



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:56 AM GMT

PDB ID : 2I2X
Title : Crystal structure of methanol:cobalamin methyltransferase complex MtaBC from *Methanosarcina barkeri*
Authors : Hagemeier, C.H.; Kruer, M.; Thauer, R.K.; Warkentin, E.; Ermler, U.
Deposited on : 2006-08-17
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

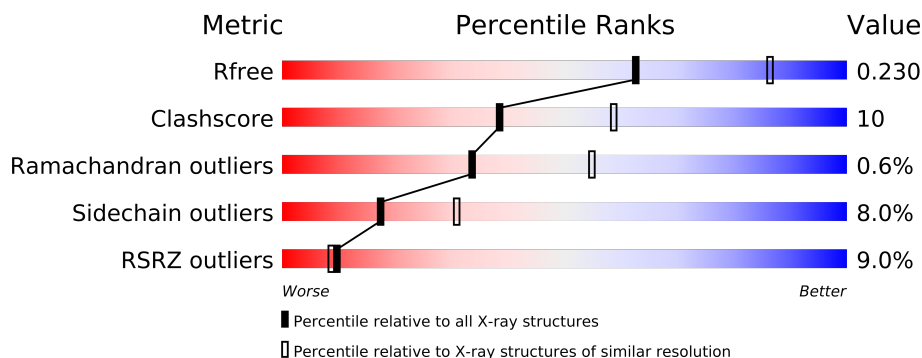
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	461	
1	C	461	
1	E	461	
1	G	461	
1	I	461	
1	K	461	
1	M	461	
1	O	461	
2	B	258	
2	D	258	
2	F	258	
2	H	258	
2	J	258	
2	L	258	

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Mol	Chain	Length	Quality of chain
2	N	258	
2	P	258	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45566 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	C	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	E	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	G	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	I	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	K	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	M	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	O	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			

- Molecule 2 is a protein called Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	D	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	F	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	H	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	J	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	L	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0
2	P	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	E	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	2	Total 2	Zn 2	0	0
3	O	1	Total 1	Zn 1	0	0
3	M	2	Total 2	Zn 2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

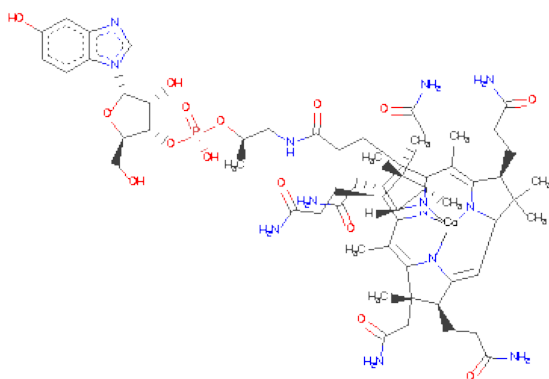
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	K 1	0	0
4	K	1	Total 1	K 1	0	0
4	E	1	Total 1	K 1	0	0
4	I	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0
4	O	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total K 1 1	0	0

- Molecule 5 is 5-HYDROXYBENZIMIDAZOLYLCOB(III)AMIDE (three-letter code: B13) (formula: $C_{60}H_{88}CoN_{13}O_{15}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	D	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	F	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	H	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	J	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	L	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	N	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	P	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		

- Molecule 6 is water.

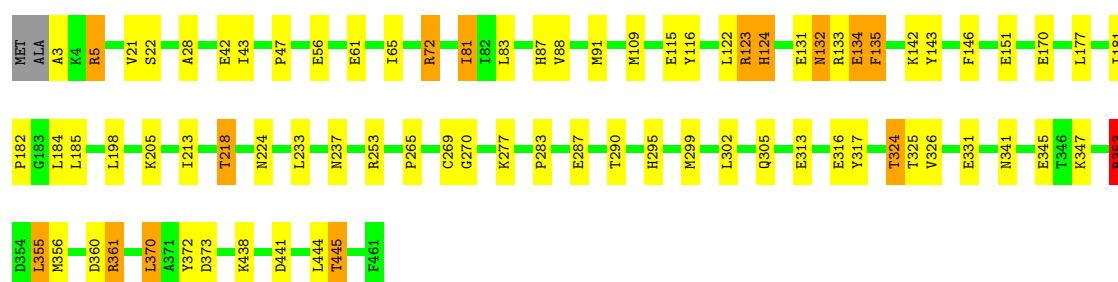
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total 162	O 162	0	0
6	B	36	Total 36	O 36	0	0
6	C	183	Total 183	O 183	0	0
6	D	27	Total 27	O 27	0	0
6	E	20	Total 20	O 20	0	0
6	F	6	Total 6	O 6	0	0
6	G	47	Total 47	O 47	0	0
6	H	1	Total 1	O 1	0	0
6	I	93	Total 93	O 93	0	0
6	J	15	Total 15	O 15	0	0
6	K	99	Total 99	O 99	0	0
6	L	18	Total 18	O 18	0	0
6	M	95	Total 95	O 95	0	0
6	N	18	Total 18	O 18	0	0
6	O	111	Total 111	O 111	0	0
6	P	15	Total 15	O 15	0	0

3 Residue-property plots

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.

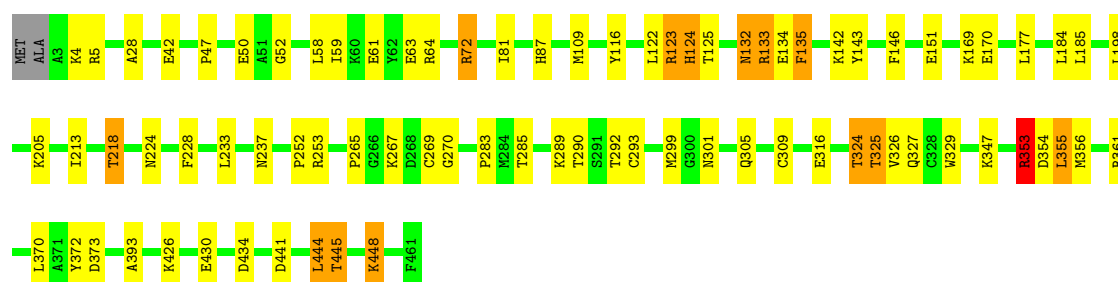
• Molecule 1: Methyltransferase 1

Chain A:



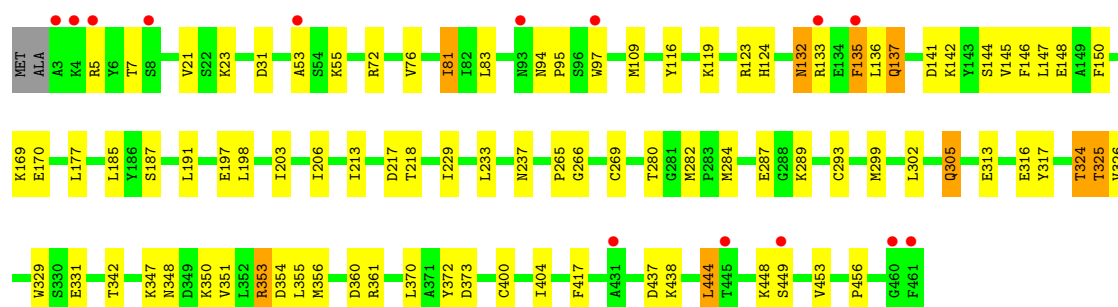
• Molecule 1: Methyltransferase 1

Chain C:



• Molecule 1: Methyltransferase 1

Chain E:



• Molecule 1: Methyltransferase 1

Age Group	Percentage
18-24	10%
25-34	85%
35-44	3%
45-54	2%
55-64	1%
65-74	1%
75-84	1%
85+	1%



Age Group	Percentage
18-24	15%
25-34	20%
35-44	25%
45-54	20%
55-64	15%
65-74	10%
75-84	5%
85+	5%



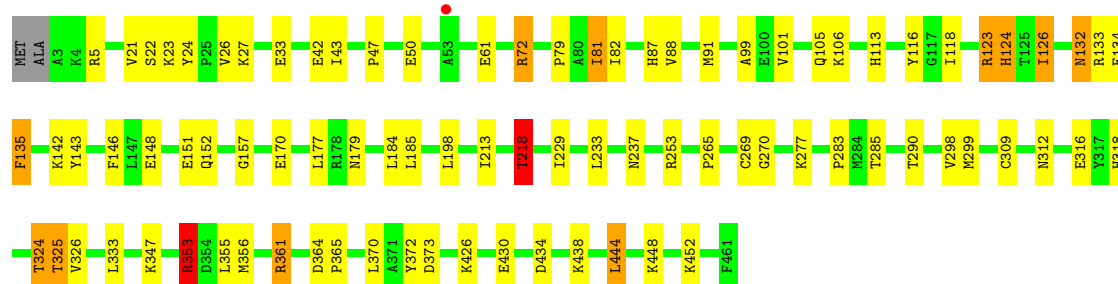
Age Group	Percentage
18-24	10%
25-34	75%
35-44	10%
45-54	3%
55-64	1%
65-74	1%
75-84	1%
85+	1%



Age Group	Percentage
18-24	15%
25-34	25%
35-44	30%
45-54	15%
55-64	10%
65-74	5%
75-84	2%
85+	1%

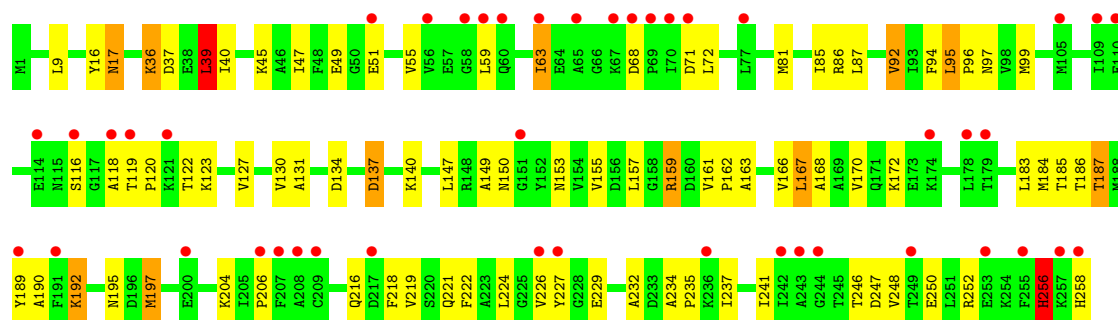


Chain O: 



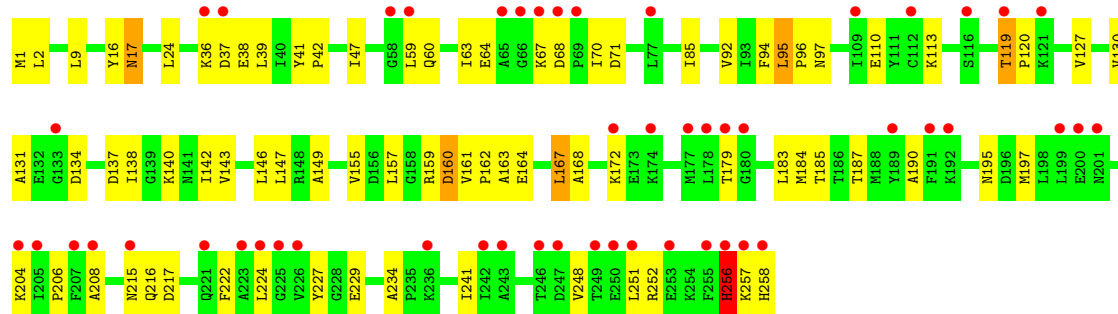
• Molecule 2: Methyltransferase 1

Chain B: 



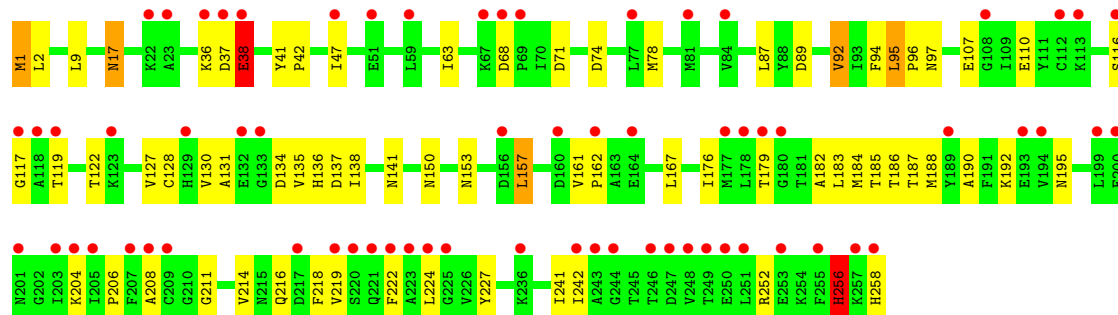
• Molecule 2: Methyltransferase 1

Chain D: 



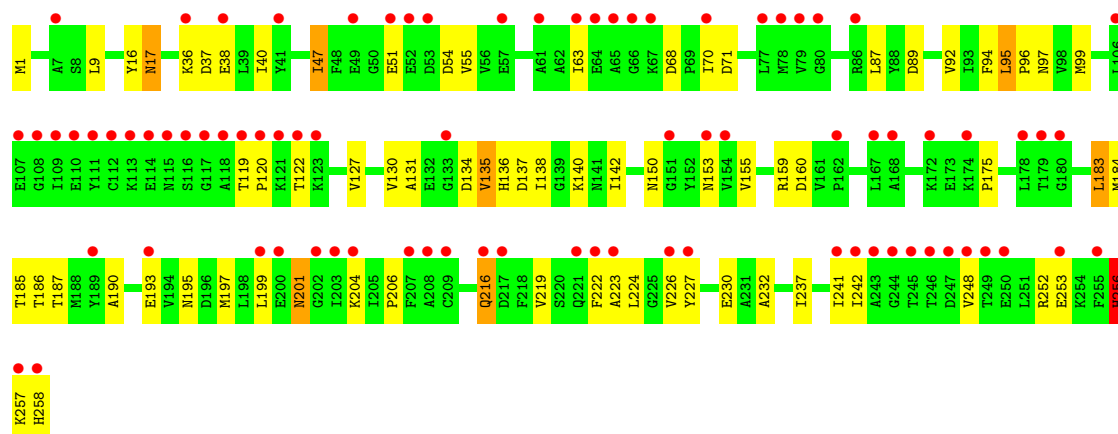
• Molecule 2: Methyltransferase 1

Chain F: 



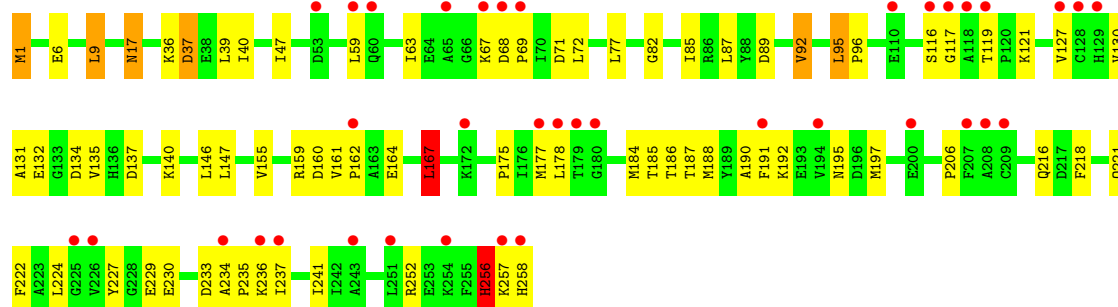
- Molecule 2: Methyltransferase 1

Chain H:



