



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2016 – 01:17 PM EST

PDB ID : 5GM1
Title : Crystal structure of methyltransferase TleD complexed with SAH
Authors : Yu, F.; Li, M.J.; Xu, C.Y.; Zhou, H.; Sun, B.; Wang, Z.J.; Xu, Q.; Xie, M.Y.;
Zuo, G.; Huang, P.; Wang, Q.S.; He, J.H.
Deposited on : 2016-07-12
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

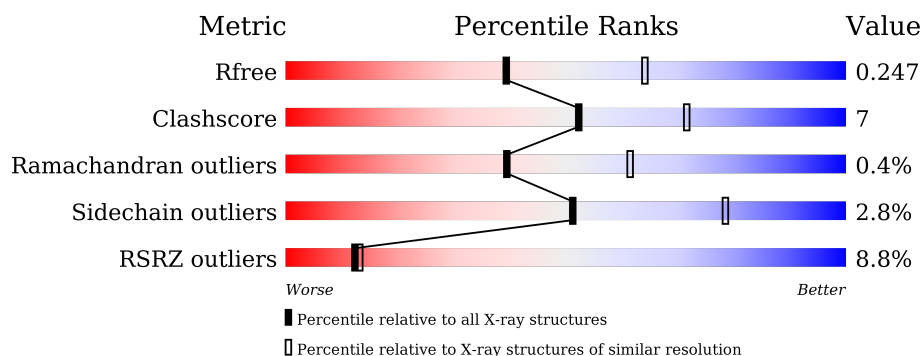
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	297	<div> <div></div> <div>79%15%5%</div> </div>
1	B	297	<div> <div></div> <div>79%14%6%</div> </div>
1	C	297	<div> <div>%</div> <div>76%17%6%</div> </div>
1	D	297	<div> <div>%</div> <div>81%12%6%</div> </div>
1	E	297	<div> <div>%</div> <div>80%13%6%</div> </div>
1	F	297	<div> <div>%</div> <div>80%14%6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	297	
1	H	297	
1	I	297	
1	J	297	
1	K	297	
1	L	297	
1	M	297	
1	N	297	
1	O	297	
1	P	297	
1	Q	297	
1	R	297	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	B	302	-	-	-	X
2	SAH	R	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40182 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 O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	B	280	Total	C	N	O	S	0	1	0
			2164	1372	367	414	11			
1	C	280	Total	C	N	O	S	0	0	0
			2157	1370	365	411	11			
1	D	280	Total	C	N	O	S	0	1	0
			2169	1375	370	413	11			
1	E	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	F	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	G	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	H	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	I	280	Total	C	N	O	S	3	1	0
			2169	1375	370	413	11			
1	J	281	Total	C	N	O	S	0	0	0
			2167	1374	368	414	11			
1	K	281	Total	C	N	O	S	0	0	0
			2166	1375	367	413	11			
1	L	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	M	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	N	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	O	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	P	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	R	281	Total	C	N	O	S	0	1	0
			2176	1379	370	416	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LEU	-	expression tag	UNP A0A077K7L1
A	291	GLU	-	expression tag	UNP A0A077K7L1
A	292	HIS	-	expression tag	UNP A0A077K7L1
A	293	HIS	-	expression tag	UNP A0A077K7L1
A	294	HIS	-	expression tag	UNP A0A077K7L1
A	295	HIS	-	expression tag	UNP A0A077K7L1
A	296	HIS	-	expression tag	UNP A0A077K7L1
A	297	HIS	-	expression tag	UNP A0A077K7L1
B	290	LEU	-	expression tag	UNP A0A077K7L1
B	291	GLU	-	expression tag	UNP A0A077K7L1
B	292	HIS	-	expression tag	UNP A0A077K7L1
B	293	HIS	-	expression tag	UNP A0A077K7L1
B	294	HIS	-	expression tag	UNP A0A077K7L1
B	295	HIS	-	expression tag	UNP A0A077K7L1
B	296	HIS	-	expression tag	UNP A0A077K7L1
B	297	HIS	-	expression tag	UNP A0A077K7L1
C	290	LEU	-	expression tag	UNP A0A077K7L1
C	291	GLU	-	expression tag	UNP A0A077K7L1
C	292	HIS	-	expression tag	UNP A0A077K7L1
C	293	HIS	-	expression tag	UNP A0A077K7L1
C	294	HIS	-	expression tag	UNP A0A077K7L1
C	295	HIS	-	expression tag	UNP A0A077K7L1
C	296	HIS	-	expression tag	UNP A0A077K7L1
C	297	HIS	-	expression tag	UNP A0A077K7L1
D	290	LEU	-	expression tag	UNP A0A077K7L1
D	291	GLU	-	expression tag	UNP A0A077K7L1
D	292	HIS	-	expression tag	UNP A0A077K7L1
D	293	HIS	-	expression tag	UNP A0A077K7L1
D	294	HIS	-	expression tag	UNP A0A077K7L1
D	295	HIS	-	expression tag	UNP A0A077K7L1
D	296	HIS	-	expression tag	UNP A0A077K7L1
D	297	HIS	-	expression tag	UNP A0A077K7L1
E	290	LEU	-	expression tag	UNP A0A077K7L1
E	291	GLU	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	292	HIS	-	expression tag	UNP A0A077K7L1
E	293	HIS	-	expression tag	UNP A0A077K7L1
E	294	HIS	-	expression tag	UNP A0A077K7L1
E	295	HIS	-	expression tag	UNP A0A077K7L1
E	296	HIS	-	expression tag	UNP A0A077K7L1
E	297	HIS	-	expression tag	UNP A0A077K7L1
F	290	LEU	-	expression tag	UNP A0A077K7L1
F	291	GLU	-	expression tag	UNP A0A077K7L1
F	292	HIS	-	expression tag	UNP A0A077K7L1
F	293	HIS	-	expression tag	UNP A0A077K7L1
F	294	HIS	-	expression tag	UNP A0A077K7L1
F	295	HIS	-	expression tag	UNP A0A077K7L1
F	296	HIS	-	expression tag	UNP A0A077K7L1
F	297	HIS	-	expression tag	UNP A0A077K7L1
G	290	LEU	-	expression tag	UNP A0A077K7L1
G	291	GLU	-	expression tag	UNP A0A077K7L1
G	292	HIS	-	expression tag	UNP A0A077K7L1
G	293	HIS	-	expression tag	UNP A0A077K7L1
G	294	HIS	-	expression tag	UNP A0A077K7L1
G	295	HIS	-	expression tag	UNP A0A077K7L1
G	296	HIS	-	expression tag	UNP A0A077K7L1
G	297	HIS	-	expression tag	UNP A0A077K7L1
H	290	LEU	-	expression tag	UNP A0A077K7L1
H	291	GLU	-	expression tag	UNP A0A077K7L1
H	292	HIS	-	expression tag	UNP A0A077K7L1
H	293	HIS	-	expression tag	UNP A0A077K7L1
H	294	HIS	-	expression tag	UNP A0A077K7L1
H	295	HIS	-	expression tag	UNP A0A077K7L1
H	296	HIS	-	expression tag	UNP A0A077K7L1
H	297	HIS	-	expression tag	UNP A0A077K7L1
I	290	LEU	-	expression tag	UNP A0A077K7L1
I	291	GLU	-	expression tag	UNP A0A077K7L1
I	292	HIS	-	expression tag	UNP A0A077K7L1
I	293	HIS	-	expression tag	UNP A0A077K7L1
I	294	HIS	-	expression tag	UNP A0A077K7L1
I	295	HIS	-	expression tag	UNP A0A077K7L1
I	296	HIS	-	expression tag	UNP A0A077K7L1
I	297	HIS	-	expression tag	UNP A0A077K7L1
J	290	LEU	-	expression tag	UNP A0A077K7L1
J	291	GLU	-	expression tag	UNP A0A077K7L1
J	292	HIS	-	expression tag	UNP A0A077K7L1
J	293	HIS	-	expression tag	UNP A0A077K7L1

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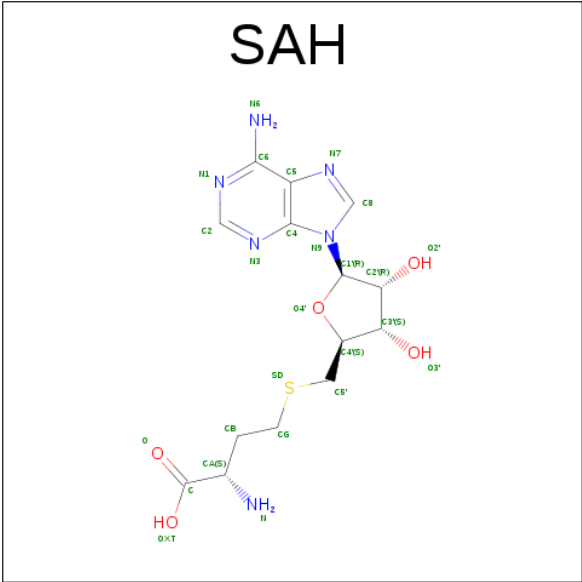
Chain	Residue	Modelled	Actual	Comment	Reference
J	294	HIS	-	expression tag	UNP A0A077K7L1
J	295	HIS	-	expression tag	UNP A0A077K7L1
J	296	HIS	-	expression tag	UNP A0A077K7L1
J	297	HIS	-	expression tag	UNP A0A077K7L1
K	290	LEU	-	expression tag	UNP A0A077K7L1
K	291	GLU	-	expression tag	UNP A0A077K7L1
K	292	HIS	-	expression tag	UNP A0A077K7L1
K	293	HIS	-	expression tag	UNP A0A077K7L1
K	294	HIS	-	expression tag	UNP A0A077K7L1
K	295	HIS	-	expression tag	UNP A0A077K7L1
K	296	HIS	-	expression tag	UNP A0A077K7L1
K	297	HIS	-	expression tag	UNP A0A077K7L1
L	290	LEU	-	expression tag	UNP A0A077K7L1
L	291	GLU	-	expression tag	UNP A0A077K7L1
L	292	HIS	-	expression tag	UNP A0A077K7L1
L	293	HIS	-	expression tag	UNP A0A077K7L1
L	294	HIS	-	expression tag	UNP A0A077K7L1
L	295	HIS	-	expression tag	UNP A0A077K7L1
L	296	HIS	-	expression tag	UNP A0A077K7L1
L	297	HIS	-	expression tag	UNP A0A077K7L1
M	290	LEU	-	expression tag	UNP A0A077K7L1
M	291	GLU	-	expression tag	UNP A0A077K7L1
M	292	HIS	-	expression tag	UNP A0A077K7L1
M	293	HIS	-	expression tag	UNP A0A077K7L1
M	294	HIS	-	expression tag	UNP A0A077K7L1
M	295	HIS	-	expression tag	UNP A0A077K7L1
M	296	HIS	-	expression tag	UNP A0A077K7L1
M	297	HIS	-	expression tag	UNP A0A077K7L1
N	290	LEU	-	expression tag	UNP A0A077K7L1
N	291	GLU	-	expression tag	UNP A0A077K7L1
N	292	HIS	-	expression tag	UNP A0A077K7L1
N	293	HIS	-	expression tag	UNP A0A077K7L1
N	294	HIS	-	expression tag	UNP A0A077K7L1
N	295	HIS	-	expression tag	UNP A0A077K7L1
N	296	HIS	-	expression tag	UNP A0A077K7L1
N	297	HIS	-	expression tag	UNP A0A077K7L1
O	290	LEU	-	expression tag	UNP A0A077K7L1
O	291	GLU	-	expression tag	UNP A0A077K7L1
O	292	HIS	-	expression tag	UNP A0A077K7L1
O	293	HIS	-	expression tag	UNP A0A077K7L1
O	294	HIS	-	expression tag	UNP A0A077K7L1
O	295	HIS	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	296	HIS	-	expression tag	UNP A0A077K7L1
O	297	HIS	-	expression tag	UNP A0A077K7L1
P	290	LEU	-	expression tag	UNP A0A077K7L1
P	291	GLU	-	expression tag	UNP A0A077K7L1
P	292	HIS	-	expression tag	UNP A0A077K7L1
P	293	HIS	-	expression tag	UNP A0A077K7L1
P	294	HIS	-	expression tag	UNP A0A077K7L1
P	295	HIS	-	expression tag	UNP A0A077K7L1
P	296	HIS	-	expression tag	UNP A0A077K7L1
P	297	HIS	-	expression tag	UNP A0A077K7L1
Q	290	LEU	-	expression tag	UNP A0A077K7L1
Q	291	GLU	-	expression tag	UNP A0A077K7L1
Q	292	HIS	-	expression tag	UNP A0A077K7L1
Q	293	HIS	-	expression tag	UNP A0A077K7L1
Q	294	HIS	-	expression tag	UNP A0A077K7L1
Q	295	HIS	-	expression tag	UNP A0A077K7L1
Q	296	HIS	-	expression tag	UNP A0A077K7L1
Q	297	HIS	-	expression tag	UNP A0A077K7L1
R	290	LEU	-	expression tag	UNP A0A077K7L1
R	291	GLU	-	expression tag	UNP A0A077K7L1
R	292	HIS	-	expression tag	UNP A0A077K7L1
R	293	HIS	-	expression tag	UNP A0A077K7L1
R	294	HIS	-	expression tag	UNP A0A077K7L1
R	295	HIS	-	expression tag	UNP A0A077K7L1
R	296	HIS	-	expression tag	UNP A0A077K7L1
R	297	HIS	-	expression tag	UNP A0A077K7L1

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	O	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	P	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	Q	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	R	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	90	Total	O	0	0
			90	90		
3	C	51	Total	O	0	0
			51	51		
3	D	35	Total	O	0	0
			35	35		
3	E	48	Total	O	0	0
			48	48		
3	F	72	Total	O	0	0
			72	72		
3	G	22	Total	O	0	0
			22	22		
3	H	19	Total	O	0	0
			19	19		
3	I	46	Total	O	0	0
			46	46		
3	J	21	Total	O	0	0
			21	21		
3	K	11	Total	O	0	0
			11	11		
3	L	21	Total	O	0	0
			21	21		
3	M	28	Total	O	0	0
			28	28		
3	N	19	Total	O	0	0
			19	19		

