Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:54 AM GMT

PDB ID	:	3CJQ
Title	:	Ribosomal protein L11 methyltransferase (PrmA) in complex with dimethylated ribosomal protein L11 in space group P212121
Authors	:	Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2008-03-13
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

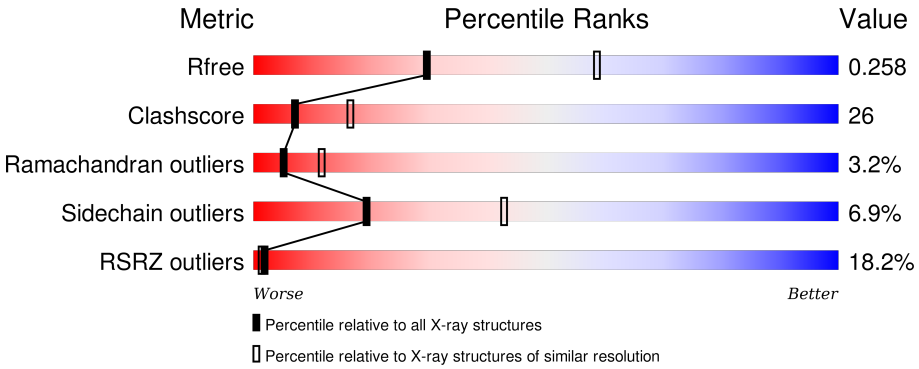
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	254	10% 76% 20% ·
1	D	254	9% 81% 14% · ·
1	G	254	18% 75% 20% · · ·
2	B	146	24% 38% 38% 7% 17%
2	E	146	16% 42% 29% 7% · 21%

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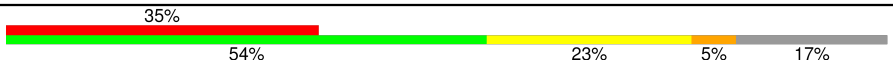
Mol	Chain	Length	Quality of chain
2	H	146	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8801 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 Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1949	1265	338	342	4			
1	D	252	Total	C	N	O	S	0	1	0
			1954	1270	338	342	4			
1	G	252	Total	C	N	O	S	5	0	0
			1941	1261	337	339	4			

- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			884	566	150	163	5			
2	E	115	Total	C	N	O	S	0	0	0
			838	540	143	150	5			
2	H	121	Total	C	N	O	S	0	0	0
			884	566	150	163	5			

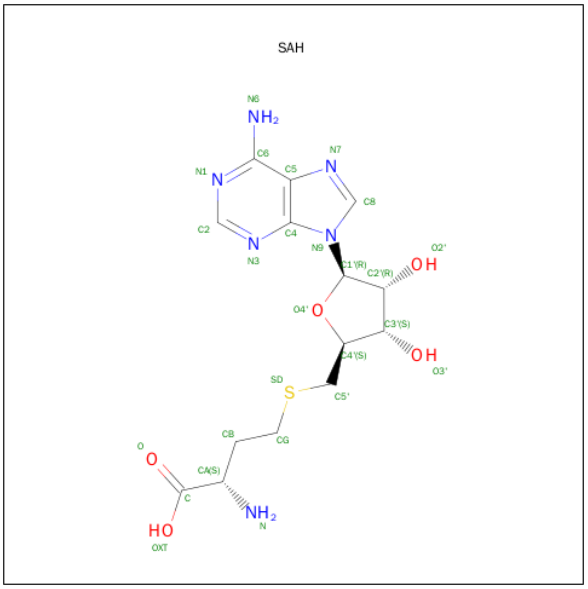
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ALA	LYS	ENGINEERED	UNP P36238
E	39	ALA	LYS	ENGINEERED	UNP P36238
H	39	ALA	LYS	ENGINEERED	UNP P36238

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

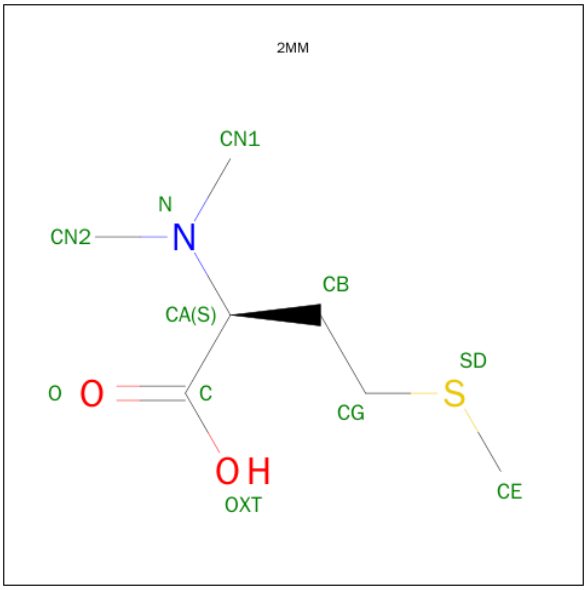
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	I	0	0
			1	1		
3	B	1	Total	I	0	0
			1	1		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is N,N-DIMETHYL-L-METHIONINE (three-letter code: 2MM) (formula: $C_7H_{15}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	E	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	H	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

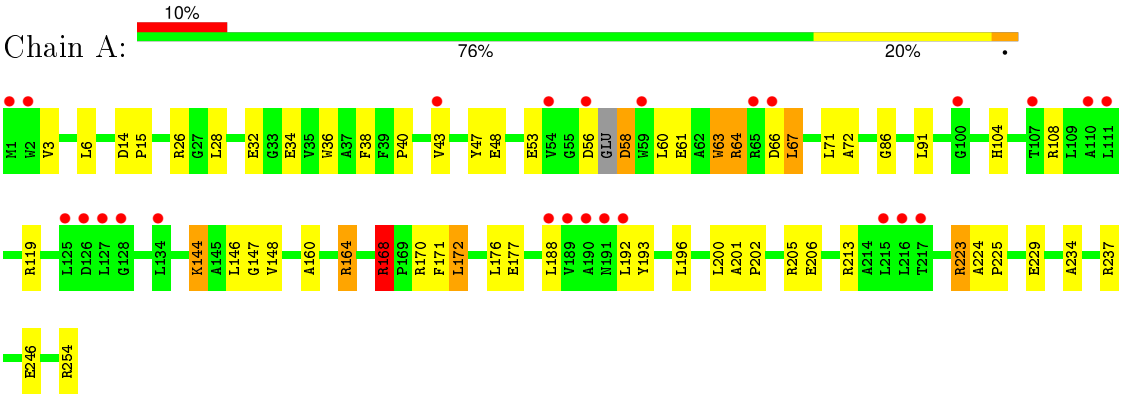
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	10	Total	O	0	0
			10	10		
6	D	88	Total	O	0	0
			88	88		
6	E	16	Total	O	0	0
			16	16		
6	G	48	Total	O	0	0
			48	48		
6	H	4	Total	O	0	0
			4	4		

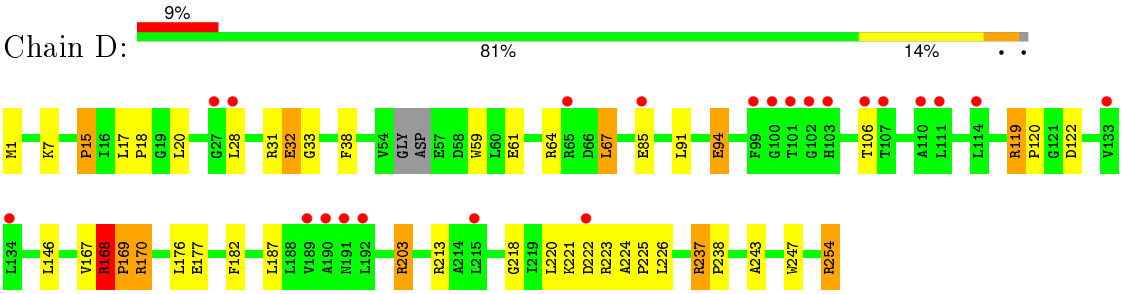
3 Residue-property plots (i)

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.