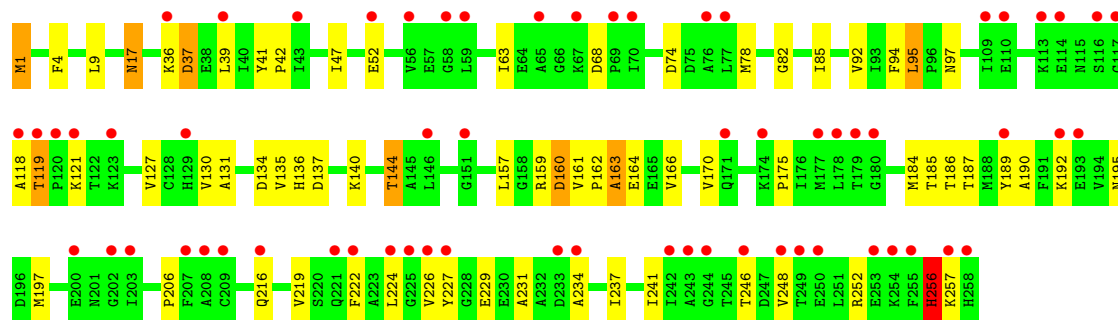
- Molecule 2: Methyltransferase 1

Chain J:



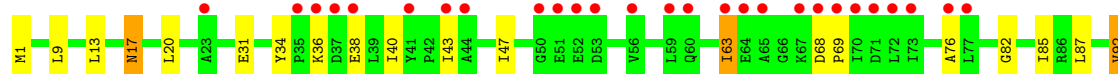
- Molecule 2: Methyltransferase 1

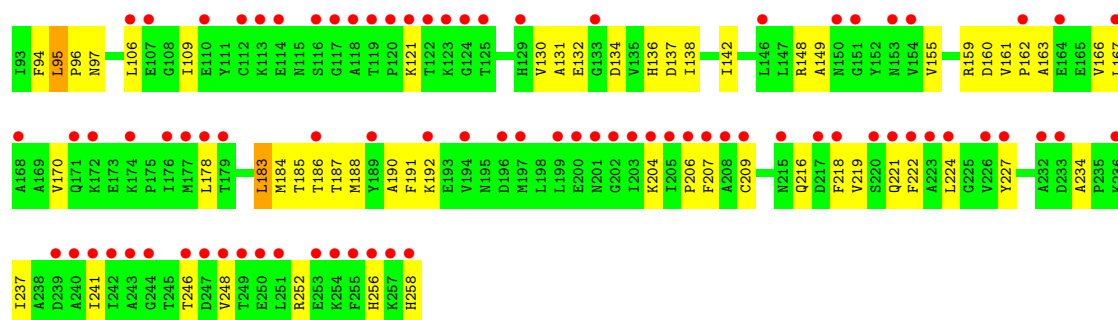
Chain L:



- Molecule 2: Methyltransferase 1

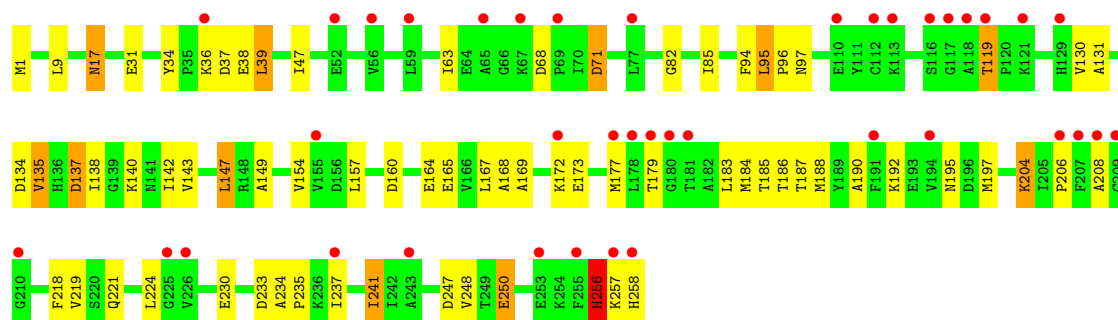
Chain N:





• Molecule 2: Methyltransferase 1

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.75Å 172.85Å 190.54Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.02 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.50) 98.5 (20.02-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.231 0.182 , 0.230	Depositor DCC
R_{free} test set	10921 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 218403 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45566	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, B13