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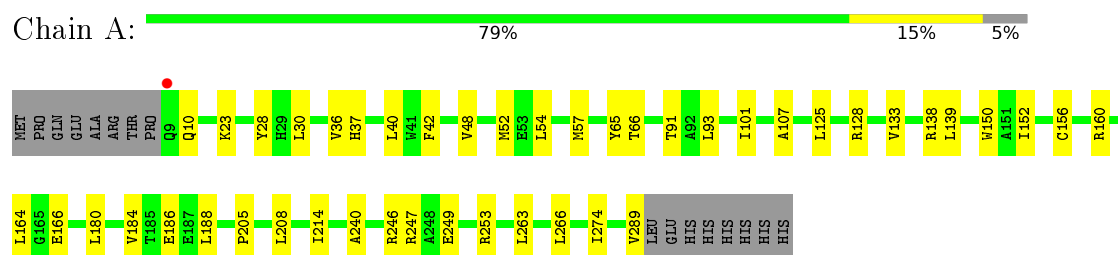
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	38	Total 38	O 38	0	0
3	P	25	Total 25	O 25	0	0
3	Q	24	Total 24	O 24	0	0
3	R	45	Total 45	O 45	0	0

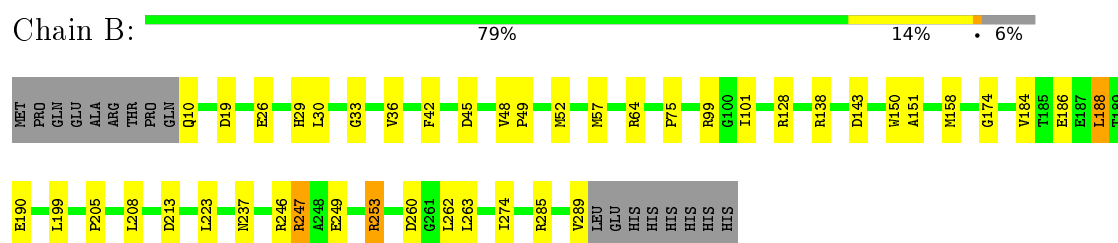
3 Residue-property plots [i](#)

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

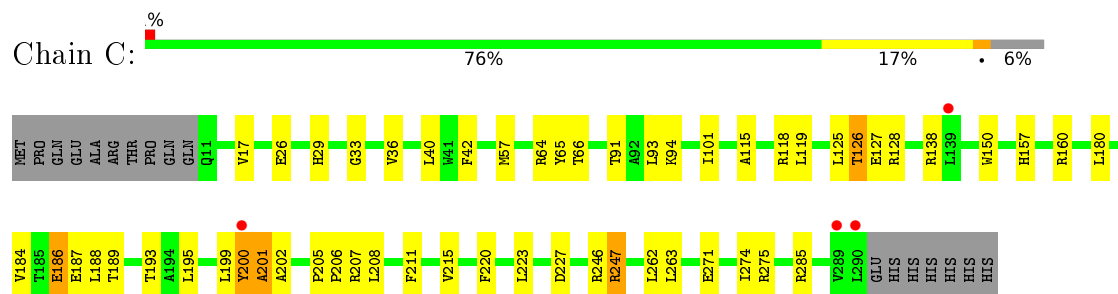
• Molecule 1: O-methyltransferase



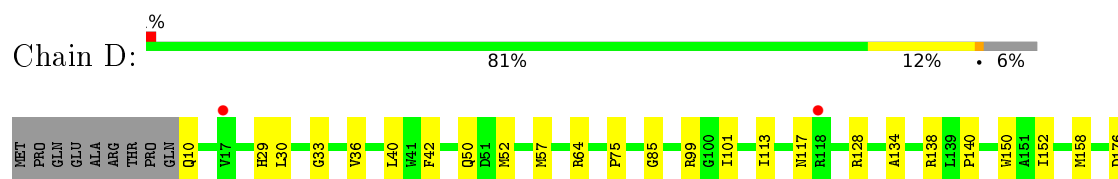
• Molecule 1: O-methyltransferase



• Molecule 1: O-methyltransferase

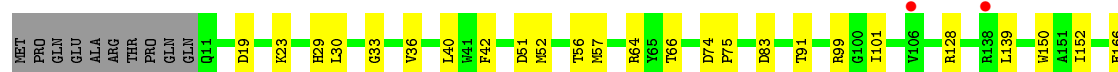
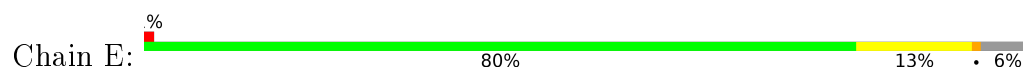


• Molecule 1: O-methyltransferase

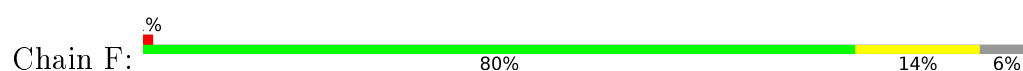




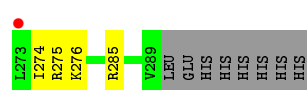
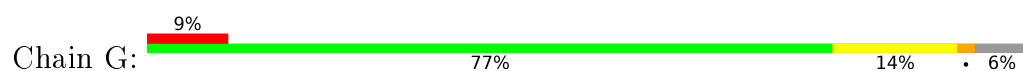
• Molecule 1: O-methyltransferase



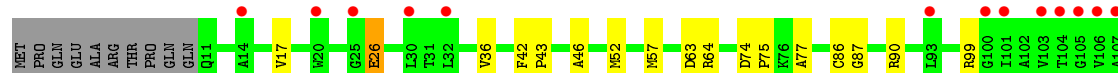
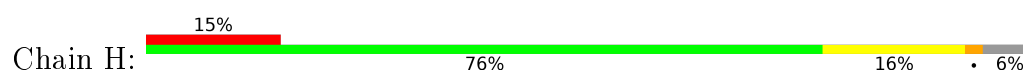
• Molecule 1: O-methyltransferase

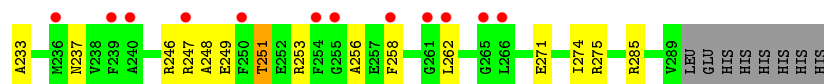


• Molecule 1: O-methyltransferase

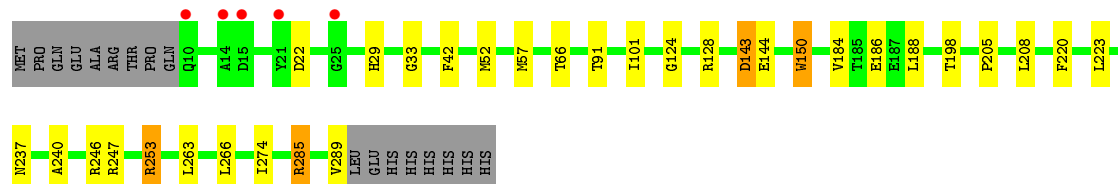
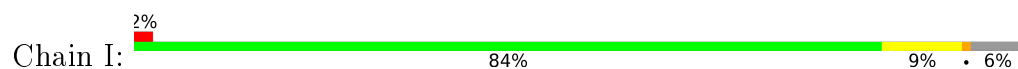


• Molecule 1: O-methyltransferase

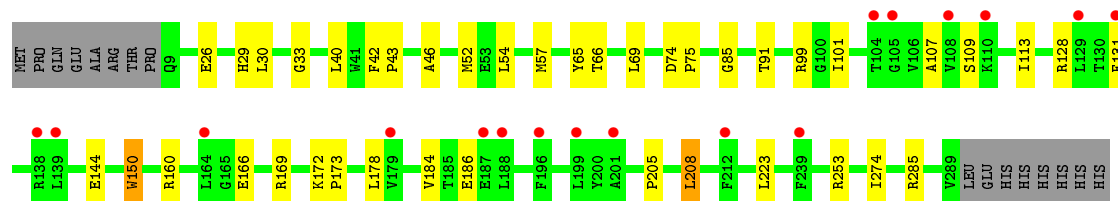
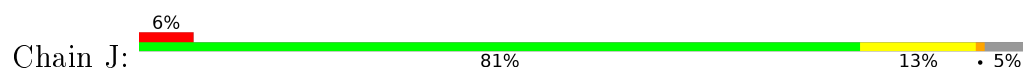




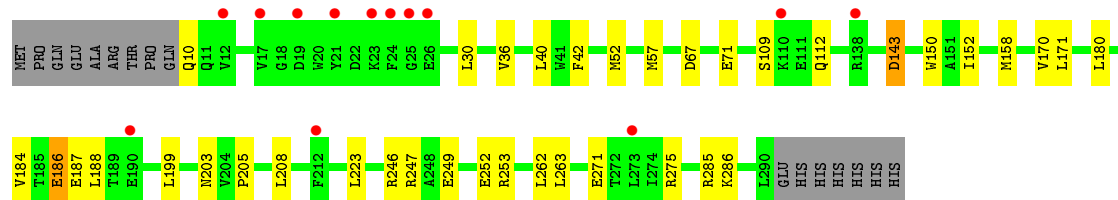
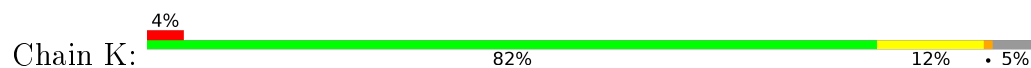
• Molecule 1: O-methyltransferase



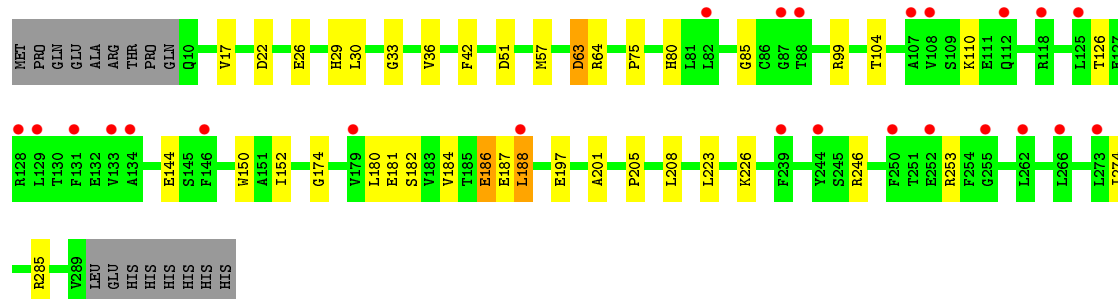
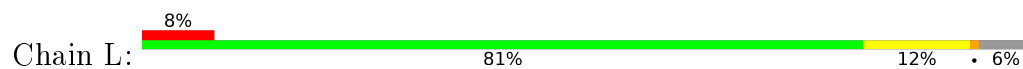
• Molecule 1: O-methyltransferase