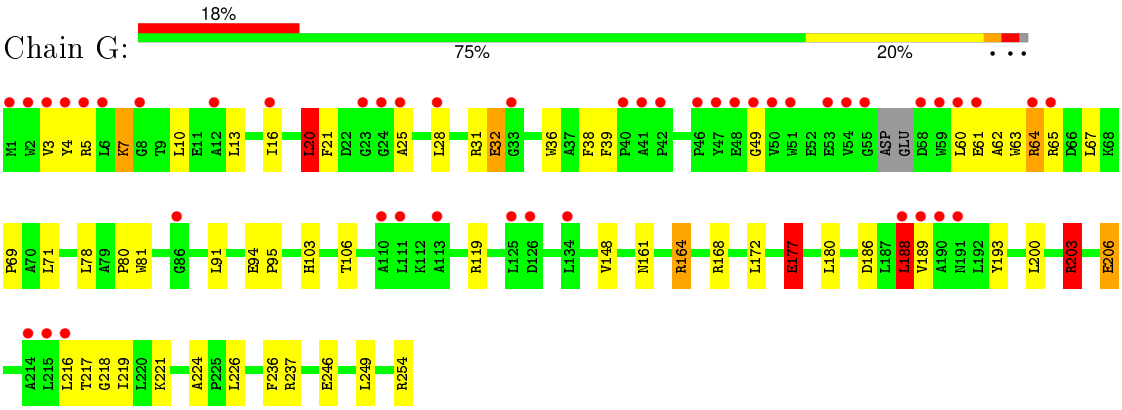
- Molecule 1: Ribosomal protein L11 methyltransferase



- Molecule 1: Ribosomal protein L11 methyltransferase

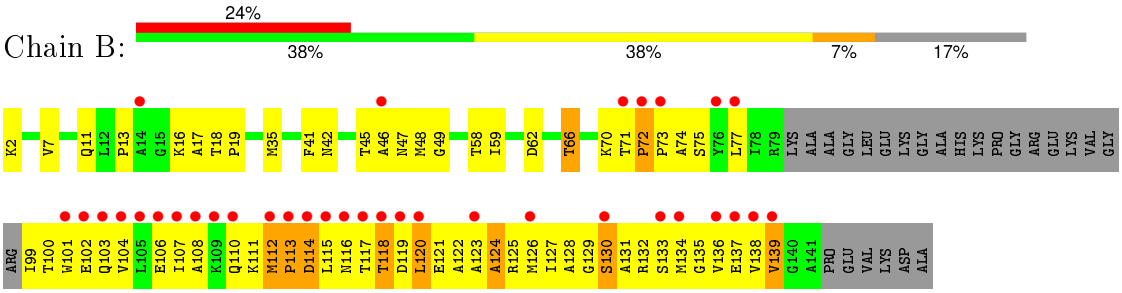


- Molecule 1: Ribosomal protein L11 methyltransferase



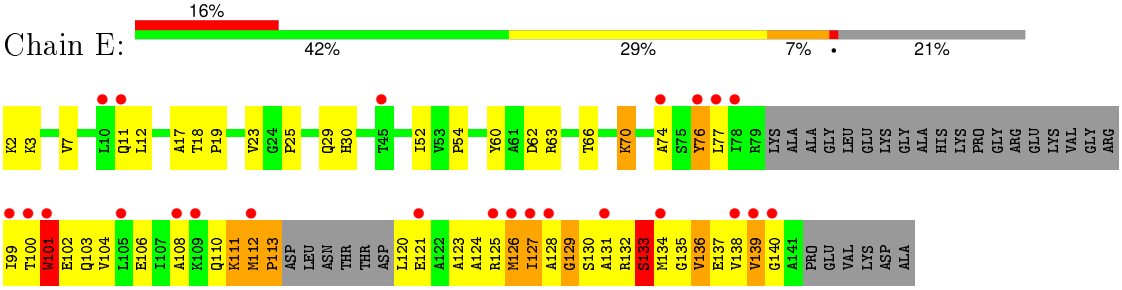
- Molecule 2: 50S ribosomal protein L11

Chain B:



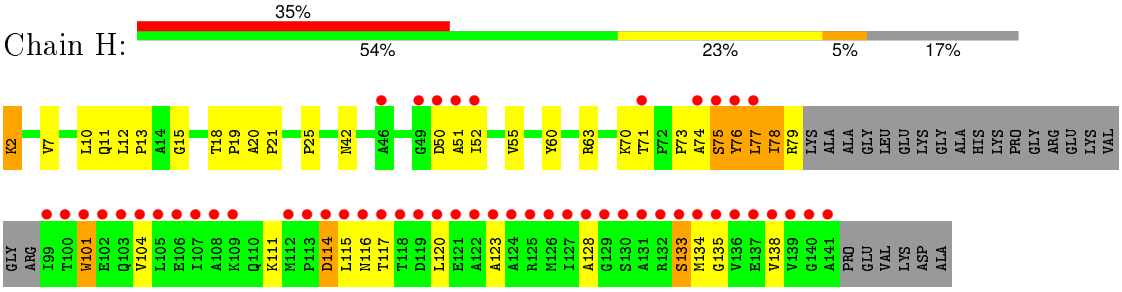
- Molecule 2: 50S ribosomal protein L11

Chain E:



- Molecule 2: 50S ribosomal protein L11

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.53Å 164.98Å 180.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 2.70 29.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.09-2.70) 99.9 (29.09-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.271 0.195 , 0.258	Depositor DCC
R_{free} test set	2207 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 43176 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8801	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, IOD, 2MM

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	1.24	7/2005 (0.3%)	1.07	4/2732 (0.1%)
1	D	1.25	6/2010 (0.3%)	1.08	8/2739 (0.3%)
1	G	1.23	9/1997 (0.5%)	1.01	7/2721 (0.3%)
2	B	0.90	0/900	0.84	0/1226
2	E	1.11	2/853 (0.2%)	0.90	1/1159 (0.1%)
2	H	1.25	3/900 (0.3%)	0.84	1/1226 (0.1%)
All	All	1.20	27/8665 (0.3%)	1.00	21/11803 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	133	SER	CB-OG	20.43	1.68	1.42
2	E	113	PRO	C-O	10.85	1.45	1.23
1	G	177	GLU	CG-CD	9.53	1.66	1.51
1	D	177	GLU	CG-CD	8.86	1.65	1.51
1	G	177	GLU	CB-CG	8.55	1.68	1.52
1	D	94	GLU	CB-CG	8.51	1.68	1.52
1	G	206	GLU	CG-CD	7.71	1.63	1.51
1	A	177	GLU	CG-CD	7.34	1.62	1.51
1	G	206	GLU	CB-CG	7.33	1.66	1.52
1	A	144	LYS	CE-NZ	7.22	1.67	1.49
2	H	2	LYS	CD-CE	7.11	1.69	1.51
1	A	206	GLU	CG-CD	6.41	1.61	1.51
1	D	85	GLU	CG-CD	6.28	1.61	1.51
1	D	168	ARG	CG-CD	6.23	1.67	1.51
1	G	246	GLU	CD-OE2	6.07	1.32	1.25
1	A	164	ARG	CG-CD	5.99	1.67	1.51
1	G	177	GLU	CD-OE1	5.94	1.32	1.25
1	A	206	GLU	CD-OE2	5.64	1.31	1.25
1	G	119	ARG	CZ-NH1	5.59	1.40	1.33
1	A	56	ASP	CG-OD1	5.45	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	114	ASP	CG-OD1	5.33	1.37	1.25
2	E	133	SER	C-O	5.22	1.33	1.23
1	G	20	LEU	C-O	5.21	1.33	1.23
1	D	177	GLU	CD-OE1	5.20	1.31	1.25
1	A	229	GLU	CG-CD	5.18	1.59	1.51
1	D	85	GLU	CB-CG	5.17	1.61	1.52
1	G	193	TYR	CD1-CE1	5.16	1.47	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	170	ARG	NE-CZ-NH1	-8.84	115.88	120.30
2	H	114	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	G	119	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	A	119	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	67	LEU	CA-CB-CG	7.66	132.91	115.30
1	D	67	LEU	CA-CB-CG	6.65	130.60	115.30
1	D	168	ARG	N-CA-CB	-6.10	99.62	110.60
1	D	122	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	169	PRO	CA-N-CD	6.00	120.10	111.70
1	G	237	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	D	168	ARG	N-CA-C	5.79	126.65	111.00
1	D	119	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	167	VAL	CG1-CB-CG2	5.52	119.73	110.90
2	E	77	LEU	CA-CB-CG	5.46	127.86	115.30
1	G	224	ALA	C-N-CD	5.43	139.81	128.40
1	G	119	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	G	188	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	A	168	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	223	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	G	203	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	186	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	1949	0	1948	31	1
1	D	1954	0	1957	38	0
1	G	1941	0	1944	45	0
2	B	884	0	906	166	0
2	E	838	0	865	125	0
2	H	884	0	906	58	0
3	B	1	0	0	0	0
3	H	1	0	0	1	0
4	A	26	0	19	0	0
4	D	26	0	19	1	0
4	G	26	0	19	0	0
5	B	10	0	14	3	0
5	E	10	0	14	2	0
5	H	10	0	14	2	0
6	A	75	0	0	2	0
6	B	10	0	0	0	0
6	D	88	0	0	3	0
6	E	16	0	0	1	1
6	G	48	0	0	6	0
6	H	4	0	0	0	0
All	All	8801	0	8625	449	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 26.