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	0.72	1/3595 (0.0%)	0.78	5/4852 (0.1%)
1	C	0.70	0/3595	0.78	5/4852 (0.1%)
1	E	0.51	0/3595	0.62	0/4852
1	G	0.54	0/3595	0.64	1/4852 (0.0%)
1	I	0.60	0/3595	0.70	3/4852 (0.1%)
1	K	0.60	0/3595	0.68	2/4852 (0.0%)
1	M	0.60	0/3595	0.69	2/4852 (0.0%)
1	O	0.62	0/3595	0.72	6/4852 (0.1%)
2	B	0.48	0/1980	0.66	1/2682 (0.0%)
2	D	0.47	0/1980	0.65	0/2682
2	F	0.46	0/1980	0.59	0/2682
2	H	0.45	0/1980	0.59	0/2682
2	J	0.47	0/1980	0.63	1/2682 (0.0%)
2	L	0.46	0/1980	0.60	0/2682
2	N	0.48	0/1980	0.61	0/2682
2	P	0.48	0/1980	0.65	0/2682
All	All	0.57	1/44600 (0.0%)	0.68	26/60272 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CG-CD	5.18	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	361	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	361	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	353	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	M	123	ARG	NE-CZ-NH2	-7.65	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	361	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	218	THR	CB-CA-C	-6.62	93.72	111.60
1	O	218	THR	CB-CA-C	-6.48	94.09	111.60
1	O	123	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	123	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	M	123	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	O	361	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	353	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	218	THR	CB-CA-C	-5.70	96.20	111.60
1	I	218	THR	CB-CA-C	-5.60	96.49	111.60
1	O	353	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	K	361	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	I	123	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	123	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	123	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	B	39	LEU	CA-CB-CG	5.23	127.32	115.30
1	K	123	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	O	123	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	J	167	LEU	CA-CB-CG	5.11	127.04	115.30
1	G	361	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	353	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	355	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3534	0	3462	49	0
1	C	3534	0	3462	56	0
1	E	3534	0	3462	54	0
1	G	3534	0	3462	63	0
1	I	3534	0	3462	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3534	0	3462	61	0
1	M	3534	0	3462	54	0
1	O	3534	0	3462	57	0
2	B	1951	0	1952	64	0
2	D	1951	0	1952	55	0
2	F	1951	0	1952	54	0
2	H	1951	0	1952	52	0
2	J	1951	0	1952	53	0
2	L	1951	0	1952	49	0
2	N	1951	0	1952	50	0
2	P	1951	0	1952	47	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	I	2	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	O	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	B	90	0	81	9	0
5	D	90	0	81	13	0
5	F	90	0	81	7	0
5	H	90	0	81	10	0
5	J	90	0	81	13	0
5	L	90	0	81	10	0
5	N	90	0	81	11	0
5	P	90	0	81	9	0
6	A	162	0	0	4	0
6	B	36	0	0	1	0
6	C	183	0	0	3	0
6	D	27	0	0	0	0
6	E	20	0	0	0	0
6	F	6	0	0	0	0
6	G	47	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1	0	0	0	0
6	I	93	0	0	3	0
6	J	15	0	0	0	0
6	K	99	0	0	4	0
6	L	18	0	0	1	0
6	M	95	0	0	4	0
6	N	18	0	0	0	0
6	O	111	0	0	4	0
6	P	15	0	0	0	0
All	All	45566	0	43960	865	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (865) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:233:ASP:O	2:P:237:ILE:HG22	1.56	1.05
1:M:353:ARG:HA	1:M:356:MET:CE	1.92	0.99
1:K:353:ARG:HA	1:K:356:MET:CE	1.95	0.97
2:L:134:ASP:HB2	2:L:187:THR:HG21	1.46	0.94
2:B:17:ASN:HD22	2:B:17:ASN:H	1.14	0.91
2:F:134:ASP:HB2	2:F:187:THR:HG21	1.54	0.90
2:H:219:VAL:HG21	2:H:227:TYR:HB2	1.54	0.89
2:F:37:ASP:O	2:F:38:GLU:HB3	1.73	0.88
2:F:68:ASP:HB3	2:F:71:ASP:HB2	1.54	0.88
2:L:184:MET:HG2	5:L:500:B13:H302	1.55	0.87
2:F:184:MET:HG2	5:F:500:B13:H302	1.58	0.85
1:A:72:ARG:NH2	6:A:681:HOH:O	2.09	0.85
2:L:219:VAL:HG21	2:L:227:TYR:HB2	1.57	0.85
1:O:218:THR:HG21	1:O:269:CYS:SG	2.17	0.85
1:E:354:ASP:OD2	2:F:1:MET:HA	1.77	0.85
1:O:316:GLU:O	1:O:325:THR:HG21	1.77	0.84
2:J:17:ASN:HD22	2:J:17:ASN:H	1.24	0.84
2:B:167:LEU:HB2	2:B:197:MET:HE1	1.58	0.84
2:H:134:ASP:HB2	2:H:187:THR:HG21	1.58	0.84
2:P:177:MET:HE1	2:P:237:ILE:HG13	1.59	0.82
2:B:226:VAL:HG11	2:B:237:ILE:HD11	1.59	0.82
1:G:218:THR:HG21	1:G:269:CYS:SG	2.18	0.82
2:D:17:ASN:H	2:D:17:ASN:HD22	1.26	0.81
1:O:229:ILE:HD11	2:P:138:ILE:HD13	1.63	0.80
5:D:500:B13:H363	5:D:500:B13:H401	1.45	0.80
2:L:137:ASP:HB2	5:L:500:B13:H522	1.47	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:GLN:HA	1:A:356:MET:CE	2.12	0.79
2:N:134:ASP:HB2	2:N:187:THR:HG21	1.65	0.79
1:I:218:THR:HG21	1:I:269:CYS:SG	2.24	0.77
1:C:316:GLU:O	1:C:325:THR:HG21	1.85	0.77
1:A:316:GLU:O	1:A:325:THR:HG21	1.84	0.77
1:A:353:ARG:HA	1:A:356:MET:HE2	1.65	0.77
1:G:353:ARG:HA	1:G:356:MET:CE	2.16	0.76
1:E:316:GLU:O	1:E:325:THR:HG21	1.85	0.76
1:A:305:GLN:HA	1:A:356:MET:HE3	1.68	0.76
1:M:218:THR:HG21	1:M:269:CYS:SG	2.24	0.76
1:O:353:ARG:HA	1:O:356:MET:CE	2.14	0.76
2:N:137:ASP:HB2	5:N:500:B13:H522	1.50	0.76
1:E:280:THR:HB	1:E:282:MET:HG3	1.69	0.75
2:B:85:ILE:HD11	2:B:149:ALA:HB1	1.67	0.75
1:E:218:THR:HG21	1:E:269:CYS:SG	2.26	0.75
1:C:324:THR:HG22	1:C:327:GLN:HG3	1.68	0.74
2:P:195:ASN:HD21	2:P:224:LEU:H	1.35	0.74
1:G:353:ARG:HD3	1:G:372:TYR:CE1	2.22	0.74
2:J:68:ASP:HB3	2:J:71:ASP:HB2	1.68	0.73
1:M:353:ARG:HA	1:M:356:MET:HE1	1.71	0.73
1:C:324:THR:CG2	1:C:326:VAL:HG22	2.18	0.73
1:C:218:THR:HG21	1:C:269:CYS:SG	2.29	0.73
2:B:17:ASN:ND2	2:B:17:ASN:H	1.86	0.73
1:K:218:THR:HG21	1:K:269:CYS:SG	2.29	0.73
1:E:444:LEU:O	1:E:448:LYS:HB2	1.89	0.73
2:B:216:GLN:HE21	2:B:258:HIS:HD2	1.34	0.73
2:H:137:ASP:HB2	5:H:500:B13:H522	1.53	0.72
1:K:316:GLU:O	1:K:325:THR:HG21	1.88	0.72
2:N:191:PHE:HE2	2:N:209:CYS:HB3	1.52	0.72
2:L:131:ALA:HB1	2:L:190:ALA:HB3	1.71	0.72
1:K:72:ARG:NH2	6:K:587:HOH:O	2.22	0.72
2:F:185:THR:HG23	5:F:500:B13:H332	1.55	0.71
2:H:17:ASN:H	2:H:17:ASN:HD22	1.39	0.71
1:K:317:TYR:HE1	1:K:324:THR:HG21	1.56	0.71
2:P:94:PHE:H	2:P:97:ASN:HD22	1.37	0.71
1:A:218:THR:HG21	1:A:269:CYS:SG	2.31	0.70
2:H:219:VAL:CG2	2:H:227:TYR:HB2	2.22	0.70
1:I:361:ARG:NH2	1:I:373:ASP:OD1	2.24	0.70
1:I:353:ARG:HA	1:I:356:MET:HE2	1.73	0.70
1:M:316:GLU:O	1:M:325:THR:HG21	1.90	0.70
2:N:219:VAL:HG21	2:N:227:TYR:HB2	1.73	0.70
2:D:85:ILE:HD11	2:D:149:ALA:O	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:137:ASP:HB2	5:D:500:B13:H522	1.57	0.69
2:P:68:ASP:HB3	2:P:71:ASP:HB2	1.72	0.69
1:K:353:ARG:HA	1:K:356:MET:HE1	1.75	0.69
2:N:17:ASN:H	2:N:17:ASN:HD22	1.38	0.69
1:K:28:ALA:HB2	1:K:213:ILE:HD12	1.74	0.69
1:G:316:GLU:O	1:G:325:THR:HG21	1.91	0.69
2:F:219:VAL:HG21	2:F:227:TYR:HB2	1.74	0.69
2:H:94:PHE:H	2:H:97:ASN:HD22	1.41	0.69
2:J:184:MET:HG2	5:J:500:B13:H302	1.73	0.69
2:B:134:ASP:OD2	2:B:187:THR:HG21	1.92	0.69
2:B:130:VAL:HG23	2:B:140:LYS:HD3	1.74	0.69
2:P:134:ASP:HB2	2:P:187:THR:HG21	1.74	0.69
2:P:17:ASN:H	2:P:17:ASN:HD22	1.39	0.69
1:I:316:GLU:O	1:I:325:THR:HG21	1.91	0.69
5:P:500:B13:H601	5:P:500:B13:H262	1.75	0.68
1:I:354:ASP:OD2	2:J:1:MET:HA	1.94	0.68
1:C:28:ALA:HB2	1:C:213:ILE:HD13	1.76	0.68
1:K:26:VAL:CG1	1:K:213:ILE:HD13	2.23	0.68
2:B:185:THR:H	5:B:500:B13:H332	1.40	0.68
2:H:195:ASN:ND2	2:H:224:LEU:HB2	2.09	0.68
2:P:206:PRO:HG2	2:P:241:ILE:HD12	1.76	0.68
1:G:16:GLU:OE2	1:M:347:LYS:NZ	2.25	0.68
2:J:131:ALA:HB1	2:J:190:ALA:HB3	1.75	0.68
1:K:305:GLN:HA	1:K:356:MET:HE3	1.76	0.67
5:L:500:B13:H262	5:L:500:B13:H601	1.76	0.67
2:B:216:GLN:HE22	2:B:258:HIS:H	1.41	0.67
1:M:361:ARG:NH2	1:M:373:ASP:OD1	2.27	0.67
2:J:192:LYS:HG2	2:J:222:PHE:CE2	2.29	0.67
2:B:168:ALA:O	2:B:172:LYS:HG2	1.94	0.67
2:F:131:ALA:HB1	2:F:190:ALA:HB3	1.76	0.67
2:D:41:TYR:HB3	2:D:42:PRO:HD3	1.76	0.67
1:G:301:ASN:HD22	1:G:304:MET:CE	2.07	0.67
1:O:132:ASN:HD22	1:O:134:GLU:H	1.43	0.66
2:F:17:ASN:H	2:F:17:ASN:HD22	1.41	0.66
1:G:426:LYS:O	1:G:430:GLU:HG3	1.95	0.66
1:I:353:ARG:HD3	1:I:372:TYR:CE1	2.30	0.66
2:P:37:ASP:O	2:P:39:LEU:N	2.25	0.66
5:F:500:B13:H601	5:F:500:B13:H252	1.76	0.66
5:H:500:B13:H252	5:H:500:B13:H601	1.75	0.66
5:B:500:B13:H361	5:B:500:B13:H351	1.77	0.66
2:D:134:ASP:HB2	2:D:187:THR:HG21	1.77	0.66
1:C:132:ASN:ND2	1:C:135:PHE:H	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:317:TYR:HE1	1:I:324:THR:HG21	1.59	0.66
1:M:123:ARG:NH2	1:M:265:PRO:O	2.28	0.66
1:I:361:ARG:HH22	1:I:373:ASP:CG	2.00	0.65
1:G:301:ASN:HD22	1:G:304:MET:HE2	1.60	0.65
1:G:417:PHE:HZ	2:H:97:ASN:HD21	1.43	0.65
1:O:43:ILE:HG22	1:O:81:ILE:HD11	1.79	0.65
2:B:192:LYS:HG2	2:B:222:PHE:HE2	1.62	0.65
1:M:353:ARG:HD3	1:M:372:TYR:CE1	2.31	0.65
2:B:206:PRO:HG2	2:B:241:ILE:HD12	1.79	0.65
2:B:166:VAL:O	2:B:170:VAL:HG23	1.97	0.65
1:G:5:ARG:HA	1:G:259:GLU:HG2	1.80	0.64
2:F:195:ASN:HD21	2:F:224:LEU:H	1.43	0.64
2:N:184:MET:HG2	5:N:500:B13:H302	1.78	0.64
2:D:185:THR:H	5:D:500:B13:H332	1.46	0.64
1:I:305:GLN:HA	1:I:356:MET:CE	2.28	0.64
2:P:85:ILE:HD11	2:P:149:ALA:HB1	1.79	0.64
1:M:353:ARG:HA	1:M:356:MET:HE2	1.79	0.64
1:A:5:ARG:HD2	6:A:657:HOH:O	1.97	0.64
6:G:530:HOH:O	2:H:1:MET:HB3	1.97	0.64
2:J:17:ASN:N	2:J:17:ASN:HD22	1.94	0.64
1:C:353:ARG:HA	1:C:356:MET:HE2	1.78	0.64
2:J:87:LEU:HB3	2:J:92:VAL:HG22	1.79	0.63
2:D:216:GLN:HE21	2:D:258:HIS:HD2	1.46	0.63
5:J:500:B13:H351	5:J:500:B13:H361	1.80	0.63
1:G:302:LEU:HB2	1:G:360:ASP:HB2	1.81	0.63
2:F:17:ASN:HD22	2:F:17:ASN:N	1.96	0.63
2:F:216:GLN:HE22	2:F:258:HIS:H	1.45	0.63
1:G:132:ASN:C	1:G:132:ASN:HD22	2.01	0.63
5:D:500:B13:H363	5:D:500:B13:N40	2.14	0.63
2:B:137:ASP:HB2	5:B:500:B13:H522	1.64	0.63
2:N:185:THR:HG23	5:N:500:B13:H332	1.64	0.62
2:B:216:GLN:HE21	2:B:258:HIS:CD2	2.16	0.62
1:G:361:ARG:HH22	1:G:373:ASP:CG	2.03	0.62
1:C:353:ARG:HA	1:C:356:MET:CE	2.29	0.62
2:D:222:PHE:O	2:D:252:ARG:NH2	2.32	0.62
6:M:611:HOH:O	2:N:138:ILE:HG12	1.99	0.62
2:P:247:ASP:HB3	2:P:250:GLU:HB2	1.81	0.62
2:P:168:ALA:O	2:P:172:LYS:HG2	1.99	0.62
2:D:131:ALA:HB1	2:D:190:ALA:HB3	1.81	0.62
2:B:192:LYS:HG2	2:B:222:PHE:CE2	2.34	0.61
2:P:185:THR:HG23	5:P:500:B13:H332	1.65	0.61
2:D:168:ALA:O	2:D:172:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:195:ASN:HD21	2:B:224:LEU:H	1.47	0.61
2:D:215:ASN:HD22	2:D:217:ASP:H	1.48	0.61
1:K:133:ARG:HD2	2:L:160:ASP:HB3	1.80	0.61
1:O:72:ARG:NH2	6:O:616:HOH:O	2.33	0.61
1:C:42:GLU:OE2	1:C:123:ARG:HD2	2.00	0.61
2:P:177:MET:CE	2:P:237:ILE:HG13	2.30	0.61
1:G:460:GLY:HA2	6:G:554:HOH:O	2.00	0.61
1:E:305:GLN:HA	1:E:356:MET:HE3	1.82	0.61
2:J:195:ASN:HD21	2:J:224:LEU:H	1.47	0.61
1:M:305:GLN:HA	1:M:356:MET:HE3	1.82	0.61
1:O:132:ASN:ND2	1:O:134:GLU:H	1.98	0.61
1:M:426:LYS:HE3	1:M:430:GLU:OE2	2.00	0.61
2:P:131:ALA:HB1	2:P:190:ALA:HB3	1.81	0.61
2:N:94:PHE:H	2:N:97:ASN:HD22	1.49	0.61
1:C:426:LYS:O	1:C:430:GLU:HG3	2.01	0.61
5:D:500:B13:H361	5:D:500:B13:H351	1.83	0.61
2:N:94:PHE:H	2:N:97:ASN:ND2	1.98	0.60
2:F:94:PHE:H	2:F:97:ASN:HD22	1.48	0.60
2:H:135:VAL:HG22	2:H:159:ARG:HE	1.66	0.60
2:L:82:GLY:HA2	2:L:85:ILE:HD12	1.81	0.60
2:N:166:VAL:O	2:N:170:VAL:HG23	2.01	0.60
1:C:289:LYS:HD3	1:C:301:ASN:ND2	2.16	0.60
1:E:237:ASN:HA	2:F:95:LEU:HB2	1.83	0.60
1:O:132:ASN:ND2	1:O:135:PHE:H	1.98	0.60
1:C:4:LYS:HG2	6:O:629:HOH:O	2.02	0.60
2:F:252:ARG:O	2:F:256:HIS:HB2	2.00	0.60
1:M:133:ARG:HH11	1:M:133:ARG:CG	2.14	0.60
1:G:224:ASN:O	1:G:228:PHE:HD2	1.84	0.60
2:J:37:ASP:HB3	2:J:40:ILE:HB	1.84	0.60
2:L:224:LEU:HA	2:L:248:VAL:HG21	1.83	0.59
1:I:312:ASN:HB3	1:I:333:LEU:HD11	1.85	0.59
1:A:42:GLU:OE2	1:A:123:ARG:HD2	2.03	0.59
2:F:179:THR:HG22	2:F:208:ALA:HB3	1.85	0.59
2:L:222:PHE:O	2:L:252:ARG:NH2	2.36	0.59
1:C:324:THR:HG23	1:C:326:VAL:HG22	1.85	0.59
2:N:224:LEU:HA	2:N:248:VAL:HG21	1.83	0.59
2:N:40:ILE:HA	2:N:43:ILE:HD12	1.85	0.59
5:H:500:B13:O58	5:H:500:B13:H532	2.02	0.59
2:N:219:VAL:CG2	2:N:227:TYR:HB2	2.33	0.59
2:B:206:PRO:HG2	2:B:241:ILE:CD1	2.33	0.58
2:J:216:GLN:HE21	2:J:258:HIS:HD2	1.49	0.58
1:K:317:TYR:CE1	1:K:324:THR:HG21	2.35	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:184:MET:HG2	5:P:500:B13:H302	1.85	0.58
2:N:137:ASP:HB2	5:N:500:B13:N52	2.18	0.58
1:E:444:LEU:CD2	1:E:448:LYS:HD2	2.32	0.58
2:J:185:THR:HG23	5:J:500:B13:H332	1.68	0.58
2:B:94:PHE:H	2:B:97:ASN:HD22	1.51	0.58
2:L:17:ASN:HD22	2:L:17:ASN:H	1.52	0.58
1:M:42:GLU:OE2	1:M:123:ARG:HD2	2.03	0.58
2:H:130:VAL:HG23	2:H:140:LYS:HD3	1.86	0.58
2:D:94:PHE:H	2:D:97:ASN:HD22	1.51	0.58
1:K:293:CYS:HB3	1:K:329:TRP:CZ2	2.39	0.58
2:J:185:THR:H	5:J:500:B13:H332	1.50	0.58
1:G:18:THR:HG23	1:G:21:VAL:HG13	1.86	0.58
1:E:132:ASN:ND2	1:E:135:PHE:H	2.02	0.58
1:I:444:LEU:HD22	1:I:448:LYS:HD2	1.85	0.58
2:B:189:TYR:O	2:B:192:LYS:HB2	2.04	0.58
2:P:234:ALA:HB3	2:P:235:PRO:HD3	1.85	0.58
1:E:373:ASP:HB3	2:F:1:MET:HE3	1.86	0.57
1:I:305:GLN:HA	1:I:356:MET:HE3	1.84	0.57
2:B:184:MET:HG2	5:B:500:B13:H302	1.84	0.57
1:I:444:LEU:O	1:I:448:LYS:HB2	2.04	0.57
1:G:353:ARG:HA	1:G:356:MET:HE3	1.84	0.57
2:H:37:ASP:O	2:H:38:GLU:HB3	2.04	0.57
2:H:185:THR:HG23	5:H:500:B13:H332	1.68	0.57
2:B:36:LYS:H	2:B:36:LYS:HD3	1.69	0.57
1:E:444:LEU:HD22	1:E:448:LYS:HD2	1.85	0.57
2:H:199:LEU:C	2:H:201:ASN:H	2.07	0.57
2:H:17:ASN:N	2:H:17:ASN:HD22	2.03	0.57
2:J:216:GLN:HE21	2:J:258:HIS:CD2	2.21	0.57
1:K:132:ASN:C	1:K:132:ASN:HD22	2.07	0.57
2:P:138:ILE:O	2:P:142:ILE:HG13	2.04	0.57
2:P:185:THR:H	5:P:500:B13:H332	1.51	0.57
1:O:42:GLU:OE2	1:O:123:ARG:HD2	2.04	0.57
2:L:130:VAL:HG12	2:L:134:ASP:HB3	1.87	0.57
5:N:500:B13:H262	5:N:500:B13:H601	1.87	0.57
1:G:231:GLY:HA3	1:G:235:ASN:ND2	2.20	0.57
2:B:195:ASN:ND2	2:B:224:LEU:H	2.03	0.57
2:H:197:MET:HG2	2:H:197:MET:O	2.04	0.57
1:K:169:LYS:HD2	5:L:500:B13:H473	1.87	0.57
2:H:184:MET:HG2	5:H:500:B13:H302	1.86	0.57
2:L:127:VAL:HG23	2:L:175:PRO:HG3	1.85	0.57
2:B:94:PHE:H	2:B:97:ASN:ND2	2.03	0.56
1:M:444:LEU:O	1:M:448:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:17:ASN:HD22	2:D:17:ASN:N	2.02	0.56
1:C:305:GLN:HA	1:C:356:MET:CE	2.35	0.56
2:B:226:VAL:HG11	2:B:237:ILE:CD1	2.31	0.56
5:D:500:B13:H601	5:D:500:B13:H262	1.87	0.56
2:N:252:ARG:O	2:N:256:HIS:HB2	2.05	0.56
2:P:188:MET:HB3	2:P:218:PHE:CZ	2.41	0.56
1:G:123:ARG:NH2	1:G:265:PRO:O	2.39	0.56
2:D:37:ASP:O	2:D:39:LEU:N	2.29	0.56