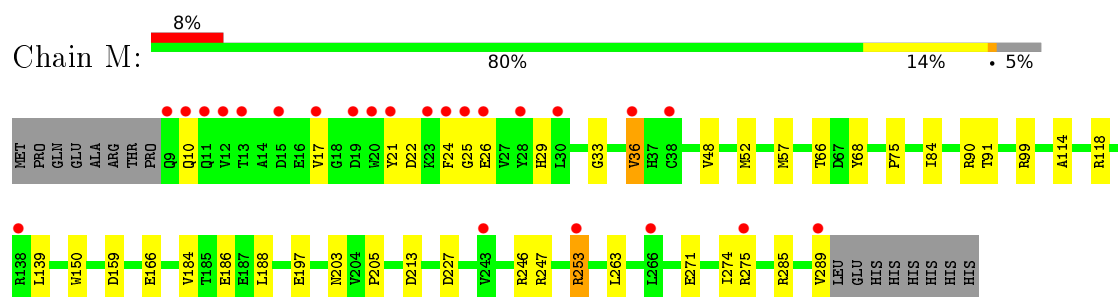
• Molecule 1: O-methyltransferase



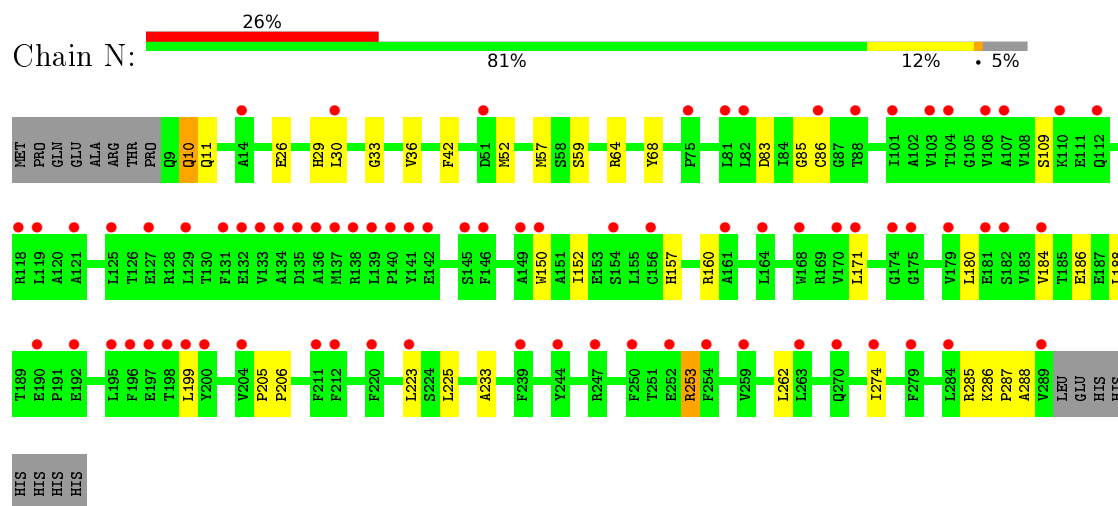
• Molecule 1: O-methyltransferase



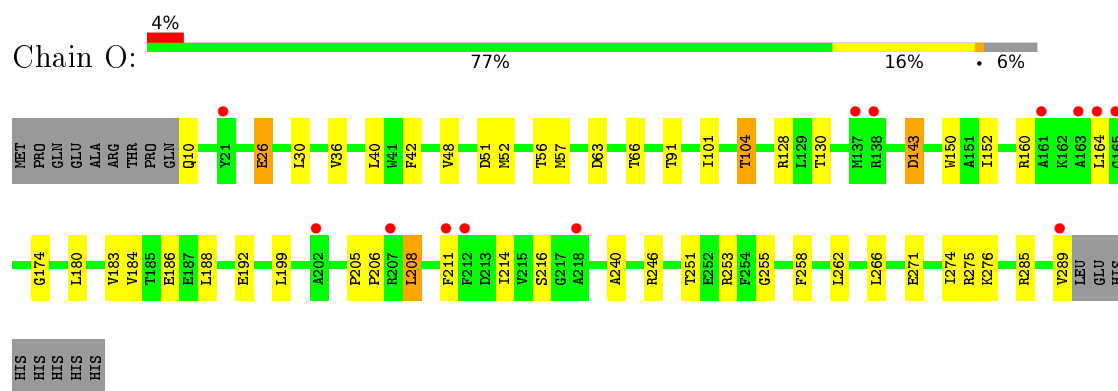
• Molecule 1: O-methyltransferase



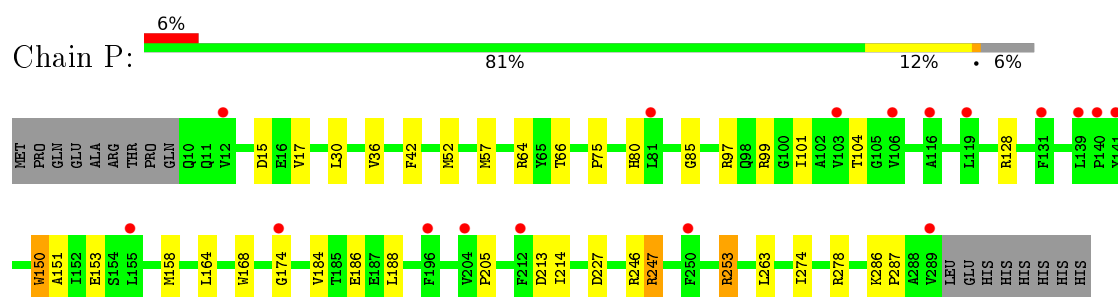
- Molecule 1: O-methyltransferase



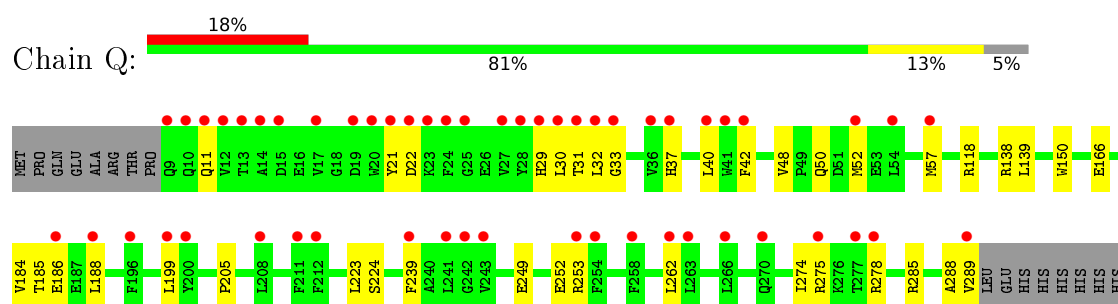
- Molecule 1: O-methyltransferase



- Molecule 1: O-methyltransferase



- Molecule 1: O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.62Å 152.90Å 154.79Å 90.00° 93.33° 90.00°	Depositor
Resolution (Å)	102.27 – 2.50 154.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (102.27-2.50) 99.0 (154.53-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.52Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.207 , 0.248 0.204 , 0.247	Depositor DCC
R_{free} test set	10308 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40182	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH

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	0.29	0/2229	0.48	0/3024
1	B	0.28	0/2209	0.46	0/2998
1	C	0.28	0/2202	0.46	0/2989
1	D	0.27	0/2214	0.45	0/3004
1	E	0.28	0/2194	0.47	0/2978
1	F	0.28	0/2203	0.47	0/2990
1	G	0.26	0/2203	0.45	0/2990
1	H	0.27	0/2194	0.44	0/2978
1	I	0.27	0/2214	0.47	0/3004
1	J	0.27	0/2212	0.44	0/3002
1	K	0.26	0/2211	0.44	0/3001
1	L	0.26	0/2203	0.44	0/2990
1	M	0.28	0/2229	0.46	0/3024
1	N	0.26	0/2229	0.44	0/3024
1	O	0.27	0/2203	0.46	0/2990
1	P	0.27	0/2203	0.45	0/2990
1	Q	0.28	0/2229	0.45	0/3024
1	R	0.26	0/2221	0.45	0/3014
All	All	0.27	0/39802	0.45	0/54014

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	2184	0	2139	29	0
1	B	2164	0	2120	31	0
1	C	2157	0	2119	33	0
1	D	2169	0	2128	25	0
1	E	2149	0	2108	26	0
1	F	2158	0	2116	30	0
1	G	2158	0	2116	33	0
1	H	2149	0	2108	41	0
1	I	2169	0	2128	23	0
1	J	2167	0	2124	30	0
1	K	2166	0	2127	25	0
1	L	2158	0	2116	26	0
1	M	2184	0	2139	36	0
1	N	2184	0	2139	34	0
1	O	2158	0	2116	33	0
1	P	2158	0	2116	32	0
1	Q	2184	0	2139	36	0
1	R	2176	0	2131	80	1
2	A	26	0	19	1	0
2	B	52	0	38	4	0
2	C	26	0	19	1	0
2	D	26	0	19	3	0
2	E	26	0	19	1	0
2	F	26	0	19	1	0
2	G	26	0	19	1	0
2	H	26	0	19	1	0
2	I	26	0	19	0	0
2	J	26	0	19	3	0
2	K	26	0	19	3	0
2	L	26	0	19	3	0
2	M	26	0	19	1	0
2	N	26	0	19	4	0
2	O	26	0	19	2	0
2	P	26	0	19	3	0
2	Q	26	0	19	0	0
2	R	26	0	19	1	0
3	A	81	0	0	2	0
3	B	90	0	0	8	0
3	C	51	0	0	7	0
3	D	35	0	0	3	0
3	E	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	72	0	0	6	0
3	G	22	0	0	6	0
3	H	19	0	0	10	0
3	I	46	0	0	8	0
3	J	21	0	0	3	0
3	K	11	0	0	4	0
3	L	21	0	0	7	0
3	M	28	0	0	10	0
3	N	19	0	0	7	0
3	O	38	0	0	4	0
3	P	25	0	0	13	0
3	Q	24	0	0	12	0
3	R	45	0	0	27	0
All	All	40182	0	38590	525	1

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 7.