All (449) 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)
2:B:99:ILE:CA	2:B:136:VAL:HG13	1.32	1.55
2:B:101:TRP:HB2	2:B:139:VAL:CG2	1.11	1.54
2:B:107:ILE:HG22	2:B:111:LYS:CD	1.44	1.47
2:E:132:ARG:O	2:E:135:GLY:CA	1.63	1.42
2:H:74:ALA:HA	2:H:77:LEU:CD1	1.50	1.41
2:H:78:ILE:CG2	2:H:79:ARG:H	1.20	1.40
2:B:132:ARG:HE	2:B:138:VAL:CG2	1.35	1.38
2:H:133:SER:CB	2:H:133:SER:OG	1.68	1.38
2:E:128:ALA:HA	2:E:131:ALA:CB	1.52	1.36
2:E:132:ARG:HG2	2:E:136:VAL:O	1.24	1.36
2:B:121:GLU:OE2	2:B:125:ARG:NH2	1.59	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:TRP:CB	2:B:139:VAL:CG2	2.01	1.36
2:E:128:ALA:O	2:E:131:ALA:N	1.60	1.32
2:B:101:TRP:CB	2:B:139:VAL:HG21	1.56	1.30
2:B:111:LYS:O	2:B:114:ASP:HB2	1.28	1.29
2:B:107:ILE:CG2	2:B:111:LYS:HD3	1.61	1.28
2:B:111:LYS:O	2:B:114:ASP:CB	1.83	1.27
2:B:132:ARG:NE	2:B:138:VAL:HG21	1.48	1.27
2:B:132:ARG:O	2:B:135:GLY:CA	1.85	1.25
2:E:136:VAL:CG1	2:E:137:GLU:H	1.47	1.23
2:H:78:ILE:HG22	2:H:79:ARG:N	1.26	1.23
2:B:117:THR:O	2:B:119:ASP:N	1.72	1.22
2:B:100:THR:O	2:B:137:GLU:O	1.56	1.21
2:B:112:MET:CE	2:B:118:THR:HA	1.71	1.19
2:E:99:ILE:CB	2:E:137:GLU:HG3	1.73	1.19
2:B:119:ASP:HB3	2:B:122:ALA:CB	1.72	1.19
2:E:132:ARG:HA	2:E:136:VAL:N	1.55	1.19
2:B:132:ARG:NE	2:B:138:VAL:CG2	2.03	1.18
2:E:136:VAL:HG12	2:E:137:GLU:N	1.52	1.18
2:B:107:ILE:O	2:B:111:LYS:HG2	1.38	1.18
2:B:99:ILE:CA	2:B:136:VAL:CG1	2.22	1.16
2:B:99:ILE:CB	2:B:136:VAL:HG13	1.75	1.16
2:H:71:THR:CG2	2:H:114:ASP:HB3	1.73	1.16
2:H:71:THR:HG21	2:H:114:ASP:HB3	1.24	1.15
2:B:112:MET:O	2:B:114:ASP:N	1.79	1.15
2:H:78:ILE:HD11	2:H:134:MET:SD	1.87	1.14
2:E:128:ALA:HA	2:E:131:ALA:HB2	1.30	1.14
2:B:101:TRP:CA	2:B:139:VAL:HG22	1.78	1.13
2:B:112:MET:HE1	2:B:118:THR:HA	1.14	1.13
2:B:112:MET:C	2:B:114:ASP:H	1.43	1.12
2:B:101:TRP:HB2	2:B:139:VAL:HG22	1.24	1.12
2:E:132:ARG:C	2:E:135:GLY:HA3	1.69	1.12
2:B:119:ASP:O	2:B:121:GLU:N	1.84	1.11
2:E:99:ILE:HA	2:E:137:GLU:CB	1.81	1.10
2:B:107:ILE:O	2:B:111:LYS:CG	1.99	1.10
2:B:119:ASP:HB3	2:B:122:ALA:HB3	1.19	1.10
2:B:132:ARG:HH21	2:B:138:VAL:HG11	1.07	1.10
2:E:128:ALA:HA	2:E:131:ALA:HB3	1.23	1.10
2:H:74:ALA:HA	2:H:77:LEU:HD11	1.23	1.10
2:E:128:ALA:O	2:E:130:SER:N	1.86	1.09
2:B:99:ILE:HA	2:B:136:VAL:CG1	1.80	1.09
2:B:111:LYS:O	2:B:114:ASP:CA	2.01	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:GLU:HG2	2:B:139:VAL:HG23	1.14	1.08
2:E:99:ILE:N	2:E:136:VAL:HG11	1.67	1.08
2:E:139:VAL:HG12	2:E:140:GLY:H	0.93	1.08
2:B:102:GLU:CG	2:B:139:VAL:HG23	1.85	1.07
2:E:99:ILE:CA	2:E:137:GLU:HB2	1.83	1.07
2:B:132:ARG:O	2:B:135:GLY:HA2	1.45	1.07
2:E:128:ALA:CA	2:E:131:ALA:HB3	1.84	1.06
2:E:132:ARG:CG	2:E:136:VAL:O	2.03	1.05
2:B:100:THR:N	2:B:136:VAL:CG1	2.19	1.05
2:B:101:TRP:CB	2:B:139:VAL:HG22	1.75	1.05
2:B:132:ARG:HH21	2:B:138:VAL:CG1	1.70	1.04
2:H:74:ALA:CA	2:H:77:LEU:CD1	2.35	1.03
2:B:132:ARG:O	2:B:135:GLY:HA3	1.58	1.02
2:B:100:THR:N	2:B:136:VAL:HG12	1.74	1.01
2:E:99:ILE:HA	2:E:137:GLU:HB2	1.03	1.01
2:B:107:ILE:O	2:B:111:LYS:CD	2.09	1.01
2:B:99:ILE:C	2:B:136:VAL:CG1	2.29	1.00
2:B:99:ILE:HA	2:B:136:VAL:HG13	1.04	1.00
2:E:123:ALA:O	2:E:127:ILE:HG13	1.62	1.00
2:E:139:VAL:HG12	2:E:140:GLY:N	1.76	1.00
2:E:102:GLU:HG2	2:E:139:VAL:HG21	1.42	1.00
2:H:74:ALA:O	2:H:76:TYR:N	1.95	0.99
2:B:112:MET:C	2:B:114:ASP:N	2.11	0.98
2:E:111:LYS:O	2:E:113:PRO:N	1.97	0.98
2:E:130:SER:O	2:E:134:MET:N	1.97	0.97
2:E:139:VAL:CG1	2:E:140:GLY:H	1.78	0.95
2:B:108:ALA:HA	2:B:111:LYS:HG2	1.48	0.95
2:E:134:MET:H	2:E:135:GLY:CA	1.80	0.93
2:B:107:ILE:HG22	2:B:111:LYS:CE	1.99	0.93
2:E:134:MET:H	2:E:135:GLY:HA3	1.32	0.92
2:H:78:ILE:CG2	2:H:79:ARG:N	1.94	0.92
2:E:111:LYS:C	2:E:113:PRO:HD2	1.90	0.92
2:B:115:LEU:HD11	2:B:127:ILE:HD11	1.52	0.92
2:E:128:ALA:CA	2:E:131:ALA:CB	2.42	0.91
2:H:76:TYR:CD2	2:H:77:LEU:N	2.38	0.91
2:H:74:ALA:HA	2:H:77:LEU:CG	2.01	0.90
2:B:99:ILE:C	2:B:136:VAL:HG13	1.92	0.90
2:E:129:GLY:O	2:E:133:SER:HB3	1.71	0.90
2:B:100:THR:H	2:B:136:VAL:HG12	1.35	0.90
2:B:111:LYS:C	2:B:114:ASP:HB2	1.92	0.90
2:B:132:ARG:NE	2:B:138:VAL:HG22	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:132:ARG:HH21	2:E:138:VAL:HB	1.38	0.88
2:B:13:PRO:HG2	2:B:16:LYS:HD2	1.55	0.88
1:G:80:PRO:HG3	1:G:164:ARG:HH12	1.40	0.87
2:E:112:MET:HB3	2:E:113:PRO:HD3	1.55	0.87
2:B:108:ALA:HA	2:B:111:LYS:CG	2.03	0.87
2:E:101:TRP:HE3	2:E:101:TRP:H	1.23	0.87
2:E:132:ARG:NH2	2:E:138:VAL:HB	1.90	0.87
2:E:99:ILE:N	2:E:136:VAL:CG1	2.38	0.86
2:B:117:THR:C	2:B:119:ASP:H	1.78	0.86
1:G:249:LEU:HA	6:G:350:HOH:O	1.74	0.86
2:B:107:ILE:C	2:B:111:LYS:HG2	1.96	0.86
2:E:132:ARG:HA	2:E:136:VAL:H	1.38	0.86
2:E:136:VAL:CG1	2:E:137:GLU:N	2.18	0.86
2:B:132:ARG:NH2	2:B:138:VAL:HG11	1.91	0.86
2:B:101:TRP:C	2:B:139:VAL:HG22	1.95	0.85
2:E:132:ARG:O	2:E:135:GLY:HA3	0.67	0.85
2:H:71:THR:HG22	2:H:114:ASP:HB3	1.59	0.85
