4
1	G	7	ASP	5.8
1	J	211	PHE	5.6
1	G	136	ALA	5.2
1	H	103	LEU	5.0
1	J	213	MET	5.0
1	I	273	ALA	5.0
1	J	244	TYR	4.7
1	J	233	LEU	4.7
1	I	197	ARG	4.6
1	F	101	GLN	4.6
1	D	239	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	97	ALA	4.4
1	H	244	TYR	4.3
1	H	71	THR	4.2
1	I	241	PRO	4.1
1	H	238	THR	4.1
1	G	26	ASN	4.0
1	I	184	TRP	4.0
1	I	156	GLY	4.0
1	H	94	LEU	4.0
1	H	186	VAL	3.9
1	I	7	ASP	3.9
1	G	139	GLN	3.9
1	I	255	ASN	3.8
1	I	155	ALA	3.7
1	I	233	LEU	3.6
1	I	143	THR	3.6
1	J	103	LEU	3.6
1	H	72	ASN	3.6
1	F	57	GLN	3.5
1	J	101	GLN	3.5
1	G	138	VAL	3.5
1	D	157	GLU	3.4
1	I	106	TRP	3.4
1	H	132	GLY	3.4
1	J	214	VAL	3.4
1	J	235	ILE	3.4
1	J	243	GLY	3.4
1	F	74	THR	3.3
1	J	26	ASN	3.3
1	I	238	THR	3.3
1	G	108	ALA	3.2
1	G	142	ALA	3.2
1	C	102	ARG	3.2
1	E	26	ASN	3.2
1	D	244	TYR	3.2
1	J	215	PHE	3.2
1	E	27	LYS	3.2
1	H	205	TYR	3.2
1	H	243	GLY	3.1
1	F	132	GLY	3.1
1	H	34	ARG	3.1
1	G	72	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	205	TYR	3.1
1	H	273	ALA	3.1
1	J	252	ALA	3.0
1	F	239	LEU	3.0
1	H	33	SER	3.0
1	F	100	GLY	3.0
1	I	206	ALA	3.0
1	J	72	ASN	3.0
1	I	274	LYS	3.0
1	F	244	TYR	3.0
1	B	55	GLN	2.9
1	J	205	TYR	2.9
1	F	95	ILE	2.9
1	I	142	ALA	2.9
1	H	201	LEU	2.9
1	J	196	PHE	2.9
1	H	108	ALA	2.9
1	I	191	ARG	2.9
1	H	106	TRP	2.8
1	G	240	LYS	2.8
1	I	176	PHE	2.8
1	F	243	GLY	2.8
1	F	133	GLN	2.8
1	F	103	LEU	2.8
1	H	239	LEU	2.8
1	J	273	ALA	2.8
1	I	190	ILE	2.8
1	F	245	LEU	2.8
1	J	239	LEU	2.8
1	A	25	SER	2.8
1	I	272	ARG	2.8
1	J	106	TRP	2.8
1	J	139	GLN	2.8
1	F	60	GLY	2.8
1	B	241	PRO	2.7
1	H	274	LYS	2.7
1	B	273	ALA	2.7
1	G	210	LYS	2.7
1	J	255	ASN	2.7
1	J	256	LEU	2.7
1	H	208	LEU	2.7
1	J	102	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	103	LEU	2.7
1	F	72	ASN	2.7
1	G	103	LEU	2.7
1	I	204	SER	2.6
1	J	94	LEU	2.6
1	G	50	LEU	2.6
1	F	238	THR	2.6
1	D	100	GLY	2.6
1	I	151	THR	2.6
1	H	213	MET	2.6
1	E	142	ALA	2.6
1	I	146	SER	2.6
1	F	263	VAL	2.6
1	B	71	THR	2.6
1	B	41	GLN	2.6
1	J	260	TYR	2.6
1	G	137	GLY	2.6
1	E	238	THR	2.6
1	D	253	LEU	2.5
1	G	143	THR	2.5
1	F	262	MET	2.5
1	J	104	ARG	2.5
1	D	57	GLN	2.5
1	E	184	TRP	2.5
1	G	216	CYS	2.5
1	E	113	GLY	2.5
1	I	8	PHE	2.5
1	J	240	LYS	2.5
1	H	215	PHE	2.5
1	I	263	VAL	2.5
1	I	210	LYS	2.4
1	J	7	ASP	2.4
1	D	208	LEU	2.4
1	I	6	ALA	2.4
1	H	240	LYS	2.4
1	G	239	LEU	2.4
1	G	117	TYR	2.4
1	I	94	LEU	2.4
1	H	198	ALA	2.4
1	G	209	GLY	2.4
1	H	90	VAL	2.4
1	B	213	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	199	LEU	2.3
1	D	211	PHE	2.3
1	H	212	ASP	2.3
1	J	105	ILE	2.3
1	B	24	GLY	2.3
1	J	258	ASP	2.3
1	G	273	ALA	2.3
1	J	23	LEU	2.3
1	G	113	GLY	2.3
1	G	211	PHE	2.3
1	I	186	VAL	2.3
1	E	212	ASP	2.3
1	B	138	VAL	2.3
1	G	107	SER	2.3
1	H	241	PRO	2.3
1	I	239	LEU	2.3
1	G	198	ALA	2.3
1	D	238	THR	2.3
1	F	211	PHE	2.3
1	I	5	ASN	2.3
1	B	185	ALA	2.3
1	I	29	TYR	2.3
1	A	26	ASN	2.3
1	B	246	PHE	2.2
1	F	273	ALA	2.2
1	J	274	LYS	2.2
1	G	201	LEU	2.2
1	F	96	LYS	2.2
1	G	141	VAL	2.2
1	J	197	ARG	2.2
1	J	266	SER	2.2
1	J	267	PRO	2.2
1	I	183	ARG	2.2
1	D	197	ARG	2.2
1	J	246	PHE	2.2
1	I	72	ASN	2.2
1	H	190	ILE	2.1
1	G	94	LEU	2.1
1	I	198	ALA	2.1
1	I	209	GLY	2.1
1	B	260	TYR	2.1
1	B	25	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	138	VAL	2.1
1	H	166	GLY	2.1
1	I	199	LEU	2.1
1	D	163	MET	2.1
1	J	156	GLY	2.1
1	I	205	TYR	2.1
1	B	94	LEU	2.1
1	G	207	SER	2.1
1	H	211	PHE	2.1
1	G	197	ARG	2.1
1	J	210	LYS	2.1
1	G	241	PRO	2.1
1	I	141	VAL	2.0
1	D	90	VAL	2.0
1	G	145	LEU	2.0
1	I	90	VAL	2.0
1	H	233	LEU	2.0
1	C	143	THR	2.0
1	C	254	ASN	2.0
1	I	216	CYS	2.0
1	J	216	CYS	2.0
1	D	137	GLY	2.0
1	C	104	ARG	2.0
1	C	253	LEU	2.0
1	F	271	TYR	2.0
1	F	98	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.