All (525) 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:G:417:HOH:O	2:H:301:SAH:SD	1.97	1.23
1:F:22:ASP:O	3:F:401:HOH:O	1.67	1.09
1:R:57:MET:SD	3:R:442:HOH:O	2.14	1.03
1:N:86:CYS:SG	3:N:411:HOH:O	2.22	0.98
1:G:166:GLU:OE1	3:G:401:HOH:O	1.82	0.95
1:L:144:GLU:OE2	3:L:401:HOH:O	1.84	0.95
1:P:213:ASP:OD1	3:P:401:HOH:O	1.89	0.91
1:D:138:ARG:NH1	3:D:401:HOH:O	2.04	0.90
2:P:301:SAH:SD	3:P:425:HOH:O	2.30	0.89
1:R:238:VAL:O	3:R:401:HOH:O	1.90	0.88
1:P:151:ALA:O	3:P:402:HOH:O	1.91	0.88
1:O:63:ASP:OD2	3:O:401:HOH:O	1.89	0.87
1:M:24:PHE:N	3:M:401:HOH:O	2.06	0.86
1:R:148:CYS:SG	3:R:434:HOH:O	2.35	0.85
3:M:423:HOH:O	2:N:301:SAH:SD	2.35	0.84
1:R:19:ASP:OD1	3:R:402:HOH:O	1.95	0.84
3:Q:421:HOH:O	1:R:57:MET:SD	2.36	0.83
1:M:227:ASP:O	3:M:403:HOH:O	1.97	0.83
1:I:144:GLU:OE2	3:I:401:HOH:O	1.95	0.82
1:H:223:LEU:HD11	1:H:285:ARG:HE	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:74:ASP:OD1	3:R:403:HOH:O	1.96	0.82
1:M:57:MET:SD	3:N:414:HOH:O	2.38	0.82
1:M:197:GLU:O	3:M:404:HOH:O	1.97	0.81
1:A:28:TYR:OH	3:A:401:HOH:O	2.00	0.80
1:P:52:MET:O	3:P:403:HOH:O	2.00	0.79
1:O:216:SER:OG	3:O:402:HOH:O	2.00	0.78
1:F:184:VAL:HG13	1:F:205:PRO:HG2	1.66	0.78
1:R:48:VAL:O	3:R:404:HOH:O	2.02	0.78
1:K:170:VAL:N	3:K:401:HOH:O	2.16	0.77
1:M:184:VAL:HG13	1:M:205:PRO:HG2	1.67	0.77
1:K:184:VAL:HG13	1:K:205:PRO:HG2	1.67	0.77
1:G:184:VAL:HG13	1:G:205:PRO:HG2	1.68	0.76
1:O:184:VAL:HG13	1:O:205:PRO:HG2	1.68	0.75
1:N:64:ARG:O	3:N:401:HOH:O	2.05	0.75
1:L:184:VAL:HG13	1:L:205:PRO:HG2	1.68	0.75
1:F:63:ASP:OD2	3:F:403:HOH:O	2.05	0.74
1:I:184:VAL:HG13	1:I:205:PRO:HG2	1.68	0.73
1:J:40:LEU:O	3:J:401:HOH:O	2.05	0.73
1:E:251:THR:HG22	1:E:256:ALA:HA	1.68	0.73
1:R:62:GLN:OE1	3:R:405:HOH:O	2.05	0.73
1:I:253:ARG:NH1	3:I:404:HOH:O	2.20	0.73
1:C:125:LEU:O	1:C:127:GLU:N	2.20	0.72
1:D:249:GLU:N	3:D:402:HOH:O	2.15	0.72
1:H:86:CYS:SG	3:H:402:HOH:O	2.46	0.72
1:J:184:VAL:HG13	1:J:205:PRO:HG2	1.71	0.72
1:O:101:ILE:O	1:O:128:ARG:NH1	2.23	0.72
1:E:184:VAL:HG13	1:E:205:PRO:HG2	1.72	0.71
1:N:287:PRO:O	3:N:402:HOH:O	2.08	0.71
1:P:184:VAL:HG13	1:P:205:PRO:HG2	1.72	0.71
1:I:124:GLY:O	3:I:402:HOH:O	2.06	0.71
1:O:285:ARG:HH21	1:Q:48:VAL:HB	1.55	0.71
1:N:68:TYR:N	3:N:401:HOH:O	2.24	0.71
1:B:247:ARG:HG3	1:B:263:LEU:HD11	1.72	0.71
1:E:64:ARG:HG2	1:F:40:LEU:HD23	1.72	0.71
1:A:23:LYS:O	1:Q:138:ARG:NH1	2.24	0.71
1:H:248:ALA:N	3:H:401:HOH:O	2.24	0.71
1:Q:185:THR:OG1	3:Q:403:HOH:O	2.10	0.70
1:B:19:ASP:OD1	3:B:401:HOH:O	2.09	0.70
1:G:52:MET:HB2	1:H:274:ILE:HG23	1.73	0.70
1:Q:252:GLU:O	3:Q:402:HOH:O	2.09	0.69
1:P:227:ASP:OD1	3:P:405:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:274:ILE:HG23	1:R:52:MET:HB2	1.73	0.69
1:C:186:GLU:O	1:C:207:ARG:NH2	2.25	0.69
1:R:82:LEU:HA	3:R:410:HOH:O	1.91	0.69
1:H:184:VAL:HG13	1:H:205:PRO:HG2	1.73	0.69
1:L:63:ASP:OD1	3:L:403:HOH:O	2.11	0.68
1:R:49:PRO:O	3:R:407:HOH:O	2.11	0.68
1:G:275:ARG:N	3:G:404:HOH:O	2.25	0.68
1:M:10:GLN:OE1	3:M:405:HOH:O	2.10	0.68
1:G:247:ARG:HG3	1:G:263:LEU:HD11	1.74	0.68
1:E:247:ARG:HG3	1:E:263:LEU:HD11	1.74	0.68
1:C:247:ARG:HG3	1:C:263:LEU:HD11	1.76	0.68
1:N:288:ALA:N	3:N:404:HOH:O	2.20	0.68
1:F:253:ARG:NH1	3:F:406:HOH:O	2.27	0.67
1:M:274:ILE:HG23	1:N:52[B]:MET:HB2	1.77	0.67
1:C:220:PHE:O	3:C:402:HOH:O	2.12	0.67
1:R:97:ARG:O	3:R:408:HOH:O	2.11	0.67
1:R:211:PHE:O	3:R:409:HOH:O	2.13	0.67
1:B:75:PRO:HG2	1:B:99:ARG:HG3	1.77	0.67
1:G:80:HIS:HE2	1:G:104:THR:HG1	1.41	0.67
1:A:30:LEU:O	1:B:246:ARG:NH2	2.27	0.67
1:K:36:VAL:HB	2:L:301:SAH:HB2	1.77	0.67
1:Q:31:THR:OG1	3:Q:404:HOH:O	2.13	0.66
1:G:101:ILE:O	1:G:128:ARG:NH1	2.28	0.66
1:D:184:VAL:HG13	1:D:205:PRO:HG2	1.77	0.66
1:I:220:PHE:O	3:I:403:HOH:O	2.13	0.66
1:M:90:ARG:NH1	3:M:402:HOH:O	1.96	0.66
1:B:10:GLN:OE1	3:B:402:HOH:O	2.14	0.66
1:N:285:ARG:NH2	3:R:404:HOH:O	2.27	0.66
1:K:247:ARG:HG3	1:K:263:LEU:HD11	1.76	0.66
1:O:30:LEU:O	1:P:246:ARG:NH2	2.28	0.66
1:M:52[B]:MET:HB2	1:N:274:ILE:HG23	1.77	0.65
1:Q:275:ARG:O	3:Q:403:HOH:O	2.14	0.65
1:Q:30:LEU:O	1:R:246:ARG:NH2	2.30	0.65
1:F:101:ILE:O	1:F:128:ARG:NH1	2.29	0.65
1:F:223:LEU:HD11	1:F:285:ARG:HE	1.60	0.65
1:M:213:ASP:OD1	3:M:406:HOH:O	2.13	0.65
1:B:184:VAL:HG11	1:B:188:LEU:HD11	1.79	0.65
1:D:199:LEU:HD22	1:D:262:LEU:HD23	1.79	0.65
1:N:184:VAL:HG13	1:N:205:PRO:HG2	1.78	0.65
1:C:184:VAL:HG13	1:C:205:PRO:HG2	1.78	0.64
1:Q:184:VAL:HG13	1:Q:205:PRO:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ILE:HD12	1:J:131:PHE:HB3	1.78	0.64
1:H:87:GLY:O	3:H:402:HOH:O	2.15	0.64
1:I:42:PHE:HZ	1:I:57:MET:HB3	1.62	0.64
1:C:274:ILE:HG23	1:D:52:MET:HB2	1.80	0.63
1:G:42:PHE:HZ	1:G:57:MET:HB3	1.62	0.63
1:G:30:LEU:O	1:H:246:ARG:NH2	2.31	0.63
1:N:152:ILE:HG23	1:N:180:LEU:HD22	1.79	0.63
1:O:199:LEU:HD22	1:O:262:LEU:HD23	1.79	0.63
1:C:227:ASP:OD1	3:C:403:HOH:O	2.16	0.62
1:N:85:GLY:O	2:N:301:SAH:N	2.33	0.62
1:H:115:ALA:HA	1:H:118:ARG:HH11	1.65	0.62
1:B:48:VAL:O	1:D:285[A]:ARG:NH2	2.33	0.62
1:F:247:ARG:NH1	3:F:409:HOH:O	2.32	0.62
1:K:246:ARG:NH2	1:L:30:LEU:O	2.32	0.62
1:B:101:ILE:O	1:B:128:ARG:NH1	2.33	0.62
1:O:26:GLU:OE1	1:P:253:ARG:NH2	2.33	0.61
1:B:184:VAL:HG13	1:B:205:PRO:HG2	1.82	0.61
1:K:52:MET:HB2	1:L:274:ILE:HG23	1.82	0.61
1:A:247:ARG:HG3	1:A:263:LEU:HD11	1.81	0.61
1:C:200:TYR:O	1:C:202:ALA:N	2.33	0.61
1:H:42:PHE:HZ	1:H:57:MET:HB3	1.66	0.61
1:Q:249:GLU:N	3:Q:410:HOH:O	2.33	0.61
1:A:253:ARG:NH1	1:B:26:GLU:OE1	2.33	0.61
1:E:42:PHE:HZ	1:E:57:MET:HB3	1.65	0.61
2:B:301:SAH:N	3:B:406:HOH:O	2.21	0.61
1:H:186:GLU:O	1:H:207:ARG:NH2	2.34	0.60
1:P:247:ARG:NH2	3:P:404:HOH:O	2.08	0.60
1:J:75:PRO:HG2	1:J:99:ARG:HG3	1.82	0.60
1:H:99:ARG:O	3:H:403:HOH:O	2.15	0.59
1:O:52:MET:HB2	1:P:274:ILE:HG23	1.84	0.59
1:H:199:LEU:HD22	1:H:262:LEU:HD23	1.84	0.59
1:L:126:THR:N	3:L:410:HOH:O	2.35	0.59
1:Q:42:PHE:HZ	1:Q:57:MET:HB3	1.67	0.59
1:R:131:PHE:N	3:R:406:HOH:O	2.08	0.59
1:O:42:PHE:HZ	1:O:57:MET:HB3	1.68	0.59
1:G:49:PRO:O	3:G:403:HOH:O	2.17	0.59
1:I:223:LEU:HD11	1:I:285:ARG:HG3	1.84	0.59
1:F:247:ARG:HG3	1:F:263:LEU:HD11	1.84	0.59
1:H:233:ALA:O	1:H:237:ASN:ND2	2.35	0.59
1:K:223:LEU:HD11	1:K:285:ARG:HE	1.66	0.58
1:R:101:ILE:O	1:R:128:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:81:LEU:O	3:R:410:HOH:O	2.17	0.58
1:Q:52[B]:MET:HB2	1:R:274:ILE:HG23	1.83	0.58
1:C:64:ARG:HG2	1:D:40:LEU:HD23	1.86	0.58
1:N:59:SER:OG	3:N:403:HOH:O	2.17	0.58
1:I:101:ILE:O	1:I:128:ARG:NH1	2.36	0.58
1:J:223:LEU:HD11	1:J:285:ARG:HE	1.67	0.58
1:P:174:GLY:N	3:P:407:HOH:O	2.36	0.58
1:D:152:ILE:HG23	1:D:180:LEU:HD22	1.84	0.57
1:P:42:PHE:HZ	1:P:57:MET:HB3	1.69	0.57
1:A:184:VAL:HG13	1:A:205:PRO:HG2	1.86	0.57
1:N:199:LEU:HD22	1:N:262:LEU:HD23	1.86	0.57
1:B:174:GLY:O	1:B:285:ARG:NH1	2.38	0.57
1:C:36:VAL:HB	2:D:301:SAH:HB2	1.86	0.57
1:Q:118:ARG:NH1	3:Q:401:HOH:O	2.03	0.57
1:P:97:ARG:NH2	3:P:411:HOH:O	2.34	0.57
1:R:232:LEU:HD22	1:R:279:PHE:CD1	2.40	0.57
1:B:260:ASP:OD1	3:B:403:HOH:O	2.18	0.57
1:G:274:ILE:HG23	1:H:52:MET:HB2	1.87	0.57
1:Q:22:ASP:OD1	1:R:109:SER:OG	2.20	0.57
1:Q:52[A]:MET:HB2	1:R:274:ILE:HG23	1.85	0.57
1:R:166:GLU:OE2	1:R:169:ARG:NH2	2.31	0.57
1:Q:40:LEU:HD23	1:R:64:ARG:HG2	1.87	0.57
1:F:251:THR:HG22	1:F:256:ALA:HA	1.87	0.56
1:K:30:LEU:O	1:L:246:ARG:NH2	2.37	0.56
1:D:85:GLY:O	2:D:301:SAH:N	2.39	0.56
1:R:152:ILE:HG23	1:R:180:LEU:HD22	1.87	0.56
1:D:42:PHE:HZ	1:D:57:MET:HB3	1.70	0.56
1:L:223:LEU:HD11	1:L:285:ARG:HE	1.70	0.56
1:L:80:HIS:HE2	1:L:104:THR:HG1	1.45	0.56
1:R:188:LEU:O	1:R:192:GLU:HB2	2.05	0.56
2:O:301:SAH:H8	1:P:17:VAL:HG11	1.86	0.56
1:M:253:ARG:NH1	1:N:26:GLU:OE1	2.39	0.56
1:P:286:LYS:O	3:P:407:HOH:O	2.18	0.56
1:R:66:THR:OG1	3:R:411:HOH:O	2.18	0.56
2:K:301:SAH:HB2	1:L:36:VAL:HB	1.88	0.56
1:E:74:ASP:OD1	1:E:99:ARG:NH1	2.36	0.56
1:I:247:ARG:HG3	1:I:263:LEU:HD11	1.87	0.56
1:R:104:THR:HB	3:R:410:HOH:O	2.05	0.56
1:R:250:PHE:HE1	3:R:422:HOH:O	1.88	0.56
1:E:30:LEU:O	1:F:246:ARG:NH2	2.39	0.56
2:L:301:SAH:N	3:L:404:HOH:O	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:LEU:HD23	1:L:64:ARG:HG2	1.89	0.55
1:H:223:LEU:HD11	1:H:285:ARG:NE	2.18	0.55
1:J:144:GLU:HG2	1:J:172:LYS:HA	1.88	0.55
1:L:152:ILE:HG23	1:L:180:LEU:HD22	1.88	0.55
1:G:157:HIS:CE1	3:H:405:HOH:O	2.60	0.55
1:O:255:GLY:O	3:O:403:HOH:O	2.17	0.55
1:E:75:PRO:HG2	1:E:99:ARG:HG3	1.88	0.55
1:A:52[B]:MET:HB2	1:B:274:ILE:HG23	1.89	0.55
1:G:66:THR:HG23	1:G:91:THR:HG23	1.87	0.55
1:A:246:ARG:HD2	1:A:249:GLU:OE1	2.07	0.55
1:B:10:GLN:N	3:B:414:HOH:O	2.38	0.55
1:H:258:PHE:HA	3:H:411:HOH:O	2.07	0.54
1:K:152:ILE:HG23	1:K:180:LEU:HD22	1.88	0.54
1:A:42:PHE:HZ	1:A:57:MET:HB3	1.73	0.54
1:H:249:GLU:N	3:H:401:HOH:O	1.97	0.54
1:R:109:SER:HB3	1:R:112:GLN:HB2	1.88	0.54
1:R:91:THR:HG21	1:R:152:ILE:HD12	1.89	0.54
1:O:183:VAL:HG11	1:O:208:LEU:HD23	1.88	0.54
1:C:199:LEU:HD22	1:C:262:LEU:HD23	1.90	0.54
1:F:42:PHE:HZ	1:F:57:MET:HB3	1.73	0.54
1:G:253:ARG:NH1	1:H:26:GLU:OE1	2.35	0.54
1:M:26:GLU:OE1	1:N:253:ARG:NH1	2.41	0.54
1:Q:239:PHE:HB2	1:R:32:LEU:HD21	1.89	0.54
1:Q:32:LEU:HG	3:Q:404:HOH:O	2.07	0.54
1:A:152:ILE:HG23	1:A:180:LEU:HD22	1.90	0.54
1:F:49:PRO:O	3:F:404:HOH:O	2.18	0.53
1:M:271:GLU:OE2	1:M:275:ARG:NE	2.41	0.53
1:A:138:ARG:NH1	3:A:409:HOH:O	2.41	0.53
1:D:101:ILE:O	1:D:128:ARG:NH1	2.41	0.53
1:H:143:ASP:OD1	1:H:169:ARG:NH1	2.38	0.53
1:N:42:PHE:HZ	1:N:57:MET:HB3	1.74	0.53
1:C:115:ALA:O	1:C:118:ARG:HG2	2.08	0.53
1:H:120:ALA:HB2	1:H:131:PHE:HE2	1.74	0.53
1:H:77:ALA:HA	3:H:403:HOH:O	2.09	0.53
1:F:285:ARG:NH2	3:F:414:HOH:O	2.42	0.53
1:J:42:PHE:HZ	1:J:57:MET:HB3	1.74	0.53
1:L:42:PHE:HZ	1:L:57:MET:HB3	1.74	0.53
1:O:274:ILE:HG23	1:P:52:MET:HB2	1.91	0.52
1:R:88:THR:O	3:R:412:HOH:O	2.19	0.52
1:C:285:ARG:NH2	3:C:411:HOH:O	2.41	0.52
3:Q:404:HOH:O	1:R:239:PHE:HD1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:MET:HB2	1:F:274:ILE:HG23	1.92	0.52
1:O:271:GLU:OE2	1:O:275:ARG:NE	2.43	0.52
1:G:158:MET:O	1:G:203:ASN:ND2	2.42	0.52
1:K:271:GLU:OE2	1:K:275:ARG:NE	2.42	0.52
1:R:184:VAL:HG13	1:R:205:PRO:HG2	1.92	0.52
1:A:246:ARG:NH2	1:B:30:LEU:O	2.41	0.52
1:I:22:ASP:OD1	1:J:109:SER:OG	2.19	0.52
1:I:247:ARG:NH1	3:I:407:HOH:O	2.42	0.52
1:M:22:ASP:OD1	1:N:109:SER:OG	2.24	0.52
1:R:74:ASP:CG	3:R:403:HOH:O	2.42	0.52
1:C:93:LEU:HD22	1:C:119:LEU:HG	1.91	0.52
1:J:101:ILE:O	1:J:128:ARG:NH1	2.43	0.52
1:J:160:ARG:N	3:J:405:HOH:O	2.42	0.52
1:I:52:MET:HB2	1:J:274:ILE:HG23	1.91	0.51
1:G:246:ARG:HH21	1:G:250:PHE:HZ	1.57	0.51
1:K:71:GLU:OE1	3:K:402:HOH:O	2.19	0.51
1:Q:21:TYR:O	3:Q:406:HOH:O	2.19	0.51
1:R:42:PHE:HZ	1:R:57:MET:HB3	1.74	0.51
1:R:187:GLU:O	1:R:188:LEU:HB2	2.11	0.51
1:M:52[A]:MET:HB2	1:N:274:ILE:HG23	1.93	0.51
1:N:83:ASP:HB3	1:N:86:CYS:HB3	1.92	0.51
1:J:65:TYR:O	1:J:69:LEU:HG	2.11	0.51
1:F:143:ASP:OD1	1:F:169:ARG:NH1	2.38	0.51
1:J:166:GLU:OE2	1:J:169:ARG:NH2	2.33	0.51
1:F:138:ARG:NH1	3:I:404:HOH:O	2.44	0.51
1:A:274:ILE:HG23	1:B:52:MET:HB2	1.91	0.50
1:G:276:LYS:N	3:G:404:HOH:O	2.34	0.50
1:M:285:ARG:HH21	1:O:48:VAL:HB	1.76	0.50
1:R:246:ARG:NH1	3:R:423:HOH:O	2.43	0.50
1:Q:139:LEU:H	1:Q:166:GLU:HG2	1.76	0.50
1:G:40:LEU:HD23	1:H:64:ARG:HG2	1.93	0.50
1:C:101:ILE:O	1:C:128:ARG:NH1	2.44	0.50
1:E:152:ILE:HG23	1:E:180:LEU:HD22	1.94	0.50
1:H:74:ASP:OD1	1:H:99:ARG:NH1	2.38	0.50
1:R:229:SER:HA	1:R:279:PHE:HB3	1.93	0.50
1:D:113:ILE:O	1:D:117:ASN:ND2	2.44	0.50
1:I:274:ILE:HG23	1:J:52:MET:HB2	1.93	0.50
1:R:19:ASP:HA	3:R:402:HOH:O	2.10	0.50
1:D:188:LEU:N	3:D:408:HOH:O	2.36	0.50
1:M:29:HIS:HA	1:M:33:GLY:O	2.11	0.50
1:O:152:ILE:HG23	1:O:180:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:LEU:HD22	1:K:262:LEU:HD23	1.94	0.49
1:L:85:GLY:O	2:L:301:SAH:N	2.44	0.49
1:E:83:ASP:OD2	3:E:401:HOH:O	2.18	0.49
1:G:152:ILE:HG23	1:G:180:LEU:HD22	1.94	0.49
1:H:87:GLY:N	3:H:402:HOH:O	2.45	0.49
1:I:246:ARG:NH2	1:J:30:LEU:O	2.46	0.49
1:M:274:ILE:HG23	1:N:52[A]:MET:HB2	1.94	0.49
1:R:73:LEU:HB2	1:R:178:LEU:HD22	1.95	0.49
1:F:139:LEU:H	1:F:166:GLU:HG2	1.77	0.49
1:M:68:TYR:OH	3:M:407:HOH:O	2.14	0.49
2:M:301:SAH:HB2	1:N:36:VAL:HB	1.95	0.49
1:R:194:ALA:O	1:R:198:THR:OG1	2.28	0.49
1:R:242:GLY:HA2	3:R:441:HOH:O	2.12	0.49
1:K:223:LEU:HD11	1:K:285:ARG:NE	2.27	0.49
1:O:164:LEU:HD12	1:O:214:ILE:HG22	1.95	0.49
1:R:170:VAL:HG23	3:R:416:HOH:O	2.11	0.49
1:H:251:THR:HG22	1:H:256:ALA:HA	1.94	0.49
1:B:49:PRO:O	1:D:285[B]:ARG:NH1	2.40	0.48
1:E:42:PHE:CZ	1:E:57:MET:HB3	2.47	0.48
1:K:67:ASP:OD2	3:K:403:HOH:O	2.20	0.48
1:L:223:LEU:HD11	1:L:285:ARG:NE	2.27	0.48
1:P:164:LEU:HD12	1:P:214:ILE:HG22	1.94	0.48
1:B:151:ALA:O	3:B:404:HOH:O	2.19	0.48
1:E:101:ILE:O	1:E:128:ARG:NH1	2.46	0.48
1:L:110:LYS:HD3	3:L:413:HOH:O	2.13	0.48
1:N:223:LEU:HD11	1:N:285:ARG:NE	2.28	0.48
1:O:104:THR:HA	1:O:130:THR:O	2.13	0.48
2:C:301:SAH:HB2	1:D:36:VAL:HB	1.95	0.48
1:M:75:PRO:HG2	1:M:99:ARG:HG3	1.96	0.48
1:G:188:LEU:N	3:G:407:HOH:O	2.38	0.48
1:E:36:VAL:HB	2:F:301:SAH:HB2	1.94	0.48
1:A:101:ILE:O	1:A:128:ARG:NH1	2.47	0.48
1:M:66:THR:HG23	1:M:91:THR:HG23	1.96	0.48
1:O:253:ARG:HH11	1:P:30:LEU:HD11	1.79	0.48
1:P:85:GLY:O	2:P:301:SAH:N	2.47	0.48
2:E:301:SAH:HB2	1:F:36:VAL:HB	1.95	0.48
1:R:183:VAL:HG11	1:R:208:LEU:HD23	1.96	0.48
1:R:85:GLY:O	2:R:301:SAH:N	2.47	0.48
1:R:88:THR:HB	3:R:412:HOH:O	2.13	0.48
1:M:246:ARG:NH2	1:N:30:LEU:O	2.47	0.47
1:R:98:GLN:HA	3:R:440:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD23	1:B:64:ARG:HG2	1.97	0.47
1:J:144:GLU:HG2	1:J:173:PRO:HD3	1.97	0.47
1:J:74:ASP:OD1	1:J:99:ARG:NH1	2.43	0.47
1:C:138:ARG:NH1	3:C:414:HOH:O	2.47	0.47
1:C:40:LEU:HD23	1:D:64:ARG:HG2	1.97	0.47
1:J:107:ALA:HA	2:J:301:SAH:N3	2.30	0.47
1:B:246:ARG:HD2	1:B:249:GLU:OE1	2.15	0.47
1:P:247:ARG:HG3	1:P:263:LEU:HD11	1.95	0.47
2:B:302:SAH:N	2:B:302:SAH:SD	2.87	0.47
1:H:197:GLU:HA	1:H:201:ALA:HA	1.97	0.47
1:M:285:ARG:NH2	1:O:48:VAL:O	2.47	0.47
1:R:168:TRP:NE1	1:R:219:GLY:O	2.48	0.47
1:D:223:LEU:HD11	1:D:285[B]:ARG:HD3	1.96	0.47
1:M:247:ARG:HG3	1:M:263:LEU:HD11	1.96	0.47
1:A:139:LEU:H	1:A:166:GLU:HG2	1.80	0.47
1:B:223:LEU:HD11	1:B:285:ARG:HE	1.78	0.47
1:K:246:ARG:HD2	1:K:249:GLU:OE1	2.14	0.47
1:L:75:PRO:HG2	1:L:99:ARG:HG3	1.96	0.47
1:N:223:LEU:HD11	1:N:285:ARG:HE	1.79	0.47
1:P:75:PRO:HG2	1:P:99:ARG:HG3	1.97	0.47
1:B:42:PHE:HZ	1:B:57:MET:HB3	1.79	0.47
1:D:50:GLN:NE2	1:F:285:ARG:HH12	2.13	0.47
1:M:36:VAL:HB	2:N:301:SAH:HB2	1.96	0.47
1:G:201:ALA:HB1	1:H:17:VAL:HG22	1.97	0.47
1:K:171:LEU:O	1:K:286:LYS:NZ	2.37	0.47
1:O:40:LEU:HD23	1:P:64:ARG:HG2	1.97	0.47
1:K:42:PHE:HZ	1:K:57:MET:HB3	1.80	0.46
1:R:91:THR:HG21	1:R:152:ILE:CD1	2.45	0.46
1:E:139:LEU:H	1:E:166:GLU:HG2	1.81	0.46
1:A:156:CYS:HA	1:A:160:ARG:NH2	2.29	0.46
1:A:48:VAL:O	1:E:285:ARG:NH2	2.48	0.46
1:C:138:ARG:CZ	3:C:414:HOH:O	2.63	0.46
2:O:301:SAH:HB2	1:P:36:VAL:HB	1.98	0.46
1:R:239:PHE:HE2	1:R:266:LEU:HD21	1.80	0.46
1:C:246:ARG:HH22	1:D:30:LEU:HB3	1.81	0.46
1:M:48:VAL:HB	1:Q:285:ARG:HH21	1.81	0.46
1:R:82:LEU:HB3	1:R:149:ALA:HB2	1.96	0.46
1:C:94:LYS:NZ	3:C:409:HOH:O	2.36	0.46
1:I:237:ASN:HD22	1:J:54:LEU:HD13	1.80	0.46
1:E:19:ASP:HB3	1:E:23:LYS:NZ	2.30	0.46
1:H:152:ILE:HG23	1:H:180:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:114:ALA:O	1:R:118:ARG:HG3	2.16	0.46
1:A:107:ALA:O	1:A:133:VAL:HA	2.16	0.46
1:B:29:HIS:HA	1:B:33:GLY:O	2.16	0.46
1:G:135:ASP:OD1	1:G:136:ALA:N	2.49	0.46
1:I:143:ASP:OD1	1:I:143:ASP:N	2.49	0.46
1:K:186:GLU:HB3	1:K:187:GLU:H	1.60	0.46
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.84	0.45
1:A:23:LYS:HG2	1:Q:138:ARG:HH22	1.81	0.45
1:E:239:PHE:HB2	1:F:32:LEU:HD21	1.98	0.45
1:M:203:ASN:OD1	1:N:11:GLN:N	2.47	0.45
1:M:25:GLY:N	3:M:401:HOH:O	1.94	0.45
1:R:188:LEU:O	1:R:189:THR:OG1	2.28	0.45
1:D:176:ASP:OD1	1:D:285[B]:ARG:HG3	2.17	0.45
1:R:232:LEU:HD22	1:R:279:PHE:HD1	1.81	0.45
1:C:65:TYR:OH	1:C:180:LEU:HD23	2.16	0.45
1:R:139:LEU:H	1:R:166:GLU:HG2	1.81	0.45
1:O:258:PHE:N	3:O:403:HOH:O	2.49	0.45
1:O:143:ASP:N	1:O:143:ASP:OD1	2.50	0.45
1:R:150:TRP:HB3	1:R:178:LEU:HB3	1.98	0.45
1:R:189:THR:O	1:R:193:THR:HG23	2.17	0.45
1:D:75:PRO:HG2	1:D:99:ARG:HG3	1.99	0.45
1:M:17:VAL:HG11	2:N:301:SAH:H8	1.98	0.45
1:B:213:ASP:OD1	3:B:405:HOH:O	2.21	0.45
1:J:223:LEU:HD11	1:J:285:ARG:NE	2.31	0.45
1:R:114:ALA:HB3	1:R:118:ARG:HH21	1.82	0.45
1:C:215:VAL:HG12	3:C:402:HOH:O	2.16	0.45
1:R:62:GLN:O	1:R:65:TYR:HB3	2.17	0.45
1:C:17:VAL:HG11	2:D:301:SAH:H8	1.99	0.45
1:I:91:THR:HG22	1:I:150:TRP:CZ2	2.52	0.45
1:F:271:GLU:OE2	1:F:275:ARG:NE	2.50	0.44
1:H:63:ASP:CG	1:H:90:ARG:HH21	2.19	0.44
1:M:84:ILE:O	3:M:408:HOH:O	2.20	0.44
1:P:66:THR:OG1	3:P:406:HOH:O	2.10	0.44
1:R:103:VAL:O	3:R:413:HOH:O	2.21	0.44
1:C:66:THR:HG23	1:C:91:THR:HG23	1.98	0.44
1:L:29:HIS:HA	1:L:33:GLY:O	2.16	0.44
1:O:51:ASP:H	1:O:56:THR:HG21	1.82	0.44
1:R:164:LEU:HD13	1:R:215:VAL:HG23	1.98	0.44
1:C:223:LEU:HD11	1:C:285:ARG:HB2	1.98	0.44
1:C:42:PHE:HZ	1:C:57:MET:HB3	1.82	0.44
1:D:134:ALA:HB1	1:D:140:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:TRP:CE2	1:E:286:LYS:HG3	2.52	0.44
1:F:223:LEU:HD11	1:F:285:ARG:NE	2.30	0.44
1:L:174:GLY:O	1:L:285:ARG:NH1	2.50	0.44
1:N:171:LEU:O	1:N:286:LYS:NZ	2.35	0.44
1:A:65:TYR:OH	1:A:180:LEU:HD23	2.17	0.44
1:J:66:THR:HG23	1:J:91:THR:HG23	2.00	0.44
1:Q:199:LEU:HD22	1:Q:262:LEU:HD23	1.99	0.44
1:H:87:GLY:O	1:H:112:GLN:HB3	2.17	0.44
1:R:215:VAL:O	1:R:218:ALA:HB3	2.18	0.44
1:E:66:THR:HG23	1:E:91:THR:HG23	2.00	0.44
1:L:188:LEU:N	3:L:412:HOH:O	2.50	0.44
1:G:186:GLU:HB3	1:G:187:GLU:H	1.64	0.44
1:O:206:PRO:HG2	1:O:211:PHE:HB2	1.98	0.44
1:R:29:HIS:HA	1:R:33:GLY:O	2.18	0.44
1:R:93:LEU:O	1:R:97:ARG:HG3	2.17	0.44
1:B:199:LEU:HD22	1:B:262:LEU:HD23	2.00	0.44
1:Q:37:HIS:O	1:R:62:GLN:NE2	2.39	0.44
1:D:181:GLU:HG3	1:D:182:SER:O	2.18	0.43
1:I:198:THR:OG1	3:I:405:HOH:O	2.21	0.43
1:K:112:GLN:OE1	2:K:301:SAH:O3'	2.24	0.43
1:P:278:ARG:NH2	3:P:413:HOH:O	2.42	0.43
1:P:101:ILE:O	1:P:128:ARG:NH1	2.51	0.43
1:Q:223:LEU:HD11	1:Q:285:ARG:HE	1.83	0.43
1:Q:278:ARG:NH1	3:Q:413:HOH:O	2.48	0.43
1:B:253:ARG:O	1:Q:138:ARG:HD3	2.18	0.43
1:M:21:TYR:HB2	1:N:109:SER:HB2	2.01	0.43
1:O:160:ARG:CZ	1:O:206:PRO:HD3	2.49	0.43
1:Q:22:ASP:HA	1:R:111:GLU:HB3	2.01	0.43
1:R:207:ARG:O	1:R:211:PHE:N	2.42	0.43
1:R:215:VAL:HA	1:R:218:ALA:HB3	2.00	0.43
1:G:156:CYS:O	1:G:203:ASN:HB2	2.18	0.43
1:K:158:MET:O	1:K:203:ASN:ND2	2.52	0.43
1:M:114:ALA:O	1:M:118:ARG:HG3	2.19	0.43
1:Q:288:ALA:N	3:Q:405:HOH:O	2.19	0.43
1:B:188:LEU:H	1:B:188:LEU:HD12	1.84	0.43
1:G:186:GLU:O	1:G:207:ARG:NH2	2.52	0.43
1:P:287:PRO:C	3:P:407:HOH:O	2.57	0.43
1:P:80:HIS:NE2	1:P:104:THR:OG1	2.38	0.43
1:N:225:LEU:O	1:Q:224:SER:HA	2.19	0.43
1:A:48:VAL:HB	1:E:285:ARG:HH21	1.84	0.43
1:C:157:HIS:ND1	1:C:201:ALA:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:ALA:HA	1:G:266:LEU:HD13	1.99	0.43
1:L:226:LYS:NZ	3:L:405:HOH:O	2.21	0.43
1:A:164:LEU:HD12	1:A:214:ILE:HG22	2.01	0.43
1:A:37:HIS:HD2	2:B:301:SAH:OXT	2.01	0.43
1:G:208:LEU:HA	1:G:208:LEU:HD22	1.91	0.43
1:Q:31:THR:HG22	1:R:246:ARG:HH21	1.84	0.43
1:B:143:ASP:N	1:B:143:ASP:OD1	2.50	0.42
1:R:53:GLU:O	1:R:57:MET:HG3	2.18	0.42
2:G:301:SAH:HB2	1:H:36:VAL:HB	1.99	0.42
1:H:271:GLU:OE2	1:H:275:ARG:NE	2.52	0.42
1:J:144:GLU:HG3	3:J:404:HOH:O	2.18	0.42
1:N:286:LYS:HA	1:N:287:PRO:HD3	1.93	0.42
1:P:168:TRP:CZ2	1:P:286:LYS:HE3	2.53	0.42
1:O:246:ARG:NH2	1:P:30:LEU:O	2.52	0.42
1:F:66:THR:HG23	1:F:91:THR:HG23	2.01	0.42
1:J:150:TRP:HB3	1:J:178:LEU:HB3	2.02	0.42
1:J:43:PRO:HG2	1:J:46:ALA:HB2	2.01	0.42
1:K:170:VAL:HG22	3:K:401:HOH:O	2.18	0.42
1:A:93:LEU:HD12	1:A:125:LEU:HD12	2.01	0.42
1:A:240:ALA:HA	1:A:266:LEU:HD13	2.02	0.42
2:A:301:SAH:HB2	1:B:36:VAL:HB	2.01	0.42
1:I:66:THR:HG23	1:I:91:THR:HG23	2.01	0.42
1:M:159:ASP:HB2	1:N:10:GLN:CD	2.40	0.42
1:Q:29:HIS:HA	1:Q:33:GLY:O	2.20	0.42
1:R:215:VAL:HG13	1:R:220:PHE:HB2	2.00	0.42
1:H:166:GLU:OE2	1:H:169:ARG:NH2	2.39	0.42
1:K:143:ASP:OD1	1:K:143:ASP:N	2.50	0.42
1:Q:11:GLN:OE1	1:R:197:GLU:HB2	2.20	0.42
1:R:181:GLU:HG2	1:R:211:PHE:CE1	2.55	0.42
1:E:51:ASP:H	1:E:56:THR:HG21	1.85	0.42
1:G:274:ILE:HG12	1:H:52:MET:HB2	2.01	0.42
1:H:75:PRO:HG2	1:H:99:ARG:HG3	2.01	0.42
1:P:153:GLU:N	3:P:402:HOH:O	2.53	0.42
1:R:171:LEU:HG	3:R:416:HOH:O	2.20	0.42
1:R:192:GLU:OE1	1:R:276:LYS:NZ	2.36	0.42
1:A:36:VAL:HB	2:B:301:SAH:HB2	2.02	0.42
1:C:211:PHE:O	1:C:215:VAL:HG23	2.19	0.42
1:C:271:GLU:OE2	1:C:275:ARG:NE	2.53	0.42
1:C:29:HIS:HA	1:C:33:GLY:O	2.19	0.42
1:I:198:THR:CB	3:I:405:HOH:O	2.68	0.42
1:J:107:ALA:HB1	2:J:301:SAH:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:THR:O	1:C:193:THR:HG23	2.20	0.42
1:G:271:GLU:OE2	1:G:275:ARG:NE	2.52	0.42
1:I:237:ASN:ND2	1:J:54:LEU:HD13	2.34	0.42
1:L:186:GLU:HB3	1:L:187:GLU:H	1.69	0.42
1:G:17:VAL:HG21	1:H:157:HIS:HB3	2.02	0.41
1:I:240:ALA:HA	1:I:266:LEU:HD13	2.02	0.41
1:I:29:HIS:HA	1:I:33:GLY:O	2.20	0.41
1:N:160:ARG:CZ	1:N:206:PRO:HD3	2.50	0.41
1:O:174:GLY:HA3	1:Q:50:GLN:OE1	2.20	0.41
1:F:156:CYS:HA	1:F:160:ARG:NH2	2.35	0.41
1:D:50:GLN:HE22	1:F:285:ARG:HH12	1.68	0.41
1:L:181:GLU:HG3	1:L:182:SER:O	2.20	0.41
1:P:150:TRP:O	1:P:150:TRP:HD1	2.02	0.41
1:R:51:ASP:H	1:R:56:THR:HG21	1.85	0.41
1:G:75:PRO:HG2	1:G:99:ARG:HG3	2.03	0.41
1:P:158:MET:HG2	2:P:301:SAH:N6	2.36	0.41
1:C:160:ARG:CZ	1:C:206:PRO:HD3	2.51	0.41
1:E:273:LEU:HD12	1:E:277:THR:OG1	2.21	0.41
1:F:195:LEU:HA	1:F:195:LEU:HD23	1.94	0.41
1:O:285:ARG:NH2	1:Q:48:VAL:O	2.53	0.41
1:E:241:LEU:HB2	1:F:241:LEU:HD13	2.02	0.41
1:Q:37:HIS:HE1	1:R:62:GLN:O	2.02	0.41
1:A:66:THR:HG23	1:A:91:THR:HG23	2.01	0.41
1:H:42:PHE:CZ	1:H:57:MET:HB3	2.52	0.41
1:J:113:ILE:HD13	1:J:113:ILE:HA	1.76	0.41
1:J:208:LEU:HA	1:J:208:LEU:HD22	1.84	0.41
2:K:301:SAH:H8	1:L:17:VAL:HG11	2.03	0.41
1:K:109:SER:OG	1:L:22:ASP:OD1	2.26	0.41
1:M:139:LEU:H	1:M:166:GLU:HG2	1.86	0.41
1:E:29:HIS:HA	1:E:33:GLY:O	2.21	0.41
1:J:29:HIS:HA	1:J:33:GLY:O	2.21	0.41
1:O:192:GLU:OE1	1:O:276:LYS:NZ	2.41	0.41
1:A:54:LEU:HD13	1:B:237:ASN:ND2	2.36	0.41
1:K:152:ILE:HG23	1:K:180:LEU:CD2	2.51	0.41
1:M:52[B]:MET:HE1	1:N:233:ALA:HB2	2.03	0.41
1:R:215:VAL:HA	1:R:218:ALA:CB	2.49	0.41
1:O:240:ALA:HA	1:O:266:LEU:HD13	2.02	0.41
1:J:85:GLY:O	2:J:301:SAH:N	2.54	0.41
1:G:223:LEU:HD11	1:G:285:ARG:HE	1.86	0.40
1:D:29:HIS:HA	1:D:33:GLY:O	2.22	0.40
1:H:208:LEU:HD22	1:H:208:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:HD23	1:F:64:ARG:HG2	2.03	0.40
1:L:197:GLU:HA	1:L:201:ALA:HA	2.02	0.40
1:N:29:HIS:HA	1:N:33:GLY:O	2.21	0.40
1:G:251:THR:HG22	1:G:256:ALA:HA	2.04	0.40
1:H:115:ALA:HA	1:H:118:ARG:HD2	2.03	0.40
1:H:43:PRO:HG2	1:H:46:ALA:HB2	2.03	0.40
1:M:17:VAL:HG21	1:N:157:HIS:HB3	2.03	0.40
1:O:66:THR:HG23	1:O:91:THR:HG23	2.03	0.40
1:R:136:ALA:HB3	1:R:158:MET:SD	2.60	0.40
1:B:138:ARG:HD2	3:B:473:HOH:O	2.21	0.40
1:F:24:PHE:O	1:F:27:VAL:HG12	2.21	0.40
1:H:188:LEU:N	3:H:406:HOH:O	2.46	0.40
1:O:251:THR:HA	1:O:255:GLY:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:126:THR:OG1	1:R:126:THR:OG1[2_555]	2.14	0.06