2:B:119:ASP:CB	2:B:122:ALA:HB3	2.06	0.85
2:E:121:GLU:HA	2:E:124:ALA:HB3	1.59	0.84
2:E:129:GLY:O	2:E:133:SER:CB	2.25	0.83
2:H:74:ALA:HA	2:H:77:LEU:HD12	1.56	0.83
2:B:102:GLU:HG2	2:B:139:VAL:CG2	2.07	0.82
2:B:119:ASP:O	2:B:122:ALA:N	2.12	0.82
1:A:168:ARG:HG2	1:D:120:PRO:HB2	1.58	0.82
1:G:203:ARG:HG3	1:G:203:ARG:HH11	1.42	0.82
2:B:99:ILE:CB	2:B:136:VAL:CG1	2.57	0.81
2:B:132:ARG:NH2	2:B:138:VAL:CG1	2.43	0.81
2:H:74:ALA:CA	2:H:77:LEU:HD12	2.08	0.81
2:E:130:SER:O	2:E:133:SER:C	2.19	0.81
2:B:103:GLN:O	2:B:106:GLU:N	2.14	0.81
2:B:119:ASP:CB	2:B:122:ALA:CB	2.57	0.80
2:H:74:ALA:CA	2:H:77:LEU:HD11	2.07	0.80
2:B:111:LYS:HG3	2:B:127:ILE:HD13	1.63	0.80
2:E:136:VAL:HG12	2:E:137:GLU:H	0.66	0.79
2:H:2:LYS:CA	5:H:1:2MM:C	2.60	0.79
2:E:111:LYS:O	2:E:112:MET:C	2.20	0.78
2:B:112:MET:HE1	2:B:118:THR:CA	2.08	0.78
2:B:132:ARG:HE	2:B:138:VAL:HG21	0.63	0.78
2:E:111:LYS:C	2:E:113:PRO:CD	2.52	0.78
1:G:7:LYS:HB2	1:G:7:LYS:NZ	1.98	0.78
1:A:146:LEU:HD11	1:A:172:LEU:HD22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ALA:CA	2:B:111:LYS:HG2	2.13	0.77
2:E:132:ARG:O	2:E:134:MET:N	2.16	0.77
2:E:99:ILE:CB	2:E:137:GLU:CG	2.61	0.77
2:B:111:LYS:O	2:B:114:ASP:C	2.24	0.76
2:E:132:ARG:C	2:E:134:MET:H	1.89	0.76
2:B:110:GLN:O	2:B:114:ASP:OD2	2.04	0.75
2:E:128:ALA:HB1	2:E:138:VAL:HG22	1.68	0.75
2:E:120:LEU:O	2:E:124:ALA:HB2	1.87	0.75
2:E:111:LYS:O	2:E:113:PRO:CD	2.35	0.74
2:B:126:MET:CE	2:B:127:ILE:HG13	2.17	0.74
1:A:164:ARG:HD3	6:A:343:HOH:O	1.88	0.74
2:B:107:ILE:CG2	2:B:111:LYS:CD	2.38	0.73
2:E:132:ARG:NE	2:E:138:VAL:HG23	2.04	0.73
2:B:107:ILE:HG22	2:B:111:LYS:HD3	0.76	0.73
1:G:28:LEU:HB2	2:H:11:GLN:HB2	1.71	0.72
2:B:119:ASP:HB3	2:B:122:ALA:HB2	1.66	0.72
2:H:74:ALA:O	2:H:77:LEU:HG	1.89	0.72
2:B:111:LYS:O	2:B:114:ASP:N	2.22	0.72
2:H:71:THR:HG21	2:H:114:ASP:CB	2.13	0.72
2:B:134:MET:N	2:B:135:GLY:HA2	2.03	0.72
2:E:132:ARG:C	2:E:135:GLY:CA	2.44	0.72
1:G:216:LEU:O	6:G:350:HOH:O	2.07	0.72
1:G:69:PRO:HB3	1:G:78:LEU:HD23	1.71	0.72
2:B:119:ASP:OD2	2:B:122:ALA:HB2	1.91	0.71
2:B:101:TRP:CD1	2:B:102:GLU:N	2.57	0.71
2:E:128:ALA:CB	2:E:131:ALA:HB3	2.20	0.71
2:H:76:TYR:HD2	2:H:77:LEU:H	1.38	0.70
1:G:80:PRO:CG	1:G:164:ARG:HH12	2.05	0.70
2:B:112:MET:O	2:B:113:PRO:C	2.29	0.69
1:D:221:LYS:HE3	6:D:371:HOH:O	1.91	0.69
2:E:124:ALA:HA	2:E:127:ILE:CD1	2.22	0.69
2:H:101:TRP:HE3	2:H:101:TRP:H	1.40	0.69
2:E:128:ALA:C	2:E:130:SER:N	2.41	0.68
1:G:80:PRO:HG3	1:G:164:ARG:NH1	2.08	0.68
2:B:107:ILE:C	2:B:111:LYS:HD3	2.14	0.68
2:H:78:ILE:HG22	2:H:79:ARG:CA	2.21	0.68
2:H:74:ALA:HA	2:H:77:LEU:HG	1.77	0.67
1:G:7:LYS:HB2	1:G:7:LYS:HZ2	1.58	0.67
2:B:132:ARG:O	2:B:134:MET:N	2.28	0.67
2:E:128:ALA:O	2:E:130:SER:C	2.30	0.67
2:B:112:MET:HE2	2:B:118:THR:HA	1.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HB2	2:B:11:GLN:HB3	1.75	0.66
2:B:101:TRP:HB2	2:B:139:VAL:HG21	0.66	0.66
1:A:148:VAL:HG12	1:A:172:LEU:CD2	2.26	0.66
1:D:94:GLU:HA	1:D:94:GLU:OE1	1.95	0.66
2:B:123:ALA:O	2:B:124:ALA:C	2.34	0.65
2:E:132:ARG:CB	2:E:136:VAL:O	2.45	0.65
2:H:74:ALA:CB	2:H:77:LEU:HD12	2.25	0.65
2:B:104:VAL:HA	2:B:107:ILE:HD12	1.77	0.65
2:E:134:MET:N	2:E:135:GLY:CA	2.52	0.65
2:B:111:LYS:CA	2:B:114:ASP:HB2	2.26	0.64
2:B:101:TRP:CG	2:B:139:VAL:HG21	2.31	0.64
2:B:107:ILE:CG2	2:B:111:LYS:NZ	2.60	0.64
2:E:103:GLN:O	2:E:106:GLU:HB3	1.98	0.64
2:B:16:LYS:O	2:B:16:LYS:HG2	1.98	0.64
1:G:177:GLU:HB3	6:G:331:HOH:O	1.97	0.64
2:B:131:ALA:O	2:B:134:MET:HB2	1.98	0.64
2:E:111:LYS:O	2:E:113:PRO:HD2	1.96	0.64
2:E:128:ALA:C	2:E:130:SER:H	1.99	0.63
2:E:132:ARG:CA	2:E:136:VAL:N	2.48	0.63
2:E:2:LYS:CA	5:E:1:2MM:C	2.76	0.63
1:D:170:ARG:HH11	1:D:170:ARG:HG3	1.64	0.63
2:B:107:ILE:CB	2:B:111:LYS:HD3	2.29	0.63
2:B:2:LYS:CA	5:B:1:2MM:C	2.76	0.62
1:A:58:ASP:OD2	1:A:58:ASP:N	2.31	0.62
2:B:102:GLU:CD	2:B:139:VAL:O	2.38	0.62
2:B:107:ILE:C	2:B:111:LYS:CD	2.67	0.62
2:E:12:LEU:HD13	2:E:17:ALA:HB2	1.81	0.62
2:H:104:VAL:HG11	2:H:128:ALA:HB2	1.81	0.62
2:E:134:MET:N	2:E:135:GLY:HA3	2.10	0.62
2:B:119:ASP:CB	2:B:122:ALA:HB2	2.26	0.61
2:E:124:ALA:HA	2:E:127:ILE:HD12	1.82	0.61
2:E:129:GLY:O	2:E:133:SER:OG	2.13	0.61
2:B:138:VAL:O	2:B:139:VAL:HG13	2.01	0.61
2:H:74:ALA:HB1	2:H:77:LEU:HD12	1.83	0.61
1:D:146:LEU:CD1	1:D:170:ARG:HB3	2.32	0.60
2:E:102:GLU:HG2	2:E:139:VAL:CG2	2.24	0.60
2:H:75:SER:O	2:H:78:ILE:HD12	2.02	0.59
1:G:61:GLU:HG3	1:G:64:ARG:NH2	2.17	0.59
2:H:74:ALA:C	2:H:76:TYR:H	2.06	0.59
1:D:170:ARG:NH1	1:D:170:ARG:HG3	2.17	0.59
1:G:103:HIS:HD2	6:G:325:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:LEU:HD12	2:H:55:VAL:HG11	1.85	0.59
1:G:148:VAL:HG12	1:G:172:LEU:HB3	1.85	0.59
2:E:137:GLU:O	2:E:138:VAL:HG22	2.02	0.59
2:E:120:LEU:O	2:E:124:ALA:CB	2.51	0.59
2:B:118:THR:C	2:B:120:LEU:H	2.06	0.59
2:E:99:ILE:HA	2:E:137:GLU:CG	2.32	0.59
2:E:137:GLU:O	2:E:138:VAL:CG2	2.51	0.58