1:E:448:LYS:HE3	1:E:456:PRO:HG2	1.86	0.56
1:A:265:PRO:HA	1:A:283:PRO:O	2.06	0.56
1:K:132:ASN:ND2	1:K:135:PHE:H	2.03	0.56
1:E:229:ILE:HD11	2:F:138:ILE:HD13	1.88	0.56
1:A:132:ASN:ND2	1:A:135:PHE:H	2.03	0.56
1:O:444:LEU:O	1:O:448:LYS:HB2	2.06	0.56
2:N:131:ALA:HB1	2:N:190:ALA:HB3	1.86	0.56
1:E:353:ARG:HD3	1:E:372:TYR:CE1	2.40	0.56
2:N:216:GLN:HE22	2:N:258:HIS:H	1.54	0.56
1:M:87:HIS:NE2	1:M:124:HIS:HD2	2.04	0.56
2:B:45:LYS:HE3	2:B:49:GLU:OE2	2.05	0.56
1:C:293:CYS:HB3	1:C:329:TRP:CZ2	2.40	0.56
1:K:354:ASP:OD2	2:L:1:MET:HA	2.06	0.56
5:F:500:B13:H351	5:F:500:B13:H361	1.88	0.55
2:J:37:ASP:O	2:J:39:LEU:N	2.30	0.55
1:K:5:ARG:NH2	6:K:611:HOH:O	2.30	0.55
2:F:137:ASP:HB3	2:F:141:ASN:ND2	2.21	0.55
2:B:68:ASP:HB3	2:B:71:ASP:HB2	1.88	0.55
1:G:444:LEU:O	1:G:448:LYS:HB2	2.06	0.55
2:D:138:ILE:HG13	5:D:500:B13:O51	2.06	0.55
1:O:312:ASN:HB3	1:O:333:LEU:HD11	1.88	0.55
1:I:123:ARG:NH2	1:I:265:PRO:O	2.40	0.55
2:J:218:PHE:O	2:J:221:GLN:HG2	2.07	0.55
2:F:176:ILE:HD13	2:F:242:ILE:HD11	1.87	0.55
6:I:562:HOH:O	2:J:96:PRO:HG2	2.07	0.55
1:A:47:PRO:HB3	1:A:61:GLU:HG2	1.88	0.55
2:P:130:VAL:HG23	2:P:140:LYS:HD3	1.88	0.55
5:B:500:B13:H262	5:B:500:B13:H601	1.89	0.55
2:J:59:LEU:HD11	2:J:77:LEU:HD21	1.88	0.55
2:N:106:LEU:HD11	2:N:148:ARG:HD3	1.88	0.55
1:O:132:ASN:C	1:O:132:ASN:HD22	2.10	0.55
2:H:222:PHE:O	2:H:252:ARG:NH2	2.39	0.55
1:O:99:ALA:HB2	1:O:152:GLN:HB3	1.89	0.54
1:O:265:PRO:HA	1:O:283:PRO:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:131:ALA:HB1	2:H:190:ALA:HB3	1.89	0.54
2:H:136:HIS:HB3	2:H:183:LEU:HD13	1.89	0.54
2:H:87:LEU:HD22	2:H:92:VAL:HG21	1.89	0.54
2:H:195:ASN:HD21	2:H:224:LEU:H	1.54	0.54
1:C:72:ARG:NH2	6:C:515:HOH:O	2.39	0.54
1:E:342:THR:HG22	1:G:355:LEU:HD12	1.90	0.54
1:G:132:ASN:ND2	1:G:134:GLU:H	2.04	0.54
2:D:127:VAL:HG13	2:D:157:LEU:HD23	1.89	0.54
1:A:353:ARG:HA	1:A:356:MET:CE	2.36	0.54
2:P:164:GLU:HA	2:P:197:MET:HE1	1.89	0.54
2:B:127:VAL:HG13	2:B:157:LEU:HD23	1.89	0.54
1:G:187:SER:HA	1:G:191:LEU:HD12	1.89	0.54
1:M:224:ASN:ND2	1:M:269:CYS:HB2	2.22	0.54
1:K:69:VAL:O	1:K:73:MET:HG2	2.08	0.54
1:I:441:ASP:O	1:I:445:THR:HG23	2.07	0.54
2:H:51:GLU:O	2:H:55:VAL:HG23	2.08	0.54
1:O:353:ARG:HD3	1:O:372:TYR:CE1	2.43	0.54
1:O:143:TYR:O	1:O:146:PHE:HB3	2.07	0.54
1:M:224:ASN:HD21	1:M:269:CYS:HB2	1.73	0.54
1:C:265:PRO:HA	1:C:283:PRO:O	2.07	0.54
1:M:43:ILE:HG22	1:M:81:ILE:HD11	1.90	0.54
1:K:444:LEU:O	1:K:448:LYS:HB2	2.08	0.54
2:L:134:ASP:OD1	2:L:136:HIS:ND1	2.32	0.53
1:E:354:ASP:HB3	2:F:2:LEU:HD12	1.90	0.53
1:O:132:ASN:HD22	1:O:134:GLU:N	2.05	0.53
2:P:218:PHE:O	2:P:221:GLN:HG2	2.08	0.53
2:L:166:VAL:O	2:L:170:VAL:HG23	2.08	0.53
2:F:192:LYS:HG2	2:F:222:PHE:CE2	2.42	0.53
1:O:353:ARG:HA	1:O:356:MET:HE3	1.88	0.53
2:D:216:GLN:HE21	2:D:258:HIS:CD2	2.26	0.53
2:D:179:THR:HG22	2:D:208:ALA:HB3	1.90	0.53
2:P:195:ASN:ND2	2:P:224:LEU:H	2.06	0.53
1:K:132:ASN:HD21	1:K:135:PHE:H	1.56	0.53
1:O:361:ARG:HH22	1:O:373:ASP:CG	2.11	0.53
1:M:131:GLU:HB2	1:M:136:LEU:HA	1.91	0.53
1:A:302:LEU:HB2	1:A:360:ASP:HB2	1.91	0.53
2:D:206:PRO:HG2	2:D:241:ILE:HD12	1.91	0.53
1:K:109:MET:HE1	1:K:122:LEU:HD13	1.91	0.53
1:G:132:ASN:HD21	1:G:134:GLU:HG2	1.74	0.53
1:M:89:GLN:NE2	1:M:90:GLN:HB3	2.24	0.53
2:L:219:VAL:CG2	2:L:227:TYR:HB2	2.35	0.52
2:D:17:ASN:ND2	2:D:17:ASN:H	2.03	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:135:VAL:CG1	2:F:135:VAL:O	2.57	0.52
5:J:500:B13:H401	5:J:500:B13:H363	1.73	0.52
2:H:230:GLU:HG3	2:H:232:ALA:H	1.74	0.52
2:H:206:PRO:HG2	2:H:241:ILE:HD12	1.90	0.52
2:B:167:LEU:HB2	2:B:197:MET:CE	2.36	0.52
1:A:3:ALA:HB2	6:A:675:HOH:O	2.09	0.52
1:M:353:ARG:CA	1:M:356:MET:HE1	2.39	0.52
1:M:435:ASP:OD2	1:M:438:LYS:HB2	2.09	0.52
1:E:331:GLU:HB3	1:G:292:THR:HG21	1.90	0.52
1:O:218:THR:HG23	1:O:270:GLY:N	2.25	0.52
1:K:290:THR:O	1:K:290:THR:HG22	2.10	0.52
2:D:215:ASN:ND2	2:D:217:ASP:H	2.08	0.52
2:N:216:GLN:HE21	2:N:258:HIS:HD2	1.55	0.52
2:H:136:HIS:CB	2:H:183:LEU:HD13	2.40	0.52
1:M:64:ARG:NE	6:M:565:HOH:O	2.42	0.52
1:I:218:THR:HG23	1:I:270:GLY:CA	2.39	0.52
2:N:191:PHE:CE2	2:N:209:CYS:HB3	2.40	0.52
1:O:132:ASN:HD21	1:O:135:PHE:H	1.58	0.52
1:M:169:LYS:HD2	5:N:500:B13:H473	1.92	0.52
1:M:99:ALA:HB2	1:M:152:GLN:HB3	1.92	0.52
1:G:229:ILE:HD11	2:H:138:ILE:HD13	1.90	0.52
1:E:324:THR:CG2	1:E:326:VAL:HG22	2.40	0.52
1:K:353:ARG:HA	1:K:356:MET:HE2	1.83	0.51
2:F:227:TYR:H	2:F:256:HIS:HE1	1.58	0.51
2:F:128:CYS:O	2:F:157:LEU:HB2	2.10	0.51
1:C:133:ARG:HD2	2:D:160:ASP:HB3	1.91	0.51
1:C:305:GLN:HA	1:C:356:MET:HE3	1.91	0.51
2:H:122:THR:HG21	2:H:153:ASN:HB2	1.92	0.51
1:G:364:ASP:CG	1:G:365:PRO:HD2	2.31	0.51
2:F:184:MET:HE1	5:F:500:B13:H353	1.92	0.51
1:I:218:THR:HG23	1:I:270:GLY:N	2.26	0.51
2:B:184:MET:HB2	2:B:187:THR:HB	1.92	0.51
2:J:37:ASP:C	2:J:39:LEU:H	2.14	0.51
2:H:95:LEU:HB3	2:H:96:PRO:HD3	1.93	0.51
1:O:23:LYS:HD3	1:O:24:TYR:CZ	2.46	0.51
1:M:132:ASN:HD21	1:M:135:PHE:H	1.59	0.51
5:B:500:B13:H252	5:B:500:B13:C61	2.41	0.51
1:A:109:MET:HE3	1:A:122:LEU:HD13	1.91	0.51
1:K:27:LYS:HG2	1:K:33:GLU:HG2	1.92	0.51
2:J:167:LEU:HG	2:J:197:MET:HG2	1.91	0.51
1:O:87:HIS:NE2	1:O:124:HIS:HD2	2.08	0.51
1:E:280:THR:HB	1:E:282:MET:CG	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:353:ARG:HA	1:O:356:MET:HE2	1.92	0.51
1:I:132:ASN:HD22	1:I:132:ASN:C	2.14	0.51
1:C:125:THR:HG21	1:C:267:LYS:HE2	1.93	0.51
1:A:109:MET:CE	1:A:122:LEU:HD13	2.41	0.51
1:A:143:TYR:O	1:A:146:PHE:HB3	2.11	0.51
1:I:109:MET:HE3	1:I:122:LEU:HD22	1.93	0.50
1:K:237:ASN:HA	2:L:95:LEU:HB2	1.92	0.50
2:L:159:ARG:O	2:L:161:VAL:N	2.44	0.50
1:K:50:GLU:CD	1:K:50:GLU:H	2.14	0.50
1:M:137:GLN:HG2	6:M:612:HOH:O	2.11	0.50
1:I:237:ASN:HA	2:J:95:LEU:HB2	1.93	0.50
2:P:179:THR:HG22	2:P:208:ALA:HB3	1.93	0.50
1:A:353:ARG:HD3	1:A:372:TYR:CE1	2.46	0.50
2:F:94:PHE:H	2:F:97:ASN:ND2	2.09	0.50
1:E:31:ASP:O	1:E:119:LYS:HG2	2.10	0.50
2:L:135:VAL:HG22	2:L:159:ARG:HE	1.77	0.50
2:N:206:PRO:HG2	2:N:241:ILE:HD12	1.92	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CE2	2.47	0.50
1:A:324:THR:CG2	1:A:326:VAL:HG22	2.42	0.50
2:P:167:LEU:HB2	2:P:197:MET:CE	2.41	0.50
2:P:167:LEU:HB2	2:P:197:MET:HE1	1.93	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CZ2	2.46	0.50
2:B:162:PRO:O	2:B:163:ALA:HB3	2.12	0.50
2:F:122:THR:HG21	2:F:153:ASN:HB2	1.94	0.50
2:D:184:MET:HG2	5:D:500:B13:H302	1.94	0.50
2:L:195:ASN:HD21	2:L:224:LEU:H	1.60	0.50
2:L:41:TYR:HB3	2:L:42:PRO:HD3	1.92	0.50
2:F:195:ASN:ND2	2:F:224:LEU:HB2	2.27	0.50
2:B:234:ALA:HB3	2:B:235:PRO:HD3	1.93	0.50
2:P:230:GLU:O	2:P:233:ASP:HB2	2.11	0.50
1:A:305:GLN:HA	1:A:356:MET:HE1	1.91	0.50
1:C:28:ALA:HB2	1:C:213:ILE:CD1	2.41	0.50
1:C:59:ILE:O	1:C:63:GLU:HG3	2.12	0.50
1:K:353:ARG:HD3	1:K:372:TYR:CE1	2.47	0.49
1:E:400:CYS:O	1:E:404:ILE:HG12	2.12	0.49
1:I:18:THR:CG2	1:I:21:VAL:HG13	2.42	0.49
2:J:195:ASN:ND2	2:J:224:LEU:HB2	2.27	0.49
1:K:361:ARG:HH22	1:K:373:ASP:CG	2.15	0.49
1:C:361:ARG:HH22	1:C:373:ASP:CG	2.15	0.49
2:J:134:ASP:OD2	2:J:187:THR:HG21	2.11	0.49
1:G:132:ASN:ND2	1:G:134:GLU:HG2	2.28	0.49
2:F:135:VAL:HG12	2:F:135:VAL:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:361:ARG:NH2	1:K:373:ASP:OD1	2.45	0.49
1:M:353:ARG:CA	1:M:356:MET:CE	2.80	0.49
2:H:223:ALA:O	2:H:248:VAL:HG11	2.13	0.49
2:P:31:GLU:HA	2:P:34:TYR:CD1	2.48	0.49
1:O:133:ARG:NH2	2:P:165:GLU:OE2	2.46	0.49
2:N:138:ILE:HG13	5:N:500:B13:C50	2.43	0.49
1:O:132:ASN:HD21	1:O:134:GLU:HG2	1.76	0.49
2:F:127:VAL:HG13	2:F:157:LEU:HD23	1.93	0.49
2:N:31:GLU:HA	2:N:34:TYR:CD1	2.48	0.49
1:A:317:TYR:HA	1:A:325:THR:HG21	1.93	0.49
2:F:116:SER:OG	2:F:117:GLY:N	2.44	0.49
2:D:185:THR:HG23	5:D:500:B13:H332	1.78	0.49
1:M:218:THR:HG23	1:M:270:GLY:N	2.27	0.49
1:K:42:GLU:OE2	1:K:123:ARG:HD2	2.12	0.49
2:B:252:ARG:HG2	2:B:256:HIS:CE1	2.48	0.49
1:O:113:HIS:HD2	1:O:118:ILE:O	1.96	0.49
2:B:17:ASN:HD22	2:B:17:ASN:N	1.95	0.49
1:I:317:TYR:CE1	1:I:324:THR:HG21	2.44	0.49
2:H:195:ASN:HD22	2:H:224:LEU:HB2	1.78	0.49
1:I:148:GLU:O	1:I:152:GLN:HG2	2.11	0.49
1:E:317:TYR:HA	1:E:325:THR:CG2	2.43	0.48
1:M:265:PRO:HA	1:M:283:PRO:O	2.12	0.48
1:K:60:LYS:HE3	1:K:64:ARG:HE	1.78	0.48
1:I:81:ILE:HD13	1:I:82:ILE:O	2.13	0.48
1:G:133:ARG:HD2	2:H:160:ASP:HB3	1.95	0.48
2:F:37:ASP:O	2:F:38:GLU:CB	2.54	0.48
5:H:500:B13:H363	5:H:500:B13:H401	1.79	0.48
1:E:136:LEU:HD21	1:E:169:LYS:HE3	1.96	0.48
1:M:237:ASN:HA	2:N:95:LEU:HB2	1.95	0.48
2:B:232:ALA:O	2:B:235:PRO:HD2	2.14	0.48
2:D:167:LEU:HB2	2:D:197:MET:HE3	1.95	0.48
1:C:52:GLY:HA2	1:C:58:LEU:HD13	1.96	0.48
6:C:686:HOH:O	2:D:138:ILE:HG12	2.13	0.48
1:K:317:TYR:HA	1:K:325:THR:CG2	2.44	0.48
2:J:137:ASP:HB2	5:J:500:B13:H522	1.78	0.48
1:M:347:LYS:HE3	6:M:616:HOH:O	2.13	0.48
1:G:132:ASN:HD21	1:G:135:PHE:H	1.61	0.48
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.95	0.48
1:E:354:ASP:CB	2:F:2:LEU:HD12	2.44	0.48
1:K:387:ASP:HB2	6:K:614:HOH:O	2.13	0.48
2:L:144:THR:HG22	6:L:518:HOH:O	2.13	0.48
1:G:22:SER:HB3	1:G:277:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:47:PRO:HB3	1:G:61:GLU:HG2	1.95	0.48
5:D:500:B13:H262	5:D:500:B13:H19	1.61	0.48
1:E:305:GLN:HA	1:E:356:MET:CE	2.44	0.48
1:E:350:LYS:HG2	1:E:353:ARG:NH2	2.29	0.48
1:I:265:PRO:HA	1:I:283:PRO:O	2.14	0.48
1:E:289:LYS:NZ	1:G:336:ASP:OD1	2.47	0.48
1:I:36:ALA:HA	6:I:568:HOH:O	2.14	0.48
2:F:130:VAL:HG12	2:F:134:ASP:HB3	1.96	0.47
1:O:324:THR:CG2	1:O:326:VAL:HG22	2.44	0.47
2:P:195:ASN:ND2	2:P:224:LEU:HB2	2.29	0.47
1:K:26:VAL:HG12	1:K:213:ILE:HD13	1.95	0.47
1:G:324:THR:HG22	1:G:327:GLN:HG3	1.96	0.47
1:M:361:ARG:HH22	1:M:373:ASP:CG	2.16	0.47
1:E:31:ASP:OD1	1:K:27:LYS:NZ	2.32	0.47
1:A:324:THR:HG23	1:A:326:VAL:HG22	1.96	0.47
1:C:132:ASN:C	1:C:132:ASN:HD22	2.18	0.47
2:N:20:LEU:HD11	1:O:116:TYR:CE1	2.49	0.47
1:A:331:GLU:HG2	1:C:292:THR:HG21	1.96	0.47
1:A:317:TYR:HA	1:A:325:THR:CG2	2.44	0.47
2:D:167:LEU:HB2	2:D:197:MET:CE	2.44	0.47
2:J:177:MET:HG2	2:J:178:LEU:N	2.29	0.47
2:N:85:ILE:HD11	2:N:149:ALA:O	2.15	0.47
1:E:361:ARG:NH2	1:E:373:ASP:OD1	2.47	0.47
2:L:189:TYR:HD2	2:L:192:LYS:HG3	1.79	0.47
1:I:301:ASN:HD22	1:I:304:MET:CE	2.27	0.47
2:J:127:VAL:HG23	2:J:175:PRO:HG3	1.96	0.47
1:K:88:VAL:HG22	1:K:91:MET:SD	2.54	0.47
2:L:52:GLU:CD	2:L:52:GLU:H	2.17	0.47
1:K:317:TYR:CE1	1:K:324:THR:CG2	2.97	0.47
1:A:224:ASN:ND2	1:A:269:CYS:HB2	2.30	0.47
2:L:189:TYR:O	2:L:192:LYS:HB2	2.15	0.47
1:I:42:GLU:OE2	1:I:123:ARG:HD2	2.15	0.47
2:L:37:ASP:O	2:L:39:LEU:N	2.43	0.47
2:H:127:VAL:HG22	2:H:155:VAL:CG1	2.45	0.47
2:L:227:TYR:CZ	2:L:229:GLU:HB3	2.49	0.47
2:J:17:ASN:H	2:J:17:ASN:ND2	2.00	0.47
1:C:218:THR:HG23	1:C:270:GLY:CA	2.45	0.47
1:I:228:PHE:CE2	5:J:500:B13:H543	2.49	0.47
2:F:95:LEU:HB3	2:F:96:PRO:HD3	1.97	0.47
2:H:138:ILE:O	2:H:142:ILE:HG13	2.14	0.47
1:O:133:ARG:HD2	2:P:160:ASP:HB3	1.97	0.47
1:E:83:LEU:HD13	1:E:109:MET:CE	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:455:LYS:HB2	1:M:458:ASN:ND2	2.29	0.47
1:O:50:GLU:CD	1:O:50:GLU:H	2.18	0.47
1:A:28:ALA:HB2	1:A:213:ILE:HD13	1.97	0.47
1:K:411:LYS:HE3	2:L:4:PHE:O	2.14	0.47
1:M:128:ASP:HA	1:M:146:PHE:CE1	2.50	0.47
1:A:65:ILE:HG23	1:A:326:VAL:HG11	1.97	0.47
1:O:356:MET:HE3	1:O:356:MET:HB2	1.60	0.47
1:G:175:ALA:HB1	1:G:180:ASP:HB3	1.96	0.47
1:E:203:ILE:O	1:E:206:ILE:HB	2.15	0.47
1:M:125:THR:HG21	1:M:267:LYS:HE2	1.96	0.47
1:G:224:ASN:HD21	1:G:269:CYS:HB2	1.79	0.47
2:H:185:THR:H	5:H:500:B13:H332	1.62	0.47
2:N:17:ASN:H	2:N:17:ASN:ND2	2.11	0.47
1:K:313:GLU:O	1:K:314:SER:HB2	2.15	0.47
2:B:116:SER:C	2:B:118:ALA:H	2.18	0.47
1:C:169:LYS:HD2	5:D:500:B13:H473	1.96	0.46
2:D:68:ASP:HB3	2:D:71:ASP:HB2	1.96	0.46
1:C:123:ARG:NH2	1:C:265:PRO:O	2.47	0.46
2:H:135:VAL:O	2:H:135:VAL:CG1	2.62	0.46
1:M:28:ALA:HB2	1:M:213:ILE:HD13	1.97	0.46
1:K:353:ARG:CA	1:K:356:MET:HE1	2.45	0.46
2:J:137:ASP:OD2	2:J:159:ARG:HD2	2.16	0.46
1:I:324:THR:CG2	1:I:326:VAL:HG22	2.45	0.46
2:F:216:GLN:NE2	2:F:258:HIS:H	2.13	0.46
2:H:37:ASP:HB3	2:H:40:ILE:HB	1.98	0.46
2:N:222:PHE:O	2:N:252:ARG:NH2	2.47	0.46
2:H:127:VAL:HG23	2:H:175:PRO:HG3	1.96	0.46
2:P:94:PHE:H	2:P:97:ASN:ND2	2.07	0.46
1:I:353:ARG:HD3	1:I:372:TYR:CZ	2.50	0.46
2:F:157:LEU:HD12	2:F:161:VAL:HG11	1.97	0.46
2:B:219:VAL:HG21	2:B:227:TYR:HB2	1.96	0.46
2:B:122:THR:HG21	2:B:153:ASN:HB2	1.98	0.46
1:G:176:VAL:HG13	1:G:177:LEU:HD13	1.97	0.46
1:G:80:ALA:HA	1:G:119:LYS:O	2.16	0.46
1:A:88:VAL:HG22	1:A:91:MET:SD	2.56	0.46
1:C:132:ASN:HD21	1:C:135:PHE:H	1.60	0.46
1:K:293:CYS:HB3	1:K:329:TRP:CE2	2.49	0.46
1:G:181:ILE:HB	1:G:182:PRO:HD3	1.98	0.46
1:K:317:TYR:HA	1:K:325:THR:HG21	1.98	0.46
1:E:132:ASN:HD22	1:E:132:ASN:C	2.19	0.46
1:E:147:LEU:HD22	1:E:206:ILE:HD11	1.97	0.46
1:O:79:PRO:HD2	6:O:595:HOH:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:192:LYS:HG2	2:L:222:PHE:HE2	1.80	0.46
2:J:116:SER:OG	2:J:117:GLY:N	2.49	0.46
2:D:159:ARG:O	2:D:161:VAL:HG23	2.15	0.46
2:L:206:PRO:HG2	2:L:241:ILE:HD12	1.96	0.46
5:N:500:B13:H262	5:N:500:B13:H19	1.69	0.46
2:H:135:VAL:O	2:H:135:VAL:HG13	2.15	0.46
2:F:185:THR:HA	2:F:188:MET:HG3	1.98	0.46
2:B:185:THR:HG23	5:B:500:B13:H332	1.80	0.46
1:M:133:ARG:HG2	1:M:133:ARG:HH11	1.80	0.46
2:D:162:PRO:O	2:D:164:GLU:N	2.49	0.46
1:O:237:ASN:HA	2:P:95:LEU:HB2	1.97	0.46
2:F:184:MET:HG2	5:F:500:B13:C30	2.38	0.46
2:F:184:MET:HB3	2:F:186:THR:HG22	1.98	0.46
5:H:500:B13:H411	5:H:500:B13:H362	1.75	0.46
2:P:17:ASN:N	2:P:17:ASN:HD22	2.10	0.46
1:C:353:ARG:HD3	1:C:372:TYR:CE1	2.51	0.46
2:B:16:TYR:CD1	1:C:116:TYR:HB3	2.50	0.46
1:K:301:ASN:HD22	1:K:304:MET:HE2	1.81	0.46
1:A:290:THR:HG22	1:A:290:THR:O	2.16	0.46
6:A:673:HOH:O	1:C:289:LYS:HE3	2.16	0.45
1:K:426:LYS:O	1:K:430:GLU:HG2	2.16	0.45
1:O:325:THR:CG2	1:O:326:VAL:N	2.79	0.45
2:B:81:MET:O	2:B:85:ILE:HD12	2.16	0.45
1:I:142:LYS:HB2	6:I:540:HOH:O	2.16	0.45
2:L:118:ALA:O	2:L:119:THR:HB	2.16	0.45
2:J:206:PRO:HG2	2:J:241:ILE:HD12	1.98	0.45
2:N:219:VAL:HG21	2:N:227:TYR:CB	2.45	0.45
2:H:252:ARG:O	2:H:256:HIS:HB2	2.17	0.45
2:D:59:LEU:O	2:D:63:ILE:HG12	2.17	0.45
2:J:135:VAL:O	2:J:135:VAL:CG1	2.64	0.45
2:P:137:ASP:HB2	5:P:500:B13:H522	1.81	0.45
1:I:143:TYR:O	1:I:146:PHE:HB3	2.16	0.45
1:G:186:TYR:O	1:G:190:CYS:HB2	2.16	0.45
1:A:295:HIS:HD2	6:B:534:HOH:O	1.99	0.45
1:I:290:THR:O	1:I:290:THR:HG22	2.16	0.45