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	281/297 (95%)	275 (98%)	4 (1%)	2 (1%)	26	46
1	B	279/297 (94%)	275 (99%)	4 (1%)	0	100	100
1	C	278/297 (94%)	269 (97%)	5 (2%)	4 (1%)	14	24
1	D	279/297 (94%)	275 (99%)	3 (1%)	1 (0%)	39	61
1	E	277/297 (93%)	275 (99%)	2 (1%)	0	100	100
1	F	278/297 (94%)	274 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	278/297 (94%)	267 (96%)	9 (3%)	2 (1%)	26	46
1	H	277/297 (93%)	269 (97%)	7 (2%)	1 (0%)	39	61
1	I	279/297 (94%)	275 (99%)	3 (1%)	1 (0%)	39	61
1	J	279/297 (94%)	273 (98%)	6 (2%)	0	100	100
1	K	279/297 (94%)	271 (97%)	7 (2%)	1 (0%)	39	61
1	L	278/297 (94%)	272 (98%)	5 (2%)	1 (0%)	39	61
1	M	281/297 (95%)	273 (97%)	7 (2%)	1 (0%)	39	61
1	N	281/297 (95%)	273 (97%)	6 (2%)	2 (1%)	26	46
1	O	278/297 (94%)	270 (97%)	7 (2%)	1 (0%)	39	61
1	P	278/297 (94%)	271 (98%)	5 (2%)	2 (1%)	26	46
1	Q	281/297 (95%)	274 (98%)	6 (2%)	1 (0%)	39	61
1	R	280/297 (94%)	269 (96%)	9 (3%)	2 (1%)	26	46
All	All	5021/5346 (94%)	4900 (98%)	99 (2%)	22 (0%)	39	61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	THR
1	C	201	ALA
1	K	188	LEU
1	O	188	LEU
1	P	188	LEU
1	Q	188	LEU
1	R	188	LEU
1	A	10	GLN
1	A	188	LEU
1	C	187	GLU
1	C	188	LEU
1	D	188	LEU
1	G	188	LEU
1	H	188	LEU
1	I	188	LEU
1	L	188	LEU
1	M	188	LEU
1	N	10	GLN
1	N	188	LEU
1	G	203	ASN
1	P	253	ARG