2:H:74:ALA:CB	2:H:77:LEU:CD1	2.80	0.58
2:B:107:ILE:C	2:B:111:LYS:CG	2.63	0.58
2:E:132:ARG:HA	2:E:135:GLY:C	2.23	0.58
2:B:112:MET:HB2	2:B:113:PRO:CD	2.33	0.58
2:B:115:LEU:CD1	2:B:127:ILE:HD11	2.31	0.58
1:G:16:ILE:O	1:G:20:LEU:HB2	2.03	0.58
2:B:119:ASP:O	2:B:120:LEU:C	2.38	0.58
2:B:132:ARG:C	2:B:134:MET:H	2.07	0.58
2:E:132:ARG:HE	2:E:138:VAL:HG23	1.68	0.58
1:D:146:LEU:HD13	1:D:170:ARG:HB3	1.86	0.58
2:E:62:ASP:O	2:E:63:ARG:HB2	2.03	0.58
2:B:58:THR:HB	2:B:66:THR:HG22	1.86	0.58
2:B:126:MET:HE3	2:B:127:ILE:HG13	1.85	0.57
2:B:134:MET:N	2:B:135:GLY:CA	2.67	0.57
2:B:132:ARG:HG2	2:B:138:VAL:CG2	2.35	0.57
2:B:132:ARG:NH2	2:B:138:VAL:HG13	2.20	0.57
2:E:128:ALA:O	2:E:129:GLY:C	2.42	0.57
1:G:203:ARG:NH1	1:G:203:ARG:HG3	2.16	0.56
2:E:132:ARG:C	2:E:134:MET:N	2.58	0.56
2:E:132:ARG:CA	2:E:136:VAL:H	2.14	0.56
2:B:73:PRO:O	2:B:74:ALA:C	2.44	0.56
2:B:110:GLN:C	2:B:114:ASP:OD2	2.44	0.56
2:H:78:ILE:HG22	2:H:79:ARG:H	0.40	0.55
1:A:61:GLU:HG3	6:A:363:HOH:O	2.06	0.55
2:E:124:ALA:HA	2:E:127:ILE:HD11	1.87	0.55
1:D:170:ARG:HH11	1:D:170:ARG:CG	2.18	0.55
2:B:111:LYS:HA	2:B:114:ASP:HB2	1.87	0.55
1:A:205:ARG:HD2	1:A:234:ALA:O	2.05	0.55
2:B:108:ALA:HA	2:B:111:LYS:HG3	1.87	0.55
2:B:101:TRP:C	2:B:139:VAL:CG2	2.71	0.55
2:B:132:ARG:HG2	2:B:138:VAL:HG23	1.89	0.55
2:B:2:LYS:N	5:B:1:2MM:CA	2.68	0.55
1:D:176:LEU:HD23	1:D:203:ARG:HB3	1.88	0.55
2:B:104:VAL:O	2:B:108:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:ALA:CA	2:H:77:LEU:HG	2.37	0.55
2:H:78:ILE:O	2:H:79:ARG:C	2.45	0.54
2:B:101:TRP:HA	2:B:139:VAL:HG22	1.80	0.54
2:B:99:ILE:C	2:B:136:VAL:HG11	2.21	0.54
2:B:104:VAL:O	2:B:108:ALA:CB	2.55	0.54
2:E:2:LYS:N	6:E:149:HOH:O	2.40	0.54
1:D:170:ARG:HD3	1:D:182:PHE:CE2	2.43	0.54
2:B:107:ILE:O	2:B:111:LYS:HD2	2.04	0.54
2:E:130:SER:O	2:E:134:MET:HB2	2.08	0.54
2:B:112:MET:HB2	2:B:113:PRO:HD3	1.90	0.54
2:E:128:ALA:HB1	2:E:138:VAL:CG2	2.36	0.53
2:B:108:ALA:N	2:B:111:LYS:HG2	2.24	0.53
2:B:111:LYS:HG3	2:B:127:ILE:CD1	2.35	0.53
2:H:134:MET:H	2:H:135:GLY:HA2	1.74	0.53
2:E:120:LEU:CD2	2:E:121:GLU:N	2.72	0.53
2:E:120:LEU:CD2	2:E:121:GLU:H	2.22	0.53
1:G:161:ASN:HA	1:G:164:ARG:HD2	1.91	0.53
2:E:99:ILE:HA	2:E:136:VAL:HG12	1.91	0.53
1:A:144:LYS:HG2	1:D:119:ARG:HD2	1.91	0.53
2:B:107:ILE:CG2	2:B:111:LYS:CE	2.80	0.52
2:B:111:LYS:C	2:B:114:ASP:CB	2.64	0.52
2:E:99:ILE:CA	2:E:137:GLU:CG	2.88	0.52
1:A:3:VAL:HG22	1:A:38:PHE:CE2	2.45	0.52
2:E:120:LEU:HD23	2:E:121:GLU:N	2.24	0.52
2:B:42:ASN:O	2:B:46:ALA:N	2.43	0.52
2:H:133:SER:CB	2:H:133:SER:HG	2.12	0.52
2:E:111:LYS:C	2:E:113:PRO:N	2.63	0.52
2:E:18:THR:HB	2:E:19:PRO:HD2	1.91	0.52
1:G:25:ALA:HB2	1:G:39:PHE:CZ	2.45	0.52
2:B:107:ILE:HG22	2:B:111:LYS:NZ	2.24	0.51
1:G:13:LEU:HD22	1:G:16:ILE:HD11	1.91	0.51
1:A:14:ASP:HB3	1:A:15:PRO:HD3	1.93	0.51
1:A:148:VAL:HG12	1:A:172:LEU:HD23	1.91	0.51
1:D:67:LEU:HD23	2:E:63:ARG:CZ	2.41	0.51
2:H:2:LYS:HE2	2:H:60:TYR:CZ	2.46	0.51
2:E:99:ILE:CA	2:E:137:GLU:HG3	2.37	0.51
1:G:203:ARG:NE	1:G:206:GLU:OE1	2.36	0.51
2:B:100:THR:H	2:B:136:VAL:CG1	2.04	0.51
2:E:128:ALA:O	2:E:130:SER:CA	2.58	0.51
2:E:132:ARG:NE	2:E:138:VAL:CG2	2.73	0.51
1:G:3:VAL:HG22	1:G:5:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:CG2	2:B:111:LYS:HZ2	2.24	0.50
2:B:132:ARG:C	2:B:134:MET:N	2.65	0.50
1:D:106:THR:HG21	1:D:218:GLY:HA2	1.93	0.50
2:B:47:ASN:O	2:B:49:GLY:N	2.42	0.50
1:G:94:GLU:HG3	1:G:95:PRO:HD2	1.94	0.50
1:A:192:LEU:HD13	1:A:196:LEU:HD23	1.92	0.50
1:G:106:THR:HG21	1:G:218:GLY:HA2	1.94	0.50
2:B:101:TRP:HD1	2:B:102:GLU:CB	2.25	0.49
2:B:132:ARG:CG	2:B:138:VAL:CG2	2.91	0.49
1:D:237:ARG:NH2	1:G:168:ARG:HH21	2.10	0.49
2:H:134:MET:H	2:H:135:GLY:CA	2.26	0.49
2:E:128:ALA:C	2:E:131:ALA:N	2.56	0.49
2:B:18:THR:HB	2:B:19:PRO:HD2	1.94	0.49
1:A:58:ASP:HB2	1:A:60:LEU:H	1.77	0.49
2:B:119:ASP:CG	2:B:122:ALA:HB2	2.34	0.48
2:E:112:MET:HB3	2:E:113:PRO:CD	2.36	0.48
1:A:72:ALA:HB2	1:A:108:ARG:HG2	1.94	0.48
2:H:2:LYS:HA	5:H:1:2MM:C	2.42	0.48
2:E:99:ILE:CA	2:E:137:GLU:CB	2.65	0.48
2:E:131:ALA:O	2:E:136:VAL:N	2.38	0.48
2:B:128:ALA:HA	2:B:131:ALA:HB3	1.94	0.48
1:G:36:TRP:HE3	1:G:38:PHE:CZ	2.31	0.48
2:B:101:TRP:CG	2:B:102:GLU:N	2.81	0.48
1:A:246:GLU:CD	1:A:246:GLU:H	2.16	0.48
2:E:130:SER:O	2:E:134:MET:CB	2.62	0.48
1:D:237:ARG:NH2	1:G:168:ARG:NH2	2.62	0.48
2:H:18:THR:C	2:H:20:ALA:H	2.17	0.47
1:A:6:LEU:O	1:A:34:GLU:HA	2.14	0.47
2:E:2:LYS:HB3	2:E:60:TYR:CE1	2.49	0.47
1:D:254:ARG:HH11	1:D:254:ARG:HG3	1.79	0.47
2:B:107:ILE:O	2:B:111:LYS:HD3	2.00	0.47
1:G:94:GLU:HG3	1:G:95:PRO:CD	2.44	0.47
2:B:107:ILE:O	2:B:111:LYS:N	2.47	0.47
1:G:63:TRP:C	1:G:65:ARG:H	2.17	0.47
2:E:137:GLU:C	2:E:138:VAL:CG2	2.83	0.47
2:E:137:GLU:C	2:E:138:VAL:HG23	2.35	0.47
1:A:148:VAL:HG12	1:A:172:LEU:HD21	1.97	0.47
2:B:111:LYS:HB2	2:B:115:LEU:HD12	1.96	0.47
2:B:132:ARG:CZ	2:B:138:VAL:CG2	2.87	0.47