2:B:161:VAL:HA	2:B:162:PRO:HD3	1.64	0.45
1:C:444:LEU:O	1:C:448:LYS:HB2	2.17	0.45
2:H:70:ILE:HD11	2:H:120:PRO:HA	1.98	0.45
5:J:500:B13:H19	5:J:500:B13:H262	1.66	0.45
1:G:292:THR:HA	1:G:295:HIS:O	2.17	0.45
1:A:116:TYR:HB3	2:D:16:TYR:CD1	2.52	0.45
1:K:356:MET:HE2	1:K:356:MET:HB2	1.56	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:163:ALA:O	2:N:166:VAL:HB	2.16	0.45
2:L:161:VAL:HA	2:L:162:PRO:HD3	1.78	0.45
1:G:361:ARG:NH2	1:G:373:ASP:OD1	2.49	0.45
2:J:59:LEU:O	2:J:63:ILE:HG12	2.16	0.45
1:I:411:LYS:HD3	2:J:6:GLU:HG2	1.98	0.45
1:K:137:GLN:NE2	1:K:142:LYS:HE2	2.31	0.45
2:N:192:LYS:HG2	2:N:222:PHE:HE2	1.81	0.45
2:H:47:ILE:HD12	2:H:55:VAL:HG22	1.98	0.45
2:F:136:HIS:CB	2:F:183:LEU:HD13	2.46	0.45
5:L:500:B13:H252	5:L:500:B13:C61	2.47	0.45
1:O:318:HIS:O	1:O:325:THR:HB	2.17	0.45
1:G:224:ASN:ND2	1:G:269:CYS:HB2	2.32	0.45
1:M:324:THR:CG2	1:M:326:VAL:HG22	2.47	0.45
2:D:252:ARG:O	2:D:256:HIS:HB2	2.17	0.45
1:G:42:GLU:OE2	1:G:123:ARG:HD2	2.17	0.45
1:O:87:HIS:NE2	1:O:124:HIS:CD2	2.85	0.45
1:G:105:GLN:NE2	1:G:124:HIS:HE1	2.15	0.45
1:A:341:ASN:O	1:A:345:GLU:HG2	2.17	0.45
1:C:224:ASN:O	1:C:228:PHE:CD2	2.70	0.45
1:E:55:LYS:HG3	1:E:97:TRP:CD2	2.52	0.45
1:A:356:MET:HB2	1:A:356:MET:HE3	1.80	0.44
2:F:222:PHE:O	2:F:252:ARG:NH2	2.50	0.44
1:C:237:ASN:HA	2:D:95:LEU:HB2	1.99	0.44
1:I:126:ILE:N	1:I:126:ILE:HD12	2.32	0.44
2:L:130:VAL:CG1	2:L:134:ASP:HB3	2.46	0.44
2:N:130:VAL:CG1	2:N:134:ASP:HB3	2.47	0.44
1:I:325:THR:CG2	1:I:326:VAL:N	2.81	0.44
2:D:248:VAL:HA	2:D:251:LEU:HD12	1.98	0.44
1:M:224:ASN:O	1:M:228:PHE:HD2	2.01	0.44
2:J:63:ILE:HG23	2:J:72:LEU:HD12	1.99	0.44
1:I:289:LYS:NZ	1:I:301:ASN:HD21	2.15	0.44
1:G:325:THR:O	1:G:329:TRP:HD1	2.01	0.44
5:J:500:B13:H362	5:J:500:B13:H411	1.81	0.44
1:O:81:ILE:HD13	1:O:82:ILE:N	2.33	0.44
2:H:95:LEU:HD22	2:H:99:MET:HG2	2.00	0.44
2:D:227:TYR:CE2	2:D:229:GLU:HB3	2.52	0.44
2:L:130:VAL:HG23	2:L:140:LYS:HD3	1.99	0.44
1:M:133:ARG:CG	1:M:133:ARG:NH1	2.80	0.44
2:L:234:ALA:O	2:L:237:ILE:HG22	2.18	0.44
1:C:87:HIS:NE2	1:C:124:HIS:HD2	2.14	0.44
1:E:302:LEU:HB2	1:E:360:ASP:HB2	1.98	0.44
2:P:204:LYS:HZ1	2:P:248:VAL:H	1.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:TYR:HE1	1:A:324:THR:HG21	1.82	0.44
2:P:82:GLY:HA2	2:P:85:ILE:HD12	2.00	0.44
2:N:162:PRO:O	2:N:163:ALA:HB3	2.18	0.44
1:K:228:PHE:HE1	1:K:295:HIS:HB2	1.82	0.44
2:B:59:LEU:HD23	2:B:72:LEU:HD13	2.00	0.44
1:C:218:THR:HG23	1:C:270:GLY:N	2.33	0.44
5:P:500:B13:H363	5:P:500:B13:H401	1.83	0.44
1:A:132:ASN:HD22	1:A:134:GLU:H	1.66	0.44
1:M:132:ASN:ND2	1:M:135:PHE:H	2.14	0.44
1:C:441:ASP:O	1:C:445:THR:HG23	2.18	0.44
2:N:13:LEU:C	2:N:13:LEU:HD12	2.38	0.44
2:N:218:PHE:O	2:N:221:GLN:HG2	2.18	0.44
2:F:188:MET:HB3	2:F:218:PHE:CZ	2.52	0.44
1:C:356:MET:HE3	1:C:356:MET:HB2	1.82	0.44
1:G:18:THR:CG2	1:G:21:VAL:HG13	2.47	0.44
1:M:64:ARG:CZ	2:P:258:HIS:OXT	2.66	0.44
1:C:237:ASN:O	2:D:96:PRO:HD3	2.18	0.44
1:K:105:GLN:O	1:K:109:MET:HG3	2.18	0.44
2:J:130:VAL:HG23	2:J:140:LYS:HD3	2.00	0.44
1:G:138:LEU:HD12	1:G:458:ASN:HB3	1.98	0.44
2:H:216:GLN:NE2	2:H:258:HIS:H	2.15	0.44
1:M:356:MET:HE2	1:M:356:MET:HB2	1.54	0.43
2:L:219:VAL:HG21	2:L:227:TYR:CB	2.38	0.43
2:N:138:ILE:O	2:N:142:ILE:HG13	2.18	0.43
1:G:324:THR:CG2	1:G:326:VAL:HG22	2.48	0.43
1:G:325:THR:HG23	1:G:326:VAL:N	2.32	0.43
2:J:227:TYR:H	2:J:256:HIS:HE1	1.66	0.43
2:B:51:GLU:O	2:B:55:VAL:HG23	2.18	0.43
1:C:293:CYS:HB3	1:C:329:TRP:CE2	2.53	0.43
1:C:355:LEU:HD13	2:D:2:LEU:CD1	2.48	0.43
1:M:301:ASN:HD22	1:M:304:MET:HE2	1.83	0.43
1:C:373:ASP:N	1:C:373:ASP:OD1	2.50	0.43
2:N:95:LEU:HB3	2:N:96:PRO:HD3	1.99	0.43
2:D:159:ARG:O	2:D:161:VAL:N	2.51	0.43
1:I:72:ARG:NH2	6:K:520:HOH:O	2.51	0.43
1:C:47:PRO:HB3	1:C:61:GLU:HG2	2.00	0.43
2:L:94:PHE:H	2:L:97:ASN:HD22	1.66	0.43
2:B:131:ALA:HB1	2:B:190:ALA:HB3	1.99	0.43
2:B:17:ASN:ND2	2:B:17:ASN:N	2.57	0.43
5:N:500:B13:H252	5:N:500:B13:C61	2.48	0.43
2:J:130:VAL:HG12	2:J:134:ASP:HB3	1.99	0.43
1:K:113:HIS:HD2	1:K:118:ILE:O	2.02	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:68:ASP:HB3	2:H:71:ASP:HB2	2.00	0.43
1:E:145:VAL:HA	1:E:148:GLU:OE1	2.18	0.43
2:D:127:VAL:HG22	2:D:155:VAL:HG13	2.00	0.43
1:A:237:ASN:O	2:B:96:PRO:HD3	2.18	0.43
2:B:95:LEU:HD22	2:B:99:MET:HG2	2.01	0.43
2:L:163:ALA:HB1	2:L:197:MET:HE1	2.01	0.43
1:O:27:LYS:HE3	1:O:33:GLU:OE2	2.19	0.43
1:A:43:ILE:HG22	1:A:81:ILE:HD11	2.01	0.43
1:G:132:ASN:ND2	1:G:135:PHE:H	2.15	0.43
2:D:95:LEU:HB3	2:D:96:PRO:HD3	2.01	0.43
2:N:87:LEU:HD22	2:N:92:VAL:HG21	2.01	0.43
2:B:37:ASP:HB3	2:B:40:ILE:HB	2.01	0.43
1:K:218:THR:HG23	1:K:270:GLY:N	2.33	0.43
2:J:127:VAL:HG22	2:J:155:VAL:CG1	2.49	0.43
2:H:216:GLN:HE21	2:H:258:HIS:HB2	1.83	0.43
1:O:106:LYS:NZ	1:O:157:GLY:O	2.51	0.43
2:F:87:LEU:HB3	2:F:92:VAL:HG22	1.99	0.43
2:J:82:GLY:HA2	2:J:85:ILE:HD12	2.01	0.43
1:E:361:ARG:HH22	1:E:373:ASP:CG	2.22	0.43
1:K:45:TYR:HB3	1:K:326:VAL:CG1	2.49	0.43
2:B:229:GLU:O	5:B:500:B13:H2R	2.19	0.43
5:H:500:B13:H19	5:H:500:B13:H262	1.85	0.43
5:J:500:B13:H472	5:J:500:B13:H481	1.96	0.43
1:E:132:ASN:HD21	1:E:135:PHE:H	1.65	0.43
1:O:105:GLN:NE2	1:O:124:HIS:HE1	2.17	0.43
2:N:82:GLY:HA2	2:N:85:ILE:HD12	2.00	0.43
2:L:206:PRO:HG2	2:L:241:ILE:CD1	2.49	0.43
1:A:361:ARG:NH2	1:A:373:ASP:OD1	2.51	0.43
1:O:26:VAL:CG1	1:O:213:ILE:HD13	2.49	0.43
2:J:17:ASN:N	2:J:17:ASN:ND2	2.62	0.42
5:D:500:B13:H411	5:D:500:B13:H362	1.73	0.42
1:A:287:GLU:OE1	1:A:313:GLU:OE2	2.36	0.42
1:O:364:ASP:CG	1:O:365:PRO:HD2	2.38	0.42
1:G:402:ASN:O	1:G:406:GLU:HG3	2.18	0.42
1:E:317:TYR:HA	1:E:325:THR:HG22	2.01	0.42
2:J:161:VAL:HA	2:J:162:PRO:HD3	1.95	0.42
2:B:224:LEU:HA	2:B:248:VAL:HG21	2.00	0.42
1:I:285:THR:OG1	1:I:309:CYS:HB2	2.19	0.42
2:J:233:ASP:O	2:J:237:ILE:HG22	2.19	0.42
2:H:242:ILE:HG22	2:H:242:ILE:O	2.19	0.42
1:G:305:GLN:HA	1:G:356:MET:HE1	2.02	0.42
2:H:224:LEU:HA	2:H:248:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:417:PHE:HZ	2:F:97:ASN:HD21	1.67	0.42
1:I:81:ILE:HD13	1:I:82:ILE:N	2.34	0.42
2:D:95:LEU:HD11	2:D:142:ILE:HG12	2.01	0.42
1:G:43:ILE:HG22	1:G:81:ILE:HD11	2.01	0.42
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.93	0.42
1:K:324:THR:CG2	1:K:326:VAL:HG22	2.49	0.42
2:B:63:ILE:H	2:B:63:ILE:HG12	1.73	0.42
1:C:64:ARG:HD2	6:C:533:HOH:O	2.19	0.42
1:O:47:PRO:HB3	1:O:61:GLU:HG2	2.01	0.42
5:N:500:B13:H401	5:N:500:B13:H8	1.84	0.42
2:J:67:LYS:HB3	2:J:68:ASP:H	1.65	0.42
2:B:130:VAL:HG12	2:B:134:ASP:HB3	2.01	0.42
2:H:256:HIS:HB3	2:H:257:LYS:H	1.59	0.42
1:G:119:LYS:HE3	6:G:561:HOH:O	2.18	0.42
2:D:161:VAL:HA	2:D:162:PRO:HD3	1.70	0.42
1:C:224:ASN:HB3	1:C:228:PHE:HE2	1.85	0.42
1:A:441:ASP:O	1:A:445:THR:HG23	2.19	0.42
1:K:436:MET:O	1:K:440:MET:HG2	2.19	0.42
1:O:426:LYS:O	1:O:430:GLU:HG3	2.19	0.42
2:J:188:MET:O	2:J:191:PHE:HB2	2.18	0.42
1:K:218:THR:HG23	1:K:270:GLY:CA	2.50	0.42
2:D:256:HIS:HB3	2:D:257:LYS:H	1.57	0.42
2:F:161:VAL:HA	2:F:162:PRO:HD3	1.73	0.42
1:I:18:THR:HG23	1:I:21:VAL:HG13	2.02	0.42
1:M:128:ASP:HA	1:M:146:PHE:HE1	1.84	0.42
1:G:88:VAL:HG22	1:G:91:MET:SD	2.59	0.42
1:G:76:VAL:O	1:G:76:VAL:HG12	2.19	0.42
1:M:353:ARG:HD3	1:M:372:TYR:CZ	2.55	0.42
5:L:500:B13:H351	5:L:500:B13:H361	2.01	0.42
2:N:132:GLU:HB3	2:N:161:VAL:O	2.20	0.42
2:L:192:LYS:HG2	2:L:222:PHE:CE2	2.54	0.42
2:F:136:HIS:HB2	2:F:183:LEU:HD13	2.02	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
2:B:37:ASP:O	2:B:39:LEU:N	2.49	0.42
1:O:22:SER:HB3	1:O:277:LYS:HE3	2.02	0.42
1:K:106:LYS:NZ	1:K:157:GLY:O	2.53	0.42
1:A:132:ASN:C	1:A:132:ASN:HD22	2.23	0.42
1:K:101:VAL:O	1:K:105:GLN:HG3	2.20	0.42
1:I:132:ASN:HD21	1:I:135:PHE:H	1.66	0.42
1:M:249:ILE:O	1:M:252:PRO:HD2	2.19	0.42
1:A:22:SER:HB3	1:A:277:LYS:HE3	2.02	0.42
5:F:500:B13:H362	5:F:500:B13:H411	1.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:17:ASN:HD22	2:L:17:ASN:N	2.15	0.42
2:D:67:LYS:HB3	2:D:68:ASP:H	1.56	0.42
1:M:289:LYS:NZ	1:M:301:ASN:HD21	2.18	0.42
2:N:234:ALA:O	2:N:237:ILE:HG22	2.20	0.42
1:O:285:THR:OG1	1:O:309:CYS:HB2	2.20	0.42
1:O:126:ILE:N	1:O:126:ILE:HD12	2.34	0.42
1:G:218:THR:HG23	1:G:270:GLY:N	2.35	0.42
2:N:130:VAL:HG12	2:N:134:ASP:HB3	2.02	0.42
2:D:134:ASP:OD2	2:D:187:THR:HG21	2.20	0.42
1:G:132:ASN:OD1	1:G:137:GLN:NE2	2.51	0.42
2:N:43:ILE:HG21	2:N:76:ALA:HB1	2.01	0.42
2:L:135:VAL:O	2:L:135:VAL:HG13	2.19	0.42
1:E:203:ILE:HA	1:E:206:ILE:HD12	2.02	0.42
1:E:187:SER:HA	1:E:191:LEU:HD12	2.01	0.42
2:D:110:GLU:HA	2:D:113:LYS:HB2	2.02	0.42
2:F:41:TYR:HB3	2:F:42:PRO:HD3	2.02	0.42
1:E:132:ASN:OD1	1:E:137:GLN:NE2	2.53	0.41
2:N:161:VAL:HA	2:N:162:PRO:HD3	1.78	0.41
2:D:130:VAL:HG23	2:D:140:LYS:HD3	2.02	0.41
1:O:452:LYS:HA	1:O:452:LYS:HD3	1.95	0.41
2:J:159:ARG:O	2:J:161:VAL:HG23	2.20	0.41
5:J:500:B13:N40	5:J:500:B13:H363	2.35	0.41
2:J:135:VAL:HB	5:J:500:B13:H421	2.02	0.41
2:F:216:GLN:HE21	2:F:258:HIS:HD2	1.68	0.41
2:J:234:ALA:HB3	2:J:235:PRO:HD3	2.01	0.41
1:A:87:HIS:NE2	1:A:124:HIS:CD2	2.89	0.41
1:G:356:MET:HE3	1:G:356:MET:HB2	1.83	0.41
5:B:500:B13:H411	5:B:500:B13:H362	1.80	0.41
2:L:226:VAL:HG11	2:L:237:ILE:HD11	2.02	0.41
1:K:106:LYS:HD3	1:K:106:LYS:HA	1.76	0.41
2:D:70:ILE:HD11	2:D:120:PRO:HG3	2.01	0.41
2:N:178:LEU:O	2:N:207:PHE:HA	2.21	0.41
2:P:147:LEU:HB3	2:P:154:VAL:HG21	2.01	0.41
2:L:74:ASP:HA	2:L:78:MET:HB2	2.02	0.41
1:E:266:GLY:HA3	1:E:284:MET:SD	2.60	0.41
2:D:195:ASN:HD22	2:D:224:LEU:HB2	1.86	0.41
2:L:185:THR:HG23	5:L:500:B13:H332	1.86	0.41
2:B:216:GLN:NE2	2:B:258:HIS:H	2.15	0.41
1:I:317:TYR:HE1	1:I:324:THR:CG2	2.30	0.41
5:P:500:B13:H411	5:P:500:B13:H362	1.74	0.41
2:B:95:LEU:HB3	2:B:96:PRO:HD3	2.03	0.41
1:E:287:GLU:OE1	1:E:313:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:143:TYR:O	1:C:146:PHE:HB3	2.21	0.41
1:C:354:ASP:OD2	2:D:1:MET:HA	2.20	0.41
1:M:452:LYS:HD3	1:M:452:LYS:HA	1.78	0.41
2:B:195:ASN:HD22	2:B:224:LEU:HB2	1.84	0.41
2:N:159:ARG:O	2:N:161:VAL:N	2.52	0.41
2:F:74:ASP:HA	2:F:78:MET:HB2	2.03	0.41
1:I:22:SER:HB3	1:I:277:LYS:HE3	2.02	0.41
1:E:146:PHE:CZ	1:E:150:PHE:HE2	2.39	0.41
2:L:256:HIS:HB3	2:L:257:LYS:H	1.57	0.41
5:H:500:B13:H472	5:H:500:B13:H481	1.88	0.41
2:F:214:VAL:HG12	2:F:227:TYR:CE1	2.55	0.41
2:J:252:ARG:O	2:J:256:HIS:HB2	2.21	0.41
1:O:126:ILE:N	1:O:126:ILE:CD1	2.84	0.41
2:N:136:HIS:CB	2:N:183:LEU:HD13	2.51	0.41
2:D:60:GLN:O	2:D:64:GLU:HG3	2.21	0.41
1:C:109:MET:HE1	1:C:122:LEU:HD13	2.01	0.41
5:L:500:B13:H262	5:L:500:B13:H19	1.83	0.41
5:L:500:B13:H18	5:L:500:B13:H621	1.71	0.41
1:A:218:THR:HG23	1:A:270:GLY:CA	2.50	0.41
2:P:135:VAL:HB	5:P:500:B13:C43	2.50	0.41
1:A:131:GLU:OE2	2:B:159:ARG:NH2	2.52	0.41
1:I:301:ASN:HD22	1:I:304:MET:HE2	1.85	0.41
2:B:87:LEU:HB3	2:B:92:VAL:HG22	2.03	0.41
1:C:290:THR:HG22	1:C:290:THR:O	2.21	0.41
2:J:159:ARG:HB3	2:J:160:ASP:H	1.63	0.41
1:I:317:TYR:CE1	1:I:324:THR:CG2	3.04	0.41
2:P:143:VAL:HG21	5:P:500:B13:C9B	2.50	0.41
1:O:132:ASN:ND2	1:O:134:GLU:HG2	2.36	0.41
2:P:37:ASP:O	2:P:37:ASP:OD2	2.39	0.41
1:A:123:ARG:NH2	1:A:265:PRO:O	2.53	0.41
2:H:193:GLU:O	2:H:197:MET:HB3	2.20	0.41
1:M:87:HIS:NE2	1:M:124:HIS:CD2	2.87	0.41
1:O:101:VAL:O	1:O:105:GLN:HG3	2.21	0.41
2:L:135:VAL:O	2:L:135:VAL:CG1	2.68	0.41
2:P:95:LEU:HB3	2:P:96:PRO:HD3	2.02	0.41
2:P:256:HIS:HB3	2:P:257:LYS:H	1.76	0.41
2:P:169:ALA:O	2:P:173:GLU:HG2	2.21	0.41
1:I:47:PRO:HB3	1:I:61:GLU:HG2	2.02	0.41
1:K:247:ARG:CZ	1:K:271:TYR:HB2	2.50	0.41
1:E:116:TYR:HB3	2:H:16:TYR:CD1	2.55	0.41
1:G:317:TYR:HA	1:G:325:THR:CG2	2.50	0.41
1:O:132:ASN:C	1:O:132:ASN:ND2	2.75	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:305:GLN:HA	1:C:356:MET:HE1	2.03	0.41
1:A:83:LEU:HB2	1:A:109:MET:HE1	2.03	0.41
2:B:159:ARG:O	2:B:161:VAL:HG23	2.21	0.41
2:D:119:THR:HA	2:D:120:PRO:HD3	1.90	0.41
2:B:247:ASP:HB3	2:B:250:GLU:HB2	2.01	0.41
2:F:182:ALA:O	2:F:211:GLY:HA3	2.21	0.41
1:C:50:GLU:H	1:C:50:GLU:CD	2.24	0.41
1:M:325:THR:CG2	1:M:326:VAL:N	2.83	0.40
2:J:132:GLU:HB3	2:J:161:VAL:O	2.21	0.40
1:E:94:ASN:HB2	1:E:97:TRP:CD1	2.56	0.40
1:O:88:VAL:HG22	1:O:91:MET:SD	2.62	0.40
2:N:63:ILE:H	2:N:63:ILE:HG12	1.74	0.40
2:L:231:ALA:HB2	5:L:500:B13:O6R	2.21	0.40
5:N:500:B13:H362	5:N:500:B13:H411	1.79	0.40
1:K:325:THR:CG2	1:K:326:VAL:N	2.85	0.40
1:K:131:GLU:OE2	2:L:159:ARG:NH2	2.54	0.40
1:C:224:ASN:HB3	1:C:228:PHE:CE2	2.56	0.40
2:F:206:PRO:HG2	2:F:241:ILE:CD1	2.51	0.40
1:E:76:VAL:O	1:E:76:VAL:HG12	2.22	0.40
2:B:218:PHE:O	2:B:221:GLN:HG2	2.21	0.40
1:G:132:ASN:HD22	1:G:134:GLU:H	1.67	0.40
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.88	0.40
1:O:290:THR:O	1:O:290:THR:HG22	2.22	0.40
1:M:285:THR:OG1	1:M:309:CYS:HB2	2.22	0.40
1:I:228:PHE:CE2	5:J:500:B13:C54	3.05	0.40
1:G:265:PRO:HA	1:G:283:PRO:O	2.21	0.40
2:J:134:ASP:HB2	2:J:187:THR:HG21	2.03	0.40
1:E:94:ASN:O	1:E:95:PRO:C	2.59	0.40
2:H:226:VAL:HG11	2:H:237:ILE:HG12	2.04	0.40
2:J:229:GLU:HG3	2:J:230:GLU:H	1.86	0.40
2:D:143:VAL:HG13	2:D:234:ALA:CB	2.52	0.40
1:O:179:ASN:HA	6:O:526:HOH:O	2.20	0.40
1:K:353:ARG:CA	1:K:356:MET:CE	2.83	0.40
2:D:138:ILE:HG13	5:D:500:B13:C50	2.52	0.40
1:M:132:ASN:C	1:M:132:ASN:HD22	2.24	0.40
2:N:87:LEU:HD22	2:N:92:VAL:CG2	2.52	0.40
1:I:362:TYR:HB2	2:J:9:LEU:HD21	2.03	0.40
1:C:285:THR:OG1	1:C:309:CYS:HB2	2.20	0.40
1:C:252:PRO:HG3	1:C:393:ALA:HA	2.04	0.40
1:E:348:ASN:O	1:E:351:VAL:HG12	2.20	0.40
1:E:123:ARG:NH2	1:E:265:PRO:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/461 (99%)	442 (97%)	15 (3%)	0	100	100
1	C	457/461 (99%)	440 (96%)	17 (4%)	0	100	100
1	E	457/461 (99%)	433 (95%)	21 (5%)	3 (1%)	30	50
1	G	457/461 (99%)	434 (95%)	22 (5%)	1 (0%)	56	79
1	I	457/461 (99%)	439 (96%)	17 (4%)	1 (0%)	56	79
1	K	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	M	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	O	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
2	B	256/258 (99%)	239 (93%)	13 (5%)	4 (2%)	14	23
2	D	256/258 (99%)	224 (88%)	28 (11%)	4 (2%)	14	23
2	F	256/258 (99%)	227 (89%)	26 (10%)	3 (1%)	19	32
2	H	256/258 (99%)	235 (92%)	18 (7%)	3 (1%)	19	32
2	J	256/258 (99%)	237 (93%)	14 (6%)	5 (2%)	11	17
2	L	256/258 (99%)	235 (92%)	15 (6%)	6 (2%)	10	14
2	N	256/258 (99%)	229 (90%)	23 (9%)	4 (2%)	14	23
2	P	256/258 (99%)	240 (94%)	13 (5%)	3 (1%)	19	32
All	All	5704/5752 (99%)	5371 (94%)	296 (5%)	37 (1%)	33	55