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Mol	Chain	Res	Type
1	R	189	THR

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	226/239 (95%)	222 (98%)	4 (2%)	66	88
1	B	224/239 (94%)	214 (96%)	10 (4%)	34	59
1	C	223/239 (93%)	216 (97%)	7 (3%)	47	75
1	D	224/239 (94%)	216 (96%)	8 (4%)	42	69
1	E	222/239 (93%)	217 (98%)	5 (2%)	58	83
1	F	223/239 (93%)	219 (98%)	4 (2%)	66	88
1	G	223/239 (93%)	215 (96%)	8 (4%)	42	69
1	H	222/239 (93%)	214 (96%)	8 (4%)	42	69
1	I	224/239 (94%)	217 (97%)	7 (3%)	47	75
1	J	224/239 (94%)	219 (98%)	5 (2%)	60	84
1	K	224/239 (94%)	217 (97%)	7 (3%)	47	75
1	L	223/239 (93%)	216 (97%)	7 (3%)	47	75
1	M	226/239 (95%)	221 (98%)	5 (2%)	60	84
1	N	226/239 (95%)	223 (99%)	3 (1%)	76	92
1	O	223/239 (93%)	214 (96%)	9 (4%)	38	64
1	P	223/239 (93%)	219 (98%)	4 (2%)	66	88
1	Q	226/239 (95%)	222 (98%)	4 (2%)	66	88
1	R	225/239 (94%)	217 (96%)	8 (4%)	42	69
All	All	4031/4302 (94%)	3918 (97%)	113 (3%)	51	78

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	TRP

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Mol	Chain	Res	Type
1	A	186	GLU
1	A	208	LEU
1	A	289	VAL
1	B	45	ASP
1	B	150	TRP
1	B	158	MET
1	B	186	GLU
1	B	188	LEU
1	B	190	GLU
1	B	208	LEU
1	B	247	ARG
1	B	253	ARG
1	B	289	VAL
1	C	26	GLU
1	C	126	THR
1	C	150	TRP
1	C	186	GLU
1	C	200	TYR
1	C	208	LEU
1	C	247	ARG
1	D	10	GLN
1	D	150	TRP
1	D	158	MET
1	D	183	VAL
1	D	186	GLU
1	D	253	ARG
1	D	285[A]	ARG
1	D	285[B]	ARG
1	E	150	TRP
1	E	183	VAL
1	E	247	ARG
1	E	251	THR
1	E	253	ARG
1	F	26	GLU
1	F	150	TRP
1	F	186	GLU
1	F	208	LEU
1	G	36	VAL
1	G	150	TRP
1	G	186	GLU
1	G	208	LEU
1	G	247	ARG

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Mol	Chain	Res	Type
1	G	251	THR
1	G	252	GLU
1	G	253	ARG
1	H	26	GLU
1	H	118	ARG
1	H	150	TRP
1	H	186	GLU
1	H	208	LEU
1	H	247	ARG
1	H	251	THR
1	H	253	ARG
1	I	143	ASP
1	I	150	TRP
1	I	186	GLU
1	I	208	LEU
1	I	253	ARG
1	I	285	ARG
1	I	289	VAL
1	J	26	GLU
1	J	150	TRP
1	J	186	GLU
1	J	208	LEU
1	J	253	ARG
1	K	10	GLN
1	K	143	ASP
1	K	150	TRP
1	K	186	GLU
1	K	208	LEU
1	K	252	GLU
1	K	253	ARG
1	L	26	GLU
1	L	51	ASP
1	L	63	ASP
1	L	150	TRP
1	L	186	GLU
1	L	208	LEU
1	L	253	ARG
1	M	36	VAL
1	M	150	TRP
1	M	186	GLU
1	M	253	ARG
1	M	289	VAL

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Mol	Chain	Res	Type
1	N	150	TRP
1	N	186	GLU
1	N	253	ARG
1	O	10	GLN
1	O	26	GLU
1	O	36	VAL
1	O	104	THR
1	O	143	ASP
1	O	150	TRP
1	O	186	GLU
1	O	208	LEU
1	O	289	VAL
1	P	15	ASP
1	P	150	TRP
1	P	186	GLU
1	P	247	ARG
1	Q	150	TRP
1	Q	186	GLU
1	Q	253	ARG
1	Q	289	VAL
1	R	126	THR
1	R	150	TRP
1	R	186	GLU
1	R	188	LEU
1	R	190	GLU
1	R	195	LEU
1	R	208	LEU
1	R	289	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	231	ASN