1:A:63:TRP:CZ3	1:A:64:ARG:HG2	2.50	0.47
2:B:101:TRP:HD1	2:B:102:GLU:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:NH1	1:D:170:ARG:CG	2.77	0.47
1:D:220:LEU:HG	5:E:1:2MM:HEB	1.97	0.46
1:G:7:LYS:CB	1:G:7:LYS:NZ	2.74	0.46
1:G:67:LEU:HD23	2:H:63:ARG:NE	2.30	0.46
2:E:112:MET:N	2:E:113:PRO:CD	2.76	0.46
1:D:31:ARG:O	1:D:32:GLU:C	2.54	0.46
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.80	0.46
1:G:31:ARG:O	1:G:32:GLU:C	2.54	0.46
2:B:99:ILE:CB	2:B:137:GLU:H	2.29	0.46
1:D:223:ARG:O	1:D:226:LEU:HB2	2.16	0.46
1:D:15:PRO:HA	2:E:134:MET:CE	2.46	0.46
2:E:123:ALA:C	2:E:125:ARG:H	2.19	0.46
1:D:59:TRP:CZ2	2:E:25:PRO:HB3	2.50	0.46
2:B:132:ARG:CD	2:B:138:VAL:CG2	2.91	0.46
2:B:71:THR:HA	2:B:72:PRO:HD3	1.71	0.46
2:E:29:GLN:HG3	2:E:30:HIS:ND1	2.31	0.46
2:H:120:LEU:O	2:H:120:LEU:HD23	2.16	0.46
1:G:219:ILE:HD12	6:G:350:HOH:O	2.16	0.45
1:D:119:ARG:HD3	6:D:364:HOH:O	2.15	0.45
1:G:67:LEU:HD23	2:H:63:ARG:HE	1.80	0.45
1:D:17:LEU:N	1:D:18:PRO:CD	2.79	0.45
1:D:222:ASP:N	1:D:222:ASP:OD2	2.49	0.45
1:D:17:LEU:HA	1:D:20:LEU:HD12	1.98	0.45
1:A:147:GLY:O	1:A:171:PHE:HA	2.16	0.45
1:A:104:HIS:HB2	2:B:62:ASP:HB3	1.98	0.45
2:H:76:TYR:CG	2:H:77:LEU:N	2.83	0.45
1:G:217:THR:HA	6:G:350:HOH:O	2.16	0.45
2:B:103:GLN:O	2:B:106:GLU:CA	2.65	0.45
1:A:47:TYR:O	1:A:48:GLU:HB2	2.17	0.45
1:G:236:PHE:CE2	1:G:254:ARG:HB3	2.52	0.45
2:E:132:ARG:CA	2:E:135:GLY:CA	2.95	0.44
2:E:123:ALA:O	2:E:127:ILE:CG1	2.48	0.44
2:E:101:TRP:CZ2	2:E:103:GLN:CB	2.99	0.44
1:G:63:TRP:CZ3	1:G:64:ARG:HG3	2.52	0.44
2:H:21:PRO:HA	2:H:25:PRO:HD2	2.00	0.44
1:G:4:TYR:OH	1:G:49:GLY:N	2.51	0.44
2:B:130:SER:O	2:B:131:ALA:C	2.56	0.44
2:E:134:MET:H	2:E:135:GLY:HA2	1.74	0.44
2:B:123:ALA:O	2:B:126:MET:N	2.51	0.44
2:H:78:ILE:HG23	2:H:79:ARG:N	2.17	0.44
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LYS:CB	2:B:115:LEU:HD12	2.47	0.44
1:D:146:LEU:HD12	1:D:170:ARG:HB3	1.99	0.44
2:H:2:LYS:N	3:H:148:IOD:I	3.21	0.44
1:G:36:TRP:HB3	1:G:38:PHE:CE1	2.53	0.44
1:A:160:ALA:O	1:A:164:ARG:HG3	2.17	0.44
2:B:138:VAL:O	2:B:139:VAL:CG1	2.65	0.43
2:B:102:GLU:OE1	2:B:139:VAL:O	2.36	0.43
2:H:117:THR:HG21	2:H:123:ALA:HB2	2.00	0.43
2:E:101:TRP:CE2	2:E:103:GLN:CB	3.00	0.43
1:D:28:LEU:HB2	2:E:11:GLN:HB2	2.00	0.43
2:B:127:ILE:O	2:B:131:ALA:N	2.25	0.43
1:A:3:VAL:HG11	1:A:36:TRP:CE3	2.53	0.43
2:E:139:VAL:CG1	2:E:140:GLY:N	2.49	0.43
1:G:63:TRP:CH2	1:G:81:TRP:CH2	3.06	0.43
1:D:224:ALA:N	1:D:225:PRO:CD	2.82	0.43
2:E:126:MET:O	2:E:127:ILE:C	2.57	0.43
1:D:168:ARG:HA	1:D:169:PRO:HD2	1.88	0.43
1:D:119:ARG:NH1	6:D:364:HOH:O	2.09	0.43
2:B:47:ASN:C	2:B:49:GLY:H	2.21	0.43
2:B:103:GLN:C	2:B:106:GLU:H	2.15	0.43
2:H:10:LEU:HB2	2:H:55:VAL:HG13	2.00	0.43
2:B:134:MET:CB	2:B:135:GLY:HA2	2.48	0.42
1:G:62:ALA:HA	1:G:65:ARG:CZ	2.49	0.42
1:G:39:PHE:CD1	1:G:39:PHE:N	2.87	0.42
1:D:254:ARG:O	1:D:254:ARG:HG3	2.18	0.42
2:E:121:GLU:CA	2:E:124:ALA:HB3	2.40	0.42
2:H:134:MET:N	2:H:135:GLY:HA2	2.33	0.42
2:B:72:PRO:HB3	2:B:73:PRO:HD3	2.01	0.42
2:H:111:LYS:O	2:H:115:LEU:HG	2.18	0.42
2:B:102:GLU:HG3	2:B:139:VAL:HG23	1.86	0.42
2:H:74:ALA:O	2:H:77:LEU:N	2.52	0.42
2:E:3:LYS:O	2:E:60:TYR:HA	2.19	0.42
2:B:103:GLN:O	2:B:106:GLU:CB	2.68	0.42
1:G:3:VAL:HG21	1:G:36:TRP:CE3	2.54	0.42
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.73	0.42
1:A:170:ARG:NH1	1:A:170:ARG:HG3	2.34	0.42
1:A:26:ARG:HH21	1:A:40:PRO:HG3	1.85	0.42
2:B:107:ILE:O	2:B:110:GLN:C	2.58	0.42
1:D:31:ARG:O	1:D:33:GLY:N	2.52	0.42
2:H:74:ALA:C	2:H:77:LEU:HG	2.40	0.42
4:D:303:SAH:H3'	2:E:2:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:ALA:O	2:H:77:LEU:CG	2.64	0.42
1:D:237:ARG:HA	1:D:238:PRO:HD3	1.92	0.42
2:B:17:ALA:HB2	2:B:41:PHE:CD2	2.55	0.42
2:B:45:THR:C	2:B:47:ASN:N	2.73	0.41
2:E:104:VAL:O	2:E:108:ALA:HB2	2.20	0.41
2:E:100:THR:N	2:E:137:GLU:HB2	2.35	0.41
1:G:21:PHE:CE1	2:H:52:ILE:HG21	2.55	0.41
2:B:128:ALA:O	2:B:129:GLY:C	2.59	0.41
1:A:193:TYR:HB3	5:B:1:2MM:HB	2.02	0.41
1:G:188:LEU:HD12	1:G:189:VAL:N	2.36	0.41
2:B:111:LYS:HB3	2:B:115:LEU:CD1	2.51	0.41
2:E:18:THR:O	2:E:23:VAL:HB	2.20	0.41
1:D:1:MET:HE2	1:D:38:PHE:HB3	2.03	0.41
2:E:132:ARG:CA	2:E:136:VAL:O	2.69	0.41
2:E:99:ILE:CA	2:E:136:VAL:CG1	2.99	0.41
1:G:63:TRP:HH2	1:G:81:TRP:CH2	2.37	0.41
1:D:243:ALA:HA	1:D:247:TRP:O	2.21	0.41
1:A:224:ALA:N	1:A:225:PRO:CD	2.83	0.41
2:B:102:GLU:O	2:B:104:VAL:N	2.54	0.40
2:B:138:VAL:HG12	2:B:139:VAL:N	2.35	0.40
2:H:15:GLY:HA2	2:H:42:ASN:HA	2.03	0.40
2:E:128:ALA:HB1	2:E:131:ALA:HB3	1.99	0.40
1:D:17:LEU:N	1:D:18:PRO:HD2	2.37	0.40
2:E:52:ILE:HD12	2:E:76:TYR:HB2	2.03	0.40
2:H:13:PRO:HA	2:H:51:ALA:O	2.21	0.40
2:B:101:TRP:HD1	2:B:102:GLU:HG3	1.87	0.40
1:D:187[B]:LEU:HD13	1:D:213:ARG:HB2	2.02	0.40
2:E:54:PRO:HG2	2:E:70:LYS:HB3	2.03	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:A:48:GLU:OE1	6:E:149:HOH:O[3_554]	2.16	0.04