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	256	HIS
2	F	256	HIS
2	H	256	HIS
2	L	37	ASP
2	L	256	HIS
2	B	256	HIS
2	D	163	ALA
1	E	53	ALA

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Mol	Chain	Res	Type
1	E	305	GLN
2	F	38	GLU
1	G	53	ALA
2	J	256	HIS
2	J	257	LYS
2	D	119	THR
2	D	160	ASP
2	H	119	THR
2	J	119	THR
2	L	119	THR
2	F	119	THR
2	J	37	ASP
2	L	160	ASP
2	L	163	ALA
2	N	69	PRO
2	P	38	GLU
2	P	119	THR
2	P	256	HIS
2	B	119	THR
2	H	201	ASN
2	J	69	PRO
2	L	68	ASP
2	N	68	ASP
2	N	186	THR
2	B	159	ARG
2	B	192	LYS
1	I	313	GLU
2	N	160	ASP
1	E	81	ILE

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	373/374 (100%)	344 (92%)	29 (8%)	18	32
1	C	373/374 (100%)	344 (92%)	29 (8%)	18	32
1	E	373/374 (100%)	339 (91%)	34 (9%)	14	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	373/374 (100%)	346 (93%)	27 (7%)	21	36
1	I	373/374 (100%)	345 (92%)	28 (8%)	19	34
1	K	373/374 (100%)	348 (93%)	25 (7%)	23	40
1	M	373/374 (100%)	344 (92%)	29 (8%)	18	32
1	O	373/374 (100%)	343 (92%)	30 (8%)	17	31
2	B	206/206 (100%)	183 (89%)	23 (11%)	9	15
2	D	206/206 (100%)	192 (93%)	14 (7%)	22	39
2	F	206/206 (100%)	189 (92%)	17 (8%)	16	29
2	H	206/206 (100%)	190 (92%)	16 (8%)	18	32
2	J	206/206 (100%)	190 (92%)	16 (8%)	18	32
2	L	206/206 (100%)	190 (92%)	16 (8%)	18	32
2	N	206/206 (100%)	189 (92%)	17 (8%)	16	29
2	P	206/206 (100%)	184 (89%)	22 (11%)	10	17
All	All	4632/4640 (100%)	4260 (92%)	372 (8%)	17	31