5.3.3 RNA ⓘ

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](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SAH	A	301	-	22,28,28	1.06	2 (9%)	18,40,40	2.97	3 (16%)
2	SAH	B	301	-	22,28,28	1.06	2 (9%)	18,40,40	3.05	3 (16%)
2	SAH	B	302	-	22,28,28	1.07	2 (9%)	18,40,40	3.03	5 (27%)
2	SAH	C	301	-	22,28,28	1.04	2 (9%)	18,40,40	3.04	2 (11%)
2	SAH	D	301	-	22,28,28	1.09	2 (9%)	18,40,40	2.90	2 (11%)
2	SAH	E	301	-	22,28,28	1.08	2 (9%)	18,40,40	2.91	3 (16%)
2	SAH	F	301	-	22,28,28	1.11	2 (9%)	18,40,40	2.85	3 (16%)
2	SAH	G	301	-	22,28,28	1.08	2 (9%)	18,40,40	2.86	2 (11%)
2	SAH	H	301	-	22,28,28	1.14	2 (9%)	18,40,40	3.26	4 (22%)
2	SAH	I	301	-	22,28,28	1.04	2 (9%)	18,40,40	2.98	3 (16%)
2	SAH	J	301	-	22,28,28	1.08	2 (9%)	18,40,40	2.93	2 (11%)
2	SAH	K	301	-	22,28,28	1.05	2 (9%)	18,40,40	2.99	2 (11%)
2	SAH	L	301	-	22,28,28	1.07	2 (9%)	18,40,40	2.86	2 (11%)
2	SAH	M	301	-	22,28,28	1.07	2 (9%)	18,40,40	2.85	2 (11%)
2	SAH	N	301	-	22,28,28	1.07	2 (9%)	18,40,40	2.93	2 (11%)
2	SAH	O	301	-	22,28,28	1.07	2 (9%)	18,40,40	2.88	3 (16%)
2	SAH	P	301	-	22,28,28	1.08	2 (9%)	18,40,40	2.77	2 (11%)
2	SAH	Q	301	-	22,28,28	1.04	2 (9%)	18,40,40	2.91	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	R	301	-	22,28,28	1.07	2 (9%)	18,40,40	2.96	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	301	-	-	0/7/31/31	0/3/3/3
2	SAH	B	301	-	-	0/7/31/31	0/3/3/3
2	SAH	B	302	-	-	0/7/31/31	0/3/3/3
2	SAH	C	301	-	-	0/7/31/31	0/3/3/3
2	SAH	D	301	-	-	0/7/31/31	0/3/3/3
2	SAH	E	301	-	-	0/7/31/31	0/3/3/3
2	SAH	F	301	-	-	0/7/31/31	0/3/3/3
2	SAH	G	301	-	-	0/7/31/31	0/3/3/3
2	SAH	H	301	-	-	0/7/31/31	0/3/3/3
2	SAH	I	301	-	-	0/7/31/31	0/3/3/3
2	SAH	J	301	-	-	0/7/31/31	0/3/3/3
2	SAH	K	301	-	-	0/7/31/31	0/3/3/3
2	SAH	L	301	-	-	0/7/31/31	0/3/3/3
2	SAH	M	301	-	-	0/7/31/31	0/3/3/3
2	SAH	N	301	-	-	0/7/31/31	0/3/3/3
2	SAH	O	301	-	-	0/7/31/31	0/3/3/3
2	SAH	P	301	-	-	0/7/31/31	0/3/3/3
2	SAH	Q	301	-	-	0/7/31/31	0/3/3/3
2	SAH	R	301	-	-	0/7/31/31	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	301	SAH	C2-N1	2.25	1.38	1.33
2	C	301	SAH	C2-N1	2.29	1.38	1.33
2	J	301	SAH	C2-N1	2.31	1.38	1.33
2	F	301	SAH	C2-N1	2.31	1.38	1.33
2	M	301	SAH	C2-N1	2.32	1.38	1.33
2	O	301	SAH	C2-N1	2.33	1.38	1.33
2	P	301	SAH	C2-N1	2.35	1.38	1.33
2	I	301	SAH	C2-N1	2.36	1.38	1.33
2	K	301	SAH	C2-N1	2.37	1.38	1.33
2	B	301	SAH	C2-N1	2.38	1.38	1.33
2	G	301	SAH	C2-N1	2.40	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	SAH	C2-N1	2.41	1.38	1.33
2	B	302	SAH	C2-N1	2.42	1.38	1.33
2	D	301	SAH	C2-N1	2.43	1.38	1.33
2	L	301	SAH	C2-N1	2.43	1.38	1.33
2	E	301	SAH	C2-N1	2.43	1.38	1.33
2	R	301	SAH	C2-N1	2.43	1.38	1.33
2	H	301	SAH	C2-N1	2.45	1.38	1.33
2	A	301	SAH	C2-N1	2.46	1.38	1.33
2	I	301	SAH	C2-N3	3.29	1.38	1.32
2	Q	301	SAH	C2-N3	3.30	1.38	1.32
2	B	301	SAH	C2-N3	3.32	1.38	1.32
2	A	301	SAH	C2-N3	3.37	1.38	1.32
2	E	301	SAH	C2-N3	3.42	1.38	1.32
2	C	301	SAH	C2-N3	3.44	1.38	1.32
2	O	301	SAH	C2-N3	3.48	1.38	1.32
2	K	301	SAH	C2-N3	3.48	1.38	1.32
2	G	301	SAH	C2-N3	3.52	1.38	1.32
2	R	301	SAH	C2-N3	3.52	1.38	1.32
2	N	301	SAH	C2-N3	3.54	1.38	1.32
2	L	301	SAH	C2-N3	3.55	1.38	1.32
2	J	301	SAH	C2-N3	3.56	1.38	1.32
2	P	301	SAH	C2-N3	3.58	1.38	1.32
2	M	301	SAH	C2-N3	3.58	1.38	1.32
2	D	301	SAH	C2-N3	3.59	1.38	1.32
2	H	301	SAH	C2-N3	3.64	1.38	1.32
2	B	302	SAH	C2-N3	3.66	1.38	1.32
2	F	301	SAH	C2-N3	3.67	1.38	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SAH	N3-C2-N1	-11.77	119.62	128.87
2	I	301	SAH	N3-C2-N1	-11.60	119.76	128.87
2	B	301	SAH	N3-C2-N1	-11.59	119.77	128.87
2	A	301	SAH	N3-C2-N1	-11.52	119.82	128.87
2	K	301	SAH	N3-C2-N1	-11.43	119.90	128.87
2	N	301	SAH	N3-C2-N1	-11.38	119.93	128.87
2	E	301	SAH	N3-C2-N1	-11.37	119.94	128.87
2	R	301	SAH	N3-C2-N1	-11.37	119.94	128.87
2	Q	301	SAH	N3-C2-N1	-11.25	120.03	128.87
2	J	301	SAH	N3-C2-N1	-11.25	120.03	128.87
2	H	301	SAH	N3-C2-N1	-11.13	120.13	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	301	SAH	N3-C2-N1	-11.11	120.15	128.87
2	D	301	SAH	N3-C2-N1	-11.10	120.15	128.87
2	G	301	SAH	N3-C2-N1	-11.03	120.21	128.87
2	O	301	SAH	N3-C2-N1	-10.90	120.31	128.87
2	F	301	SAH	N3-C2-N1	-10.81	120.38	128.87
2	L	301	SAH	N3-C2-N1	-10.77	120.41	128.87
2	B	302	SAH	N3-C2-N1	-10.74	120.43	128.87
2	P	301	SAH	N3-C2-N1	-10.60	120.54	128.87
2	L	301	SAH	C5'-SD-CG	-4.34	89.25	102.42
2	B	301	SAH	C5'-SD-CG	-4.21	89.65	102.42
2	H	301	SAH	C5'-SD-CG	-4.19	89.69	102.42
2	K	301	SAH	C5'-SD-CG	-4.13	89.88	102.42
2	D	301	SAH	C5'-SD-CG	-4.07	90.05	102.42
2	O	301	SAH	C5'-SD-CG	-4.00	90.28	102.42
2	C	301	SAH	C5'-SD-CG	-3.98	90.34	102.42
2	J	301	SAH	C5'-SD-CG	-3.95	90.42	102.42
2	B	302	SAH	C4'-O4'-C1'	-3.93	105.48	109.64
2	R	301	SAH	C5'-SD-CG	-3.89	90.61	102.42
2	F	301	SAH	C5'-SD-CG	-3.89	90.62	102.42
2	G	301	SAH	C5'-SD-CG	-3.83	90.77	102.42
2	Q	301	SAH	C5'-SD-CG	-3.73	91.08	102.42
2	M	301	SAH	C5'-SD-CG	-3.70	91.18	102.42
2	N	301	SAH	C5'-SD-CG	-3.70	91.20	102.42
2	A	301	SAH	C5'-SD-CG	-3.56	91.61	102.42
2	P	301	SAH	C5'-SD-CG	-3.49	91.82	102.42
2	B	302	SAH	C5'-SD-CG	-3.39	92.11	102.42
2	E	301	SAH	C5'-SD-CG	-3.33	92.32	102.42
2	I	301	SAH	C5'-SD-CG	-2.91	93.60	102.42
2	I	301	SAH	C1'-N9-C4	-2.49	124.03	126.81
2	H	301	SAH	C5'-C4'-C3'	-2.18	109.34	114.98
2	A	301	SAH	C1'-N9-C4	-2.10	124.47	126.81
2	B	301	SAH	C1'-N9-C4	-2.05	124.52	126.81
2	E	301	SAH	C1'-N9-C4	-2.04	124.53	126.81
2	B	302	SAH	O4'-C4'-C5'	2.05	114.44	108.85
2	F	301	SAH	O4'-C1'-N9	2.18	112.22	108.11
2	O	301	SAH	O4'-C1'-N9	2.30	112.45	108.11
2	B	302	SAH	O4'-C1'-N9	3.68	115.05	108.11
2	H	301	SAH	O4'-C1'-N9	5.39	118.29	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SAH	1	0
2	B	301	SAH	3	0
2	B	302	SAH	1	0
2	C	301	SAH	1	0
2	D	301	SAH	3	0
2	E	301	SAH	1	0
2	F	301	SAH	1	0
2	G	301	SAH	1	0
2	H	301	SAH	1	0
2	J	301	SAH	3	0
2	K	301	SAH	3	0
2	L	301	SAH	3	0
2	M	301	SAH	1	0
2	N	301	SAH	4	0
2	O	301	SAH	2	0
2	P	301	SAH	3	0
2	R	301	SAH	1	0

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	281/297 (94%)	0.16	1 (0%) 93 93	29, 46, 71, 105	0
1	B	280/297 (94%)	0.15	0 100 100	32, 49, 77, 95	0
1	C	280/297 (94%)	0.31	4 (1%) 78 80	38, 61, 87, 101	0
1	D	280/297 (94%)	0.19	3 (1%) 82 84	40, 61, 86, 101	0
1	E	279/297 (93%)	0.19	3 (1%) 82 84	30, 56, 77, 94	0
1	F	280/297 (94%)	0.19	2 (0%) 89 90	28, 49, 75, 102	0
1	G	280/297 (94%)	0.77	26 (9%) 11 11	53, 85, 122, 138	0
1	H	279/297 (93%)	1.05	46 (16%) 2 2	64, 99, 123, 137	0
1	I	280/297 (94%)	0.18	5 (1%) 71 75	25, 47, 96, 132	1 (0%)
1	J	281/297 (94%)	0.54	17 (6%) 25 28	35, 85, 113, 133	0
1	K	281/297 (94%)	0.54	13 (4%) 36 41	46, 76, 117, 127	0
1	L	280/297 (94%)	0.70	24 (8%) 13 14	51, 88, 120, 147	0
1	M	281/297 (94%)	0.58	24 (8%) 13 14	40, 63, 141, 169	0
1	N	281/297 (94%)	1.42	76 (27%) 1 1	50, 107, 137, 152	0
1	O	280/297 (94%)	0.45	13 (4%) 36 41	36, 70, 100, 124	0
1	P	280/297 (94%)	0.48	17 (6%) 25 27	42, 78, 105, 116	0
1	Q	281/297 (94%)	1.11	53 (18%) 2 1	36, 77, 159, 191	0
1	R	281/297 (94%)	2.11	118 (41%) 0 0	73, 115, 149, 173	0
All	All	5045/5346 (94%)	0.62	445 (8%) 12 13	25, 70, 124, 191	1 (0%)

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	11	GLN	19.2
1	M	9	GLN	11.9
1	R	250	PHE	8.8