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	249/254 (98%)	231 (93%)	16 (6%)	2 (1%)	24	51
1	D	249/254 (98%)	237 (95%)	10 (4%)	2 (1%)	24	51
1	G	248/254 (98%)	233 (94%)	12 (5%)	3 (1%)	16	39
2	B	117/146 (80%)	86 (74%)	20 (17%)	11 (9%)	1	1
2	E	109/146 (75%)	84 (77%)	15 (14%)	10 (9%)	1	1
2	H	117/146 (80%)	92 (79%)	18 (15%)	7 (6%)	2	3
All	All	1089/1200 (91%)	963 (88%)	91 (8%)	35 (3%)	5	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLY
2	B	75	SER
2	B	113	PRO
2	B	118	THR
2	B	120	LEU
2	E	112	MET
2	E	127	ILE
2	E	129	GLY
2	E	133	SER
1	G	10	LEU
1	G	64	ARG
2	H	73	PRO
2	H	75	SER
2	H	77	LEU
2	H	78	ILE
2	H	101	TRP
1	A	32	GLU
2	B	48	MET
2	B	124	ALA
2	B	133	SER

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Mol	Chain	Res	Type
2	B	139	VAL
2	E	74	ALA
2	E	136	VAL
2	E	139	VAL
2	B	77	LEU
1	D	32	GLU
2	E	111	LYS
1	G	32	GLU
2	B	112	MET
2	H	19	PRO
2	H	50	ASP
2	E	101	TRP
2	E	126	MET
2	B	72	PRO
1	D	15	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/189 (100%)	171 (91%)	17 (9%)	12	27
1	D	189/189 (100%)	181 (96%)	8 (4%)	36	68
1	G	187/189 (99%)	174 (93%)	13 (7%)	19	42
2	B	90/109 (83%)	82 (91%)	8 (9%)	12	27
2	E	84/109 (77%)	78 (93%)	6 (7%)	18	41
2	H	90/109 (83%)	85 (94%)	5 (6%)	26	54
All	All	828/894 (93%)	771 (93%)	57 (7%)	19	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	53	GLU
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	63	TRP
1	A	64	ARG
1	A	66	ASP
1	A	67	LEU
1	A	71	LEU
1	A	91	LEU
1	A	168	ARG
1	A	172	LEU
1	A	188	LEU
1	A	200	LEU
1	A	213	ARG
1	A	223	ARG
1	A	237	ARG
1	A	254	ARG
2	B	7	VAL
2	B	35	MET
2	B	59	ILE
2	B	66	THR
2	B	70	LYS
2	B	114	ASP
2	B	116	ASN
2	B	130	SER
1	D	7	LYS
1	D	61	GLU
1	D	64	ARG
1	D	91	LEU
1	D	168	ARG
1	D	203	ARG
1	D	237	ARG
1	D	254	ARG
2	E	7	VAL
2	E	66	THR
2	E	70	LYS
2	E	76	TYR
2	E	101	TRP
2	E	110	GLN
1	G	7	LYS
1	G	20	LEU
1	G	60	LEU
1	G	71	LEU
1	G	91	LEU
1	G	164	ARG