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	21	VAL
1	A	72	ARG
1	A	81	ILE
1	A	115	GLU
1	A	124	HIS
1	A	132	ASN
1	A	133	ARG
1	A	134	GLU
1	A	135	PHE
1	A	142	LYS
1	A	151	GLU
1	A	170	GLU
1	A	177	LEU
1	A	184	LEU
1	A	185	LEU
1	A	198	LEU
1	A	205	LYS
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	253	ARG
1	A	299	MET
1	A	324	THR
1	A	347	LYS
1	A	353	ARG
1	A	355	LEU
1	A	370	LEU
1	A	438	LYS
1	A	444	LEU
1	A	445	THR
2	B	9	LEU
2	B	17	ASN
2	B	36	LYS
2	B	39	LEU
2	B	47	ILE
2	B	63	ILE
2	B	86	ARG
2	B	92	VAL
2	B	95	LEU
2	B	120	PRO
2	B	123	LYS
2	B	137	ASP
2	B	147	LEU
2	B	150	ASN
2	B	155	VAL
2	B	167	LEU
2	B	183	LEU
2	B	186	THR
2	B	187	THR
2	B	197	MET
2	B	204	LYS
2	B	246	THR
2	B	256	HIS
1	C	5	ARG
1	C	72	ARG
1	C	81	ILE
1	C	124	HIS
1	C	132	ASN
1	C	133	ARG
1	C	134	GLU
1	C	135	PHE
1	C	142	LYS

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Mol	Chain	Res	Type
1	C	151	GLU
1	C	170	GLU
1	C	177	LEU
1	C	184	LEU
1	C	185	LEU
1	C	198	LEU
1	C	205	LYS
1	C	233	LEU
1	C	253	ARG
1	C	299	MET
1	C	324	THR
1	C	325	THR
1	C	347	LYS
1	C	353	ARG
1	C	355	LEU
1	C	370	LEU
1	C	434	ASP
1	C	444	LEU
1	C	445	THR
1	C	448	LYS
2	D	9	LEU
2	D	17	ASN
2	D	24	LEU
2	D	36	LYS
2	D	38	GLU
2	D	47	ILE
2	D	92	VAL
2	D	95	LEU
2	D	146	LEU
2	D	147	LEU
2	D	167	LEU
2	D	183	LEU
2	D	204	LYS
2	D	256	HIS
1	E	5	ARG
1	E	7	THR
1	E	21	VAL
1	E	23	LYS
1	E	72	ARG
1	E	81	ILE
1	E	124	HIS
1	E	132	ASN

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Mol	Chain	Res	Type
1	E	133	ARG
1	E	135	PHE
1	E	137	GLN
1	E	141	ASP
1	E	142	LYS
1	E	144	SER
1	E	170	GLU
1	E	177	LEU
1	E	185	LEU
1	E	197	GLU
1	E	198	LEU
1	E	213	ILE
1	E	217	ASP
1	E	233	LEU
1	E	299	MET
1	E	324	THR
1	E	325	THR
1	E	347	LYS
1	E	353	ARG
1	E	355	LEU
1	E	370	LEU
1	E	437	ASP
1	E	438	LYS
1	E	444	LEU
1	E	449	SER
1	E	453	VAL
2	F	1	MET
2	F	9	LEU
2	F	17	ASN
2	F	36	LYS
2	F	38	GLU
2	F	47	ILE
2	F	63	ILE
2	F	89	ASP
2	F	92	VAL
2	F	95	LEU
2	F	107	GLU
2	F	110	GLU
2	F	150	ASN
2	F	157	LEU
2	F	167	LEU
2	F	204	LYS

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Mol	Chain	Res	Type
2	F	256	HIS
1	G	5	ARG
1	G	21	VAL
1	G	72	ARG
1	G	81	ILE
1	G	124	HIS
1	G	132	ASN
1	G	135	PHE
1	G	141	ASP
1	G	142	LYS
1	G	170	GLU
1	G	177	LEU
1	G	184	LEU
1	G	185	LEU
1	G	198	LEU
1	G	213	ILE
1	G	233	LEU
1	G	299	MET
1	G	311	SER
1	G	324	THR
1	G	347	LYS
1	G	355	LEU
1	G	359	SER
1	G	370	LEU
1	G	413	GLU
1	G	434	ASP
1	G	441	ASP
1	G	444	LEU
2	H	9	LEU
2	H	17	ASN
2	H	36	LYS
2	H	47	ILE
2	H	54	ASP
2	H	63	ILE
2	H	89	ASP
2	H	95	LEU
2	H	135	VAL
2	H	150	ASN
2	H	183	LEU
2	H	186	THR
2	H	204	LYS
2	H	216	GLN

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Mol	Chain	Res	Type
2	H	253	GLU
2	H	256	HIS
1	I	5	ARG
1	I	21	VAL
1	I	72	ARG
1	I	81	ILE
1	I	124	HIS
1	I	132	ASN
1	I	133	ARG
1	I	134	GLU
1	I	135	PHE
1	I	142	LYS
1	I	170	GLU
1	I	177	LEU
1	I	184	LEU
1	I	185	LEU
1	I	198	LEU
1	I	233	LEU
1	I	253	ARG
1	I	299	MET
1	I	324	THR
1	I	325	THR
1	I	347	LYS
1	I	353	ARG
1	I	355	LEU
1	I	370	LEU
1	I	430	GLU
1	I	444	LEU
1	I	445	THR
1	I	448	LYS
2	J	1	MET
2	J	9	LEU
2	J	17	ASN
2	J	36	LYS
2	J	47	ILE
2	J	89	ASP
2	J	92	VAL
2	J	95	LEU
2	J	121	LYS
2	J	146	LEU
2	J	147	LEU
2	J	164	GLU

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Mol	Chain	Res	Type
2	J	167	LEU
2	J	186	THR
2	J	236	LYS
2	J	256	HIS
1	K	5	ARG
1	K	21	VAL
1	K	81	ILE
1	K	106	LYS
1	K	124	HIS
1	K	132	ASN
1	K	133	ARG
1	K	135	PHE
1	K	142	LYS
1	K	170	GLU
1	K	177	LEU
1	K	184	LEU
1	K	185	LEU
1	K	198	LEU
1	K	233	LEU
1	K	253	ARG
1	K	298	VAL
1	K	299	MET
1	K	324	THR
1	K	325	THR
1	K	347	LYS
1	K	353	ARG
1	K	355	LEU
1	K	370	LEU
1	K	444	LEU
2	L	1	MET
2	L	9	LEU
2	L	17	ASN
2	L	36	LYS
2	L	47	ILE
2	L	63	ILE
2	L	92	VAL
2	L	95	LEU
2	L	121	LYS
2	L	144	THR
2	L	157	LEU
2	L	164	GLU
2	L	186	THR

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Mol	Chain	Res	Type
2	L	216	GLN
2	L	246	THR
2	L	256	HIS
1	M	5	ARG
1	M	21	VAL
1	M	22	SER
1	M	81	ILE
1	M	131	GLU
1	M	132	ASN
1	M	133	ARG
1	M	135	PHE
1	M	142	LYS
1	M	151	GLU
1	M	170	GLU
1	M	177	LEU
1	M	184	LEU
1	M	185	LEU
1	M	198	LEU
1	M	218	THR
1	M	233	LEU
1	M	253	ARG
1	M	298	VAL
1	M	299	MET
1	M	324	THR
1	M	325	THR
1	M	347	LYS
1	M	353	ARG
1	M	355	LEU
1	M	370	LEU
1	M	430	GLU
1	M	438	LYS
1	M	444	LEU
2	N	1	MET
2	N	9	LEU
2	N	17	ASN
2	N	36	LYS
2	N	38	GLU
2	N	47	ILE
2	N	63	ILE
2	N	92	VAL
2	N	95	LEU
2	N	109	ILE

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Mol	Chain	Res	Type
2	N	121	LYS
2	N	155	VAL
2	N	167	LEU
2	N	183	LEU
2	N	188	MET
2	N	204	LYS
2	N	246	THR
1	O	5	ARG
1	O	21	VAL
1	O	72	ARG
1	O	81	ILE
1	O	124	HIS
1	O	126	ILE
1	O	132	ASN
1	O	135	PHE
1	O	142	LYS
1	O	148	GLU
1	O	151	GLU
1	O	170	GLU
1	O	177	LEU
1	O	184	LEU
1	O	185	LEU
1	O	198	LEU
1	O	218	THR
1	O	233	LEU
1	O	253	ARG
1	O	298	VAL
1	O	299	MET
1	O	324	THR
1	O	325	THR
1	O	347	LYS
1	O	353	ARG
1	O	355	LEU
1	O	370	LEU
1	O	434	ASP
1	O	438	LYS
1	O	444	LEU
2	P	1	MET
2	P	9	LEU
2	P	17	ASN
2	P	36	LYS
2	P	39	LEU

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Mol	Chain	Res	Type
2	P	47	ILE
2	P	63	ILE
2	P	71	ASP
2	P	95	LEU
2	P	119	THR
2	P	135	VAL
2	P	137	ASP
2	P	147	LEU
2	P	157	LEU
2	P	183	LEU
2	P	186	THR
2	P	192	LYS
2	P	204	LYS
2	P	219	VAL
2	P	241	ILE
2	P	250	GLU
2	P	256	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	124	HIS
1	A	132	ASN
1	A	137	GLN
1	A	156	ASN
1	A	222	GLN
1	A	295	HIS
1	A	301	ASN
2	B	17	ASN
2	B	60	GLN
2	B	97	ASN
2	B	195	ASN
2	B	201	ASN
2	B	216	GLN
2	B	258	HIS
1	C	105	GLN
1	C	113	HIS
1	C	124	HIS
1	C	132	ASN
1	C	222	GLN
1	C	301	ASN

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Mol	Chain	Res	Type
2	D	17	ASN
2	D	97	ASN
2	D	195	ASN
2	D	215	ASN
2	D	216	GLN
2	D	258	HIS
1	E	105	GLN
1	E	124	HIS
1	E	132	ASN
1	E	137	GLN
1	E	301	ASN
2	F	17	ASN
2	F	97	ASN
2	F	195	ASN
2	F	215	ASN
2	F	216	GLN
2	F	256	HIS
1	G	89	GLN
1	G	105	GLN
1	G	113	HIS
1	G	124	HIS
1	G	132	ASN
1	G	137	GLN
1	G	222	GLN
1	G	235	ASN
1	G	295	HIS
1	G	301	ASN
2	H	17	ASN
2	H	97	ASN
2	H	195	ASN
2	H	201	ASN
2	H	216	GLN
2	H	256	HIS
1	I	105	GLN
1	I	113	HIS
1	I	124	HIS
1	I	132	ASN
1	I	137	GLN
1	I	222	GLN
1	I	295	HIS
1	I	301	ASN
2	J	17	ASN

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Mol	Chain	Res	Type
2	J	97	ASN
2	J	195	ASN
2	J	256	HIS
2	J	258	HIS
1	K	105	GLN
1	K	113	HIS
1	K	124	HIS
1	K	132	ASN
1	K	137	GLN
1	K	156	ASN
1	K	222	GLN
1	K	295	HIS
1	K	301	ASN
1	K	348	ASN
2	L	17	ASN
2	L	97	ASN
2	L	195	ASN
2	L	215	ASN
2	L	216	GLN
2	L	256	HIS
1	M	89	GLN
1	M	93	ASN
1	M	105	GLN
1	M	113	HIS
1	M	124	HIS
1	M	132	ASN
1	M	222	GLN
1	M	295	HIS
1	M	301	ASN
2	N	17	ASN
2	N	60	GLN
2	N	97	ASN
2	N	195	ASN
2	N	215	ASN
2	N	216	GLN
1	O	105	GLN
1	O	113	HIS
1	O	124	HIS
1	O	132	ASN
1	O	137	GLN
1	O	156	ASN
1	O	301	ASN

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Mol	Chain	Res	Type
1	O	348	ASN
2	P	17	ASN
2	P	60	GLN
2	P	97	ASN
2	P	195	ASN
2	P	216	GLN
2	P	258	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 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	$\# Z > 2$
5	B13	B	500	2	100,100,100	2.05	19 (19%)	150,164,164	1.93	29 (19%)
5	B13	D	500	2	100,100,100	2.12	23 (23%)	150,164,164	1.98	36 (24%)
5	B13	F	500	2	100,100,100	2.10	22 (22%)	150,164,164	1.96	39 (26%)
5	B13	H	500	2	100,100,100	2.15	19 (19%)	150,164,164	1.99	32 (21%)
5	B13	J	500	2,6	100,100,100	2.02	19 (19%)	150,164,164	1.93	31 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	B13	L	500	2,6	100,100,100	2.10	22 (22%)	150,164,164	1.98	40 (26%)
5	B13	N	500	2	100,100,100	2.04	19 (19%)	150,164,164	2.00	36 (24%)
5	B13	P	500	2	100,100,100	2.01	20 (20%)	150,164,164	2.01	39 (26%)

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
5	B13	B	500	2	-	0/56/223/223	0/1/11/11
5	B13	D	500	2	-	0/56/223/223	0/1/11/11
5	B13	F	500	2	-	0/56/223/223	0/1/11/11
5	B13	H	500	2	-	0/56/223/223	0/1/11/11
5	B13	J	500	2,6	-	0/56/223/223	0/1/11/11
5	B13	L	500	2,6	-	0/56/223/223	0/1/11/11
5	B13	N	500	2	-	0/56/223/223	0/1/11/11
5	B13	P	500	2	-	0/56/223/223	0/1/11/11