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Mol	Chain	Res	Type	RSRZ
1	M	17	VAL	8.5
1	R	243	VAL	8.3
1	Q	25	GLY	8.2
1	M	21	TYR	8.1
1	Q	20	TRP	8.0
1	R	179	VAL	7.6
1	R	239	PHE	7.5
1	K	21	TYR	7.5
1	Q	27	VAL	7.5
1	R	82	LEU	7.4
1	N	134	ALA	7.4
1	Q	9	GLN	7.4
1	M	15	ASP	7.3
1	R	55	VAL	7.1
1	M	25	GLY	6.8
1	Q	15	ASP	6.7
1	M	10	GLN	6.7
1	N	211	PHE	6.4
1	R	260	ASP	6.3
1	R	104	THR	6.3
1	R	204	VAL	6.3
1	R	106	VAL	6.2
1	R	164	LEU	6.1
1	R	160	ARG	6.0
1	R	208	LEU	5.9
1	K	17	VAL	5.9
1	Q	12	VAL	5.8
1	R	125	LEU	5.8
1	R	149	ALA	5.8
1	R	207	ARG	5.7
1	Q	17	VAL	5.7
1	N	131	PHE	5.7
1	R	200	TYR	5.6
1	Q	30	LEU	5.5
1	R	148	CYS	5.5
1	Q	253	ARG	5.4
1	R	196	PHE	5.4
1	M	19	ASP	5.3
1	R	181	GLU	5.3
1	H	131	PHE	5.3
1	N	175	GLY	5.2
1	G	196	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	R	108	VAL	5.1
1	N	146	PHE	5.1
1	G	21	TYR	5.1
1	R	66	THR	5.0
1	N	121	ALA	5.0
1	Q	37	HIS	4.9
1	N	104	THR	4.9
1	L	252	GLU	4.8
1	R	258	PHE	4.8
1	N	200	TYR	4.8
1	O	289	VAL	4.8
1	R	205	PRO	4.7
1	Q	21	TYR	4.7
1	N	112	GLN	4.7
1	H	133	VAL	4.7
1	Q	254	PHE	4.6
1	Q	32	LEU	4.6
1	R	73	LEU	4.5
1	M	28	TYR	4.4
1	L	250	PHE	4.4
1	R	272	THR	4.3
1	R	84	ILE	4.3
1	R	212	PHE	4.3
1	N	150	TRP	4.2
1	R	266	LEU	4.2
1	R	49	PRO	4.2
1	N	199	LEU	4.2
1	R	95	ALA	4.2
1	R	42	PHE	4.2
1	Q	29	HIS	4.2
1	Q	36	VAL	4.2
1	N	125	LEU	4.2
1	N	101	ILE	4.1
1	J	138	ARG	4.1
1	H	250	PHE	4.1
1	R	171	LEU	4.1
1	M	11	GLN	4.1
1	N	250	PHE	4.0
1	R	155	LEU	4.0
1	R	153	GLU	4.0
1	Q	24	PHE	4.0
1	Q	270[A]	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	Q	188	LEU	4.0
1	R	129	LEU	3.9
1	L	88	THR	3.9
1	R	247	ARG	3.9
1	L	131	PHE	3.9
1	R	139	LEU	3.9
1	J	105	GLY	3.9
1	M	20	TRP	3.9
1	N	190	GLU	3.9
1	O	218	ALA	3.8
1	Q	28	TYR	3.8
1	N	239	PHE	3.8
1	Q	19	ASP	3.8
1	R	241	LEU	3.8
1	H	196	PHE	3.8
1	R	75	PRO	3.8
1	H	110	LYS	3.8
1	N	289	VAL	3.8
1	P	139	LEU	3.8
1	R	236	MET	3.7
1	R	138	ARG	3.7
1	R	246	ARG	3.7
1	N	204	VAL	3.7
1	Q	10	GLN	3.7
1	Q	13	THR	3.7
1	Q	52[A]	MET	3.7
1	G	20	TRP	3.7
1	G	199	LEU	3.7
1	N	259	VAL	3.7
1	N	212	PHE	3.6
1	R	151	ALA	3.6
1	H	197	GLU	3.6
1	N	140	PRO	3.6
1	Q	258	PHE	3.6
1	N	270[A]	GLN	3.6
1	R	70	ILE	3.6
1	N	139	LEU	3.6
1	G	17	VAL	3.6
1	H	105	GLY	3.5
1	G	262	LEU	3.5
1	R	177	LEU	3.5
1	R	128	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	R	147	ASP	3.5
1	N	164	LEU	3.5
1	Q	186	GLU	3.5
1	O	211	PHE	3.5
1	Q	266	LEU	3.5
1	R	232	LEU	3.5
1	R	186	GLU	3.5
1	H	119	LEU	3.5
1	Q	275	ARG	3.5
1	R	146	PHE	3.5
1	E	289	VAL	3.5
1	Q	31	THR	3.4
1	R	261	GLY	3.4
1	E	138	ARG	3.4
1	J	188	LEU	3.4
1	L	188	LEU	3.4
1	H	25	GLY	3.4
1	Q	33	GLY	3.4
1	N	220	PHE	3.4
1	G	244	TYR	3.4
1	R	116	ALA	3.4
1	H	265	GLY	3.3
1	Q	212	PHE	3.3
1	I	10	GLN	3.3
1	N	129	LEU	3.3
1	H	126	THR	3.3
1	N	254	PHE	3.3
1	R	161	ALA	3.3
1	N	196	PHE	3.3
1	R	141	TYR	3.3
1	N	195	LEU	3.3
1	Q	199	LEU	3.3
1	R	168	TRP	3.3
1	R	262	LEU	3.2
1	I	15	ASP	3.2
1	Q	23	LYS	3.2
1	N	149	ALA	3.2
1	R	130	THR	3.2
1	Q	211	PHE	3.2
1	G	266	LEU	3.2
1	J	129	LEU	3.2
1	H	106	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	289	VAL	3.2
1	R	69	LEU	3.2
1	R	85	GLY	3.2
1	Q	243	VAL	3.2
1	R	275	ARG	3.2
1	N	279	PHE	3.1
1	N	86	CYS	3.1
1	R	240	ALA	3.1
1	R	57	MET	3.1
1	K	212	PHE	3.1
1	R	101	ILE	3.1
1	R	157	HIS	3.1
1	K	26	GLU	3.1
1	G	195	LEU	3.1
1	N	171	LEU	3.1
1	R	256	ALA	3.1
1	H	103	VAL	3.1
1	G	36	VAL	3.1
1	O	137	MET	3.0
1	G	188	LEU	3.0
1	R	54	LEU	3.0
1	J	187	GLU	3.0
1	N	252	GLU	3.0
1	Q	14	ALA	3.0
1	N	106	VAL	3.0
1	N	184	VAL	3.0
1	R	270[A]	GLN	3.0
1	N	274	ILE	3.0
1	C	290	LEU	3.0
1	N	119	LEU	3.0
1	O	161	ALA	3.0
1	R	274	ILE	3.0
1	R	102	ALA	3.0
1	N	192	GLU	3.0
1	J	212	PHE	3.0
1	J	164	LEU	3.0
1	A	9	GLN	3.0
1	Q	242	GLY	3.0
1	Q	262	LEU	2.9
1	R	96	ALA	2.9
1	O	138	ARG	2.9
1	R	81	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	12	VAL	2.9
1	Q	57	MET	2.9
1	N	182	SER	2.9
1	H	121	ALA	2.9
1	Q	200	TYR	2.9
1	H	30	LEU	2.9
1	H	132	GLU	2.9
1	N	141	TYR	2.9
1	R	110	LYS	2.9
1	R	50	GLN	2.9
1	R	225	LEU	2.9
1	L	244	TYR	2.9
1	O	21	TYR	2.9
1	R	126	THR	2.8
1	R	136	ALA	2.8
1	D	289	VAL	2.8
1	H	247	ARG	2.8
1	N	137	MET	2.8
1	H	101	ILE	2.8
1	K	12	VAL	2.8
1	P	196	PHE	2.8
1	Q	196	PHE	2.8
1	R	279	PHE	2.8
1	N	179	VAL	2.8
1	G	242	GLY	2.8
1	N	103	VAL	2.8
1	H	200	TYR	2.8
1	H	262	LEU	2.8
1	N	135	ASP	2.8
1	G	243	VAL	2.7
1	O	165	GLY	2.7
1	G	253	ARG	2.7
1	N	174	GLY	2.7
1	H	134	ALA	2.7
1	L	108	VAL	2.7
1	N	198	THR	2.7
1	N	223	LEU	2.7
1	H	240	ALA	2.7
1	M	266	LEU	2.7
1	N	82	LEU	2.7
1	K	25	GLY	2.7
1	M	36	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	30	LEU	2.7
1	H	236	MET	2.7
1	R	156	CYS	2.7
1	Q	239	PHE	2.7
1	R	131	PHE	2.7
1	R	284	LEU	2.7
1	R	244	TYR	2.7
1	G	260	ASP	2.7
1	G	212	PHE	2.6
1	N	138	ARG	2.6
1	H	32	LEU	2.6
1	L	125	LEU	2.6
1	P	119	LEU	2.6
1	Q	241	LEU	2.6
1	P	212	PHE	2.6
1	K	138	ARG	2.6
1	M	275	ARG	2.6
1	R	150	TRP	2.6
1	K	190	GLU	2.6
1	Q	42	PHE	2.6
1	I	25	GLY	2.6
1	M	38	CYS	2.6
1	H	194	ALA	2.6
1	G	28	TYR	2.6
1	R	123	HIS	2.6
1	N	247	ARG	2.6
1	H	151	ALA	2.6
1	P	106	VAL	2.6
1	P	204	VAL	2.6
1	P	250	PHE	2.6
1	I	21	TYR	2.6
1	N	14	ALA	2.5
1	Q	277	THR	2.5
1	M	138	ARG	2.5
1	R	97	ARG	2.5
1	N	142	GLU	2.5
1	O	212	PHE	2.5
1	R	210	GLU	2.5
1	C	200	TYR	2.5
1	G	202	ALA	2.5
1	R	107	ALA	2.5
1	N	81	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	184	VAL	2.5
1	G	191	PRO	2.5
1	L	107	ALA	2.5
1	J	199	LEU	2.5
1	L	273	LEU	2.5
1	N	244	TYR	2.5
1	N	263	LEU	2.5
1	R	190	GLU	2.5
1	G	13	THR	2.5
1	H	20	TRP	2.4
1	Q	22	ASP	2.4
1	H	195	LEU	2.4
1	P	103	VAL	2.4
1	Q	40	LEU	2.4
1	Q	263	LEU	2.4
1	R	178	LEU	2.4
1	R	112	GLN	2.4
1	R	137	MET	2.4
1	N	136	ALA	2.4
1	P	116	ALA	2.4
1	R	120	ALA	2.4
1	R	154	SER	2.4
1	J	110	LYS	2.4
1	K	23	LYS	2.4
1	M	23	LYS	2.4
1	R	289	VAL	2.4
1	N	107	ALA	2.4
1	N	110	LYS	2.4
1	R	162	LYS	2.4
1	R	198	THR	2.4
1	P	155	LEU	2.4
1	H	100	GLY	2.4
1	R	221	HIS	2.4
1	P	81	LEU	2.4
1	J	108	VAL	2.4
1	R	52	MET	2.4
1	R	80	HIS	2.4
1	K	19	ASP	2.4
1	N	88	THR	2.4
1	N	156	CYS	2.4
1	N	284	LEU	2.4
1	J	179	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	170	VAL	2.3
1	R	159	ASP	2.3
1	N	161	ALA	2.3
1	R	183	VAL	2.3
1	H	254	PHE	2.3
1	H	258	PHE	2.3
1	R	280	PHE	2.3
1	L	134	ALA	2.3
1	R	65	TYR	2.3
1	R	216	SER	2.3
1	H	14	ALA	2.3
1	N	132	GLU	2.3
1	R	62	GLN	2.3
1	N	75	PRO	2.3
1	F	138	ARG	2.3
1	R	265	GLY	2.3
1	G	240	ALA	2.3
1	R	127	GLU	2.3
1	P	289	VAL	2.3
1	H	261	GLY	2.3
1	N	145	SER	2.3
1	O	202	ALA	2.3
1	R	187	GLU	2.3
1	L	133	VAL	2.2
1	Q	289	VAL	2.2
1	L	146	PHE	2.2
1	H	188	LEU	2.2
1	L	118	ARG	2.2
1	D	17	VAL	2.2
1	M	243	VAL	2.2
1	N	133	VAL	2.2
1	G	142	GLU	2.2
1	J	239	PHE	2.2
1	P	131	PHE	2.2
1	L	129	LEU	2.2
1	L	255	GLY	2.2
1	N	51	ASP	2.2
1	L	179	VAL	2.2
1	G	256	ALA	2.2
1	H	255	GLY	2.2
1	L	87	GLY	2.2
1	R	68	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	207	ARG	2.2
1	R	133	VAL	2.2
1	I	14	ALA	2.2
1	H	239	PHE	2.2
1	J	131	PHE	2.2
1	L	112	GLN	2.2
1	R	30	LEU	2.2
1	E	106	VAL	2.2
1	H	130	THR	2.2
1	K	24	PHE	2.2
1	C	139	LEU	2.2
1	H	123	HIS	2.2
1	Q	41	TRP	2.2
1	R	11	GLN	2.2
1	L	128	ARG	2.2
1	M	24	PHE	2.2
1	Q	54	LEU	2.2
1	N	127	GLU	2.2
1	R	9	GLN	2.1
1	N	168	TRP	2.1
1	M	13	THR	2.1
1	G	273	LEU	2.1
1	L	262	LEU	2.1
1	N	154	SER	2.1
1	M	253	ARG	2.1
1	N	181	GLU	2.1
1	N	197	GLU	2.1
1	H	104	THR	2.1
1	H	93	LEU	2.1
1	L	82	LEU	2.1
1	O	164	LEU	2.1
1	D	118	ARG	2.1
1	J	139	LEU	2.1
1	F	289	VAL	2.1
1	H	107	ALA	2.1
1	O	163	ALA	2.1
1	P	12	VAL	2.1
1	K	273	LEU	2.1
1	L	239	PHE	2.1
1	M	26	GLU	2.1
1	H	199	LEU	2.1
1	P	174	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	192	GLU	2.1
1	N	118	ARG	2.1
1	P	141	TYR	2.1
1	R	51	ASP	2.1
1	H	266	LEU	2.1
1	L	266	LEU	2.1
1	Q	208	LEU	2.1
1	H	137	MET	2.0
1	R	94	LYS	2.0
1	R	86	CYS	2.0
1	J	201	ALA	2.0
1	C	289	VAL	2.0
1	N	30	LEU	2.0
1	R	199	LEU	2.0
1	G	211	PHE	2.0
1	H	150	TRP	2.0
1	P	140	PRO	2.0
1	H	112	GLN	2.0
1	J	104	THR	2.0
1	K	110	LYS	2.0
1	Q	278	ARG	2.0
1	J	196	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SAH	B	302	26/26	0.71	0.25	3.17	105,107,108,108	0
2	SAH	B	301	26/26	0.94	0.20	1.23	49,51,52,53	0
2	SAH	R	301	26/26	0.54	0.42	0.81	118,121,122,123	0
2	SAH	H	301	26/26	0.78	0.29	0.54	98,102,105,106	0
2	SAH	Q	301	26/26	0.94	0.18	0.51	61,62,64,65	0
2	SAH	O	301	26/26	0.91	0.21	0.50	80,82,83,83	0
2	SAH	K	301	26/26	0.88	0.20	0.43	75,79,80,81	0
2	SAH	P	301	26/26	0.88	0.22	0.33	72,74,75,75	0
2	SAH	C	301	26/26	0.94	0.19	0.25	61,63,64,64	0
2	SAH	M	301	26/26	0.96	0.18	0.25	57,61,62,62	0
2	SAH	F	301	26/26	0.98	0.17	0.19	34,35,36,37	0
2	SAH	E	301	26/26	0.97	0.18	0.10	48,49,50,50	0
2	SAH	J	301	26/26	0.87	0.22	0.10	88,89,91,91	0
2	SAH	L	301	26/26	0.91	0.26	0.00	85,87,89,89	0
2	SAH	G	301	26/26	0.93	0.19	-0.10	74,75,77,77	0
2	SAH	N	301	26/26	0.69	0.29	-0.19	105,107,108,108	0
2	SAH	D	301	26/26	0.95	0.15	-0.48	57,58,59,59	0
2	SAH	I	301	26/26	0.98	0.15	-0.73	34,36,37,38	0
2	SAH	A	301	26/26	0.98	0.15	-1.08	36,38,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.