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Mol	Chain	Res	Type
1	G	177	GLU
1	G	180	LEU
1	G	188	LEU
1	G	200	LEU
1	G	203	ARG
1	G	221	LYS
1	G	226	LEU
2	H	7	VAL
2	H	70	LYS
2	H	76	TYR
2	H	116	ASN
2	H	138	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	11	GLN
2	E	30	HIS
2	E	110	GLN
2	H	29	GLN
2	H	110	GLN
2	H	116	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
4	SAH	A	303	-	20,28,28	1.32	2 (10%)	19,40,40	2.69	6 (31%)
5	2MM	B	1	2	7,9,10	0.55	0	6,10,12	2.37	2 (33%)
4	SAH	D	303	-	20,28,28	0.80	1 (5%)	19,40,40	3.16	5 (26%)
5	2MM	E	1	2	7,9,10	0.59	0	6,10,12	1.74	2 (33%)
4	SAH	G	303	-	20,28,28	2.06	6 (30%)	19,40,40	2.86	9 (47%)
5	2MM	H	1	2	7,9,10	0.59	0	6,10,12	2.80	2 (33%)

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
4	SAH	A	303	-	-	0/7/31/31	0/3/3/3
5	2MM	B	1	2	-	0/6/10/12	0/0/0/0
4	SAH	D	303	-	-	0/7/31/31	0/3/3/3
5	2MM	E	1	2	-	0/6/10/12	0/0/0/0
4	SAH	G	303	-	-	0/7/31/31	0/3/3/3
5	2MM	H	1	2	-	0/6/10/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	303	SAH	C3'-C4'	-2.09	1.47	1.53
4	A	303	SAH	O4'-C4'	-2.07	1.40	1.45
4	D	303	SAH	C2-N3	2.13	1.36	1.32
4	G	303	SAH	O2'-C2'	2.21	1.48	1.43
4	G	303	SAH	O3'-C3'	2.26	1.48	1.43
4	A	303	SAH	C2-N3	3.05	1.37	1.32
4	G	303	SAH	C2-N1	3.07	1.39	1.33
4	G	303	SAH	C5'-SD	4.31	1.89	1.81
4	G	303	SAH	C2-N3	5.02	1.41	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	303	SAH	N3-C2-N1	-11.31	120.23	128.89
4	A	303	SAH	N3-C2-N1	-8.48	122.40	128.89
4	G	303	SAH	C1'-N9-C4	-5.83	118.15	126.94
4	G	303	SAH	N3-C2-N1	-5.29	124.84	128.89
4	A	303	SAH	C5'-SD-CG	-4.45	89.05	102.41
5	B	1	2MM	CB-CA-C	-4.44	105.56	111.59
4	D	303	SAH	C2'-C1'-N9	-3.81	108.47	114.29
4	A	303	SAH	CB-CG-SD	-3.61	106.61	113.57
4	G	303	SAH	O3'-C3'-C4'	-3.60	100.24	111.05
4	G	303	SAH	O2'-C2'-C3'	-2.97	102.18	111.83
4	D	303	SAH	C4'-C5'-SD	-2.82	104.82	113.53
4	A	303	SAH	O4'-C1'-N9	-2.80	102.24	108.10
4	G	303	SAH	C5'-C4'-C3'	-2.67	108.05	114.98
4	A	303	SAH	C1'-N9-C4	-2.50	123.16	126.94
4	A	303	SAH	C4-C5-N7	-2.28	107.38	109.48
4	D	303	SAH	N6-C6-N1	-2.17	114.55	119.20
4	G	303	SAH	O4'-C4'-C3'	-2.08	100.96	105.15
5	E	1	2MM	CB-CA-C	2.10	114.44	111.59
5	B	1	2MM	CG-CB-CA	3.05	117.91	113.22
4	G	303	SAH	C2'-C3'-C4'	3.23	109.25	102.61
5	E	1	2MM	CG-CB-CA	3.58	118.72	113.22
4	G	303	SAH	N6-C6-N1	3.60	126.92	119.20
4	D	303	SAH	C4'-O4'-C1'	3.65	113.73	109.72
5	H	1	2MM	CE-SD-CG	3.93	113.80	100.37
4	G	303	SAH	C4'-O4'-C1'	4.82	115.01	109.72
5	H	1	2MM	CG-CB-CA	5.33	121.42	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	2MM	3	0
4	D	303	SAH	1	0
5	E	1	2MM	2	0
5	H	1	2MM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	253/254 (99%)	0.46	25 (9%) 9 7	38, 48, 80, 99	0
1	D	252/254 (99%)	0.44	22 (8%) 13 10	38, 48, 79, 83	0
1	G	252/254 (99%)	0.85	46 (18%) 2 1	38, 48, 81, 100	2 (0%)
2	B	121/146 (82%)	1.59	35 (28%) 1 0	58, 70, 96, 98	50 (41%)
2	E	115/146 (78%)	1.05	24 (20%) 1 1	57, 71, 96, 99	37 (32%)
2	H	121/146 (82%)	2.71	51 (42%) 0 0	59, 72, 99, 100	7 (5%)
All	All	1114/1200 (92%)	0.97	203 (18%) 2 1	38, 60, 86, 100	96 (8%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	104	VAL	13.7
2	H	105	LEU	12.6
2	B	101	TRP	12.5
2	B	104	VAL	11.3
2	H	137	GLU	10.7
2	E	105	LEU	10.2
2	H	134	MET	9.7
2	B	112	MET	9.7
2	E	108	ALA	9.0
2	H	112	MET	8.6
2	H	101	TRP	8.6
2	H	125	ARG	8.6
2	H	118	THR	8.5
2	B	105	LEU	8.2
2	H	113	PRO	8.1
1	G	41	ALA	8.1
2	B	118	THR	8.0
2	H	100	THR	7.8
2	H	108	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
2	H	141	ALA	7.7
2	H	126	MET	7.5
2	B	108	ALA	7.4
2	H	127	ILE	7.3
2	E	109	LYS	7.2
2	H	109	LYS	7.1
2	H	106	GLU	7.1
2	H	114	ASP	7.1
2	H	135	GLY	7.0
2	E	134	MET	7.0
2	B	110	GLN	6.9
2	H	121	GLU	6.9
2	H	107	ILE	6.7
2	H	123	ALA	6.6
2	B	117	THR	6.6
2	B	109	LYS	6.5
2	H	99	ILE	6.4
2	H	119	ASP	6.3
2	B	136	VAL	6.2
2	H	117	THR	6.1
1	G	23	GLY	6.0
2	H	128	ALA	6.0
1	A	189	VAL	5.7
2	H	139	VAL	5.7
2	H	102	GLU	5.5
1	G	190	ALA	5.5
1	G	2	TRP	5.4
2	E	139	VAL	5.3
2	B	107	ILE	5.3
2	H	138	VAL	5.2
1	G	24	GLY	5.2
2	E	100	THR	5.1
2	H	129	GLY	5.0
2	H	133	SER	4.9
2	H	51	ALA	4.7
1	G	189	VAL	4.7
2	H	103	GLN	4.7
1	A	191	ASN	4.6
1	A	107	THR	4.6
2	E	125	ARG	4.5
2	B	72	PRO	4.4
1	A	188	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	74	ALA	4.4
2	B	76	TYR	4.4
2	H	76	TYR	4.4
2	B	102	GLU	4.4
2	H	122	ALA	4.4
2	H	50	ASP	4.3
2	B	116	ASN	4.3
2	H	120	LEU	4.2
1	G	188	LEU	4.2
1	G	4	TYR	4.2
2	H	132	ARG	4.1
1	G	51	TRP	4.1
1	A	190	ALA	4.0
1	G	50	VAL	4.0
1	G	3	VAL	3.9
2	H	136	VAL	3.9
2	B	71	THR	3.9
1	G	110	ALA	3.9
2	E	112	MET	3.8
1	D	191	ASN	3.8
2	B	133	SER	3.8
2	B	138	VAL	3.7
2	B	106	GLU	3.7
2	B	123	ALA	3.7
2	H	140	GLY	3.7
2	E	121	GLU	3.7
1	G	55	GLY	3.7
2	H	130	SER	3.7
1	D	85	GLU	3.7
1	D	65	ARG	3.6
1	G	86	GLY	3.6
2	H	124	ALA	3.6
1	A	126	ASP	3.6
1	G	6	LEU	3.5
1	G	28	LEU	3.5
1	G	48	GLU	3.5
1	G	58	ASP	3.5
1	G	61	GLU	3.5
2	B	119	ASP	3.4
1	A	100	GLY	3.4
1	D	100	GLY	3.4
1	D	28	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	3.3
2	B	134	MET	3.3
1	G	134	LEU	3.3
2	E	126	MET	3.3
2	B	114	ASP	3.3
1	G	216	LEU	3.2
1	G	53	GLU	3.2
2	E	77	LEU	3.2
1	D	192	LEU	3.1
2	B	120	LEU	3.1
1	A	56	ASP	3.1
2	B	126	MET	3.1
2	H	52	ILE	3.1
1	A	134	LEU	3.1
2	E	99	ILE	3.1
1	G	49	GLY	3.1
1	G	60	LEU	3.1
1	D	189	VAL	3.1
1	G	191	ASN	3.0
2	H	49	GLY	3.0
1	A	54	VAL	3.0
1	D	190	ALA	3.0
2	E	128	ALA	3.0
1	G	64	ARG	3.0
1	G	16	ILE	2.9
1	A	59	TRP	2.9
1	G	59	TRP	2.9
1	A	127	LEU	2.9
1	G	5	ARG	2.9
1	G	42	PRO	2.9
1	A	2	TRP	2.9
1	A	1	MET	2.9
1	A	110	ALA	2.8
2	H	71	THR	2.8
2	B	130	SER	2.8
2	E	127	ILE	2.8
2	H	116	ASN	2.8
1	D	134	LEU	2.8
1	G	33	GLY	2.8
1	G	46	PRO	2.8
2	B	137	GLU	2.8
1	D	107	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	2.8
1	D	27	GLY	2.8
1	A	125	LEU	2.7
1	G	65	ARG	2.7
1	G	215	LEU	2.7
2	H	131	ALA	2.7
2	E	138	VAL	2.7
1	A	65	ARG	2.7
1	D	111	LEU	2.6
1	G	47	TYR	2.6
2	E	76	TYR	2.6
1	A	66	ASP	2.6
1	D	110	ALA	2.6
1	G	25	ALA	2.6
2	H	77	LEU	2.6
1	G	12	ALA	2.5
2	B	139	VAL	2.5
1	G	8	GLY	2.5
1	D	101	THR	2.5
2	H	115	LEU	2.5
2	E	45	THR	2.5
1	A	215	LEU	2.4
1	G	125	LEU	2.4
2	E	131	ALA	2.4
2	H	75	SER	2.4
2	B	73	PRO	2.4
1	D	114	LEU	2.4
1	D	133	VAL	2.4
1	A	192	LEU	2.4
1	A	43	VAL	2.4
2	E	74	ALA	2.4
1	G	126	ASP	2.4
1	G	113	ALA	2.3
1	A	216	LEU	2.3
2	B	77	LEU	2.3
1	G	54	VAL	2.3
2	E	101	TRP	2.3
2	E	10	LEU	2.3
1	D	99	PHE	2.3
2	B	14	ALA	2.3
2	H	46	ALA	2.3
2	B	113	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	78	ILE	2.2
2	B	46	ALA	2.2
2	E	11	GLN	2.2
2	E	140	GLY	2.2
1	G	1	MET	2.2
1	D	215	LEU	2.2
2	B	115	LEU	2.1
2	B	103	GLN	2.1
1	G	111	LEU	2.1
1	D	103	HIS	2.1
1	A	217	THR	2.1
1	G	40	PRO	2.1
1	D	222	ASP	2.1
1	D	106	THR	2.0
1	G	214	ALA	2.0
1	A	128	GLY	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, 95^{th} 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(Å^2)	Q<0.9
5	2MM	H	1	10/11	0.95	0.21	-0.18	51,52,62,64	0
5	2MM	B	1	10/11	0.93	0.18	-0.94	49,53,66,67	0
5	2MM	E	1	10/11	0.93	0.16	-1.12	45,50,57,64	0
4	SAH	A	303	26/26	0.95	0.14	-1.36	33,42,48,51	0
4	SAH	G	303	26/26	0.96	0.11	-1.63	35,39,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SAH	D	303	26/26	0.97	0.09	-1.92	32,41,44,47	0
3	IOD	B	148	1/1	1.00	0.02	-	59,59,59,59	1
3	IOD	H	148	1/1	0.99	0.04	-	81,81,81,81	1

6.5 Other polymers (i)

There are no such residues in this entry.