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	500	B13	C15-C14	10.32	1.41	1.33
5	D	500	B13	C15-C14	10.00	1.41	1.33
5	F	500	B13	C15-C14	9.65	1.41	1.33
5	L	500	B13	C15-C14	9.31	1.40	1.33
5	N	500	B13	C15-C14	8.70	1.40	1.33
5	B	500	B13	C5R-C4R	-8.53	1.21	1.52
5	D	500	B13	C5R-C4R	-8.51	1.22	1.52
5	B	500	B13	C15-C14	8.48	1.40	1.33
5	P	500	B13	C5R-C4R	-8.40	1.22	1.52
5	J	500	B13	C5R-C4R	-8.40	1.22	1.52
5	L	500	B13	C5R-C4R	-8.39	1.22	1.52
5	H	500	B13	C5R-C4R	-8.31	1.22	1.52
5	F	500	B13	C5R-C4R	-8.30	1.22	1.52
5	N	500	B13	C5R-C4R	-8.27	1.22	1.52
5	J	500	B13	C15-C14	7.92	1.39	1.33
5	P	500	B13	C15-C14	7.44	1.39	1.33
5	P	500	B13	C4-C5	-6.33	1.43	1.51
5	J	500	B13	C4-C5	-5.65	1.44	1.51
5	B	500	B13	O5B-C5B	5.63	1.51	1.37
5	H	500	B13	C4-C5	-5.54	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	500	B13	O5B-C5B	5.50	1.51	1.37
5	H	500	B13	O5B-C5B	5.49	1.51	1.37
5	J	500	B13	C11-C10	-5.45	1.36	1.50
5	B	500	B13	C11-C10	-5.45	1.36	1.50
5	N	500	B13	O5B-C5B	5.43	1.51	1.37
5	H	500	B13	C11-C10	-5.43	1.37	1.50
5	F	500	B13	O5B-C5B	5.39	1.50	1.37
5	F	500	B13	C11-C10	-5.34	1.37	1.50
5	D	500	B13	O5B-C5B	5.22	1.50	1.37
5	L	500	B13	C11-C10	-5.16	1.37	1.50
5	D	500	B13	C11-C10	-5.13	1.37	1.50
5	P	500	B13	C11-C10	-5.13	1.37	1.50
5	L	500	B13	C4-C5	-5.10	1.44	1.51
5	N	500	B13	C11-C10	-5.07	1.37	1.50
5	B	500	B13	C4-C5	-5.02	1.44	1.51
5	J	500	B13	O5B-C5B	4.97	1.49	1.37
5	D	500	B13	C4-C5	-4.92	1.44	1.51
5	P	500	B13	O5B-C5B	4.90	1.49	1.37
5	F	500	B13	C4-C5	-4.60	1.45	1.51
5	N	500	B13	C4-C5	-4.51	1.45	1.51
5	N	500	B13	C5-C6	4.15	1.37	1.33
5	L	500	B13	C5-C6	4.09	1.36	1.33
5	J	500	B13	C2B-N1B	4.04	1.42	1.36
5	F	500	B13	C2B-N1B	4.02	1.42	1.36
5	H	500	B13	C2B-N1B	3.98	1.42	1.36
5	D	500	B13	C2B-N1B	3.89	1.42	1.36
5	H	500	B13	C6B-C5B	3.84	1.47	1.38
5	D	500	B13	C35-C5	3.75	1.56	1.50
5	B	500	B13	C2B-N1B	3.72	1.42	1.36
5	L	500	B13	C35-C5	3.66	1.56	1.50
5	P	500	B13	C2B-N1B	3.61	1.42	1.36
5	N	500	B13	C6B-C5B	3.60	1.46	1.38
5	D	500	B13	C6B-C5B	3.58	1.46	1.38
5	J	500	B13	C35-C5	3.57	1.56	1.50
5	L	500	B13	C6B-C5B	3.56	1.46	1.38
5	F	500	B13	C6B-C5B	3.55	1.46	1.38
5	F	500	B13	C5-C6	3.52	1.36	1.33
5	J	500	B13	O8R-C5R	3.47	1.57	1.42
5	L	500	B13	C2B-N1B	3.46	1.41	1.36
5	H	500	B13	O8R-C5R	3.43	1.57	1.42
5	B	500	B13	C35-C5	3.43	1.56	1.50
5	N	500	B13	C2B-N1B	3.42	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	500	B13	C6B-C5B	3.42	1.46	1.38
5	F	500	B13	O8R-C5R	3.39	1.57	1.42
5	N	500	B13	O8R-C5R	3.38	1.57	1.42
5	B	500	B13	C6B-C5B	3.35	1.46	1.38
5	D	500	B13	O8R-C5R	3.34	1.56	1.42
5	L	500	B13	O8R-C5R	3.33	1.56	1.42
5	P	500	B13	O8R-C5R	3.33	1.56	1.42
5	N	500	B13	C35-C5	3.32	1.56	1.50
5	B	500	B13	O8R-C5R	3.32	1.56	1.42
5	H	500	B13	C35-C5	3.23	1.55	1.50
5	P	500	B13	C35-C5	3.14	1.55	1.50
5	F	500	B13	C35-C5	3.13	1.55	1.50
5	P	500	B13	C6B-C5B	3.11	1.45	1.38
5	H	500	B13	C36-C7	3.03	1.60	1.54
5	D	500	B13	C25-C2	3.03	1.60	1.54
5	B	500	B13	C55-C17	2.95	1.60	1.55
5	B	500	B13	C16-C15	-2.95	1.43	1.51
5	F	500	B13	O6R-C1R	2.93	1.45	1.41
5	P	500	B13	C5-C6	2.90	1.36	1.33
5	J	500	B13	C25-C2	2.87	1.60	1.54
5	L	500	B13	O6R-C1R	2.81	1.45	1.41
5	F	500	B13	C36-C7	2.80	1.59	1.54
5	H	500	B13	O6R-C1R	2.80	1.45	1.41
5	D	500	B13	C5-C6	2.78	1.36	1.33
5	N	500	B13	C36-C7	2.76	1.59	1.54
5	J	500	B13	C36-C7	2.76	1.59	1.54
5	L	500	B13	C55-C17	2.74	1.59	1.55
5	P	500	B13	C55-C17	2.71	1.59	1.55
5	P	500	B13	C8B-N1B	-2.69	1.35	1.39
5	B	500	B13	C20-C1	2.69	1.61	1.53
5	N	500	B13	C55-C17	2.64	1.59	1.55
5	P	500	B13	C17-C16	2.64	1.60	1.55
5	F	500	B13	C20-C1	2.63	1.61	1.53
5	H	500	B13	C55-C17	2.61	1.59	1.55
5	J	500	B13	C20-C1	2.59	1.61	1.53
5	P	500	B13	C25-C2	2.58	1.59	1.54
5	F	500	B13	C7-C6	2.58	1.60	1.54
5	P	500	B13	C20-C1	2.58	1.61	1.53
5	N	500	B13	C20-C1	2.56	1.61	1.53
5	N	500	B13	C7-C6	2.55	1.60	1.54
5	D	500	B13	C2R-C3R	-2.55	1.47	1.53
5	N	500	B13	O6R-C1R	2.55	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	500	B13	C55-C17	2.54	1.59	1.55
5	H	500	B13	C17-C16	2.53	1.60	1.55
5	H	500	B13	C20-C1	2.53	1.61	1.53
5	B	500	B13	C25-C2	2.52	1.59	1.54
5	F	500	B13	C25-C2	2.52	1.59	1.54
5	D	500	B13	C8B-N1B	-2.51	1.36	1.39
5	H	500	B13	C5-C6	2.51	1.35	1.33
5	D	500	B13	C55-C17	2.49	1.59	1.55
5	L	500	B13	C20-C1	2.48	1.61	1.53
5	F	500	B13	C55-C17	2.48	1.59	1.55
5	D	500	B13	C36-C7	2.47	1.59	1.54
5	L	500	B13	C36-C7	2.46	1.59	1.54
5	J	500	B13	O6R-C1R	2.45	1.45	1.41
5	B	500	B13	C8B-N1B	-2.44	1.36	1.39
5	L	500	B13	C2R-C3R	-2.44	1.47	1.53
5	D	500	B13	C60-C61	-2.44	1.45	1.51
5	P	500	B13	C36-C7	2.42	1.59	1.54
5	N	500	B13	C25-C2	2.39	1.59	1.54
5	B	500	B13	C17-C16	2.39	1.59	1.55
5	P	500	B13	O6R-C1R	2.30	1.44	1.41
5	D	500	B13	C14-N23	2.30	1.41	1.33
5	J	500	B13	C8B-N1B	-2.29	1.36	1.39
5	L	500	B13	C25-C2	2.26	1.59	1.54
5	B	500	B13	C5-C6	2.25	1.35	1.33
5	N	500	B13	P-O4	-2.24	1.45	1.55
5	H	500	B13	P-O4	-2.23	1.45	1.55
5	D	500	B13	P-O4	-2.23	1.45	1.55
5	D	500	B13	C20-C1	2.23	1.60	1.53
5	J	500	B13	C2R-C3R	-2.23	1.47	1.53
5	H	500	B13	C25-C2	2.22	1.59	1.54
5	B	500	B13	C36-C7	2.21	1.58	1.54
5	L	500	B13	C14-N23	2.21	1.40	1.33
5	L	500	B13	P-O4	-2.20	1.45	1.55
5	P	500	B13	P-O4	-2.19	1.45	1.55
5	L	500	B13	C8B-N1B	-2.18	1.36	1.39
5	D	500	B13	C53-C15	2.17	1.54	1.50
5	D	500	B13	C7-C6	2.17	1.59	1.54
5	D	500	B13	C16-C15	-2.16	1.45	1.51
5	H	500	B13	C7-C6	2.16	1.59	1.54
5	H	500	B13	C2R-C3R	-2.15	1.48	1.53
5	J	500	B13	P-O4	-2.15	1.45	1.55
5	N	500	B13	C2R-C3R	-2.15	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	B13	P-O4	-2.14	1.45	1.55
5	L	500	B13	C7-C6	2.13	1.59	1.54
5	F	500	B13	P-O4	-2.12	1.45	1.55
5	D	500	B13	C4B-C5B	2.12	1.41	1.37
5	F	500	B13	C17-C16	2.11	1.59	1.55
5	F	500	B13	C13-C14	2.06	1.56	1.52
5	P	500	B13	C16-C15	-2.06	1.45	1.51
5	P	500	B13	C48-C13	2.05	1.59	1.54
5	J	500	B13	C14-N23	2.05	1.40	1.33
5	B	500	B13	O6R-C1R	2.05	1.44	1.41
5	N	500	B13	C17-C16	2.05	1.59	1.55
5	L	500	B13	C17-C16	2.05	1.59	1.55
5	L	500	B13	C13-C14	2.05	1.56	1.52
5	J	500	B13	C16-C15	-2.03	1.45	1.51
5	F	500	B13	C16-C15	-2.01	1.45	1.51
5	F	500	B13	C4B-C5B	2.01	1.41	1.37
5	F	500	B13	C8B-N1B	-2.00	1.36	1.39

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	500	B13	C2B-N1B-C1R	-8.58	109.48	126.38
5	F	500	B13	O6R-C4R-C5R	8.08	126.41	109.15
5	N	500	B13	O6R-C4R-C5R	8.06	126.38	109.15
5	B	500	B13	O6R-C4R-C5R	8.02	126.29	109.15
5	H	500	B13	C2B-N1B-C1R	-7.81	111.01	126.38
5	J	500	B13	O6R-C4R-C5R	7.69	125.58	109.15
5	P	500	B13	O6R-C4R-C5R	7.64	125.48	109.15
5	L	500	B13	O6R-C4R-C5R	7.59	125.36	109.15
5	D	500	B13	O6R-C4R-C5R	7.57	125.33	109.15
5	J	500	B13	C2B-N1B-C1R	-7.51	111.59	126.38
5	L	500	B13	C2B-N1B-C1R	-7.34	111.93	126.38
5	B	500	B13	O6R-C1R-N1B	7.32	115.25	108.44
5	H	500	B13	O6R-C4R-C5R	7.31	124.78	109.15
5	F	500	B13	O6R-C1R-N1B	6.89	114.85	108.44
5	D	500	B13	O6R-C1R-N1B	6.88	114.84	108.44
5	B	500	B13	C2B-N1B-C1R	-6.83	112.94	126.38
5	L	500	B13	O6R-C1R-N1B	6.80	114.77	108.44
5	P	500	B13	C2B-N1B-C1R	-6.71	113.17	126.38
5	F	500	B13	C2B-N1B-C1R	-6.65	113.29	126.38
5	D	500	B13	C2B-N1B-C1R	-6.30	113.97	126.38
5	B	500	B13	C4R-O6R-C1R	-6.26	102.95	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	500	B13	O6R-C1R-N1B	6.19	114.20	108.44
5	H	500	B13	C1R-N1B-C8B	6.08	135.62	125.85
5	N	500	B13	O6R-C1R-N1B	5.96	113.99	108.44
5	J	500	B13	O6R-C1R-N1B	5.92	113.94	108.44
5	P	500	B13	O6R-C1R-N1B	5.61	113.66	108.44
5	J	500	B13	C4R-O6R-C1R	-5.57	103.70	109.75
5	L	500	B13	C4R-O6R-C1R	-5.54	103.73	109.75
5	P	500	B13	C4R-O6R-C1R	-5.52	103.75	109.75
5	D	500	B13	C4R-O6R-C1R	-5.44	103.84	109.75
5	L	500	B13	C1R-N1B-C8B	5.36	134.46	125.85
5	D	500	B13	C1R-N1B-C8B	5.36	134.46	125.85
5	J	500	B13	C1R-N1B-C8B	5.31	134.38	125.85
5	F	500	B13	C1R-N1B-C8B	5.01	133.89	125.85
5	H	500	B13	C5R-C4R-C3R	4.89	132.03	114.88
5	B	500	B13	C1R-N1B-C8B	4.84	133.62	125.85
5	N	500	B13	C1R-N1B-C8B	4.83	133.61	125.85
5	J	500	B13	C5R-C4R-C3R	4.81	131.76	114.88
5	H	500	B13	C60-C18-C17	4.74	122.74	114.50
5	B	500	B13	O7R-C2R-C3R	4.66	124.90	111.20
5	N	500	B13	C4R-O6R-C1R	-4.62	104.73	109.75
5	P	500	B13	C1R-N1B-C8B	4.58	133.20	125.85
5	P	500	B13	C5R-C4R-C3R	4.57	130.92	114.88
5	L	500	B13	C5R-C4R-C3R	4.57	130.92	114.88
5	F	500	B13	C5R-C4R-C3R	4.54	130.81	114.88
5	H	500	B13	O34-C32-C31	-4.53	107.80	121.06
5	N	500	B13	O7R-C2R-C3R	4.47	124.36	111.20
5	P	500	B13	O7R-C2R-C3R	4.45	124.30	111.20
5	N	500	B13	C53-C15-C14	-4.35	117.02	124.17
5	F	500	B13	O34-C32-C31	-4.35	108.33	121.06
5	H	500	B13	O7R-C2R-C3R	4.35	123.99	111.20
5	F	500	B13	C4R-O6R-C1R	-4.30	105.08	109.75
5	D	500	B13	C5R-C4R-C3R	4.29	129.93	114.88
5	B	500	B13	C5R-C4R-C3R	4.29	129.92	114.88
5	D	500	B13	O34-C32-C31	-4.16	108.87	121.06
5	N	500	B13	C5R-C4R-C3R	4.16	129.47	114.88
5	B	500	B13	O34-C32-C31	-4.13	108.95	121.06
5	L	500	B13	O34-C32-C31	-4.12	108.98	121.06
5	H	500	B13	C53-C15-C14	-4.12	117.40	124.17
5	P	500	B13	O34-C32-C31	-4.08	109.11	121.06
5	F	500	B13	O7R-C2R-C3R	4.05	123.12	111.20
5	J	500	B13	O7R-C2R-C3R	3.99	122.94	111.20
5	N	500	B13	O34-C32-C31	-3.99	109.38	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	500	B13	O7R-C2R-C3R	3.95	122.83	111.20
5	P	500	B13	C7-C37-C38	3.95	126.89	114.57
5	P	500	B13	C5B-C4B-C9B	-3.93	116.41	119.17
5	J	500	B13	O34-C32-C31	-3.88	109.69	121.06
5	N	500	B13	C3-C4-C5	3.84	125.50	117.91
5	P	500	B13	C53-C15-C14	-3.78	117.95	124.17
5	D	500	B13	O7R-C2R-C3R	3.76	122.25	111.20
5	F	500	B13	C60-C18-C17	3.72	120.98	114.50
5	H	500	B13	C7-C37-C38	3.72	126.19	114.57
5	P	500	B13	C3-C4-N21	3.70	113.69	104.63
5	H	500	B13	C4R-O6R-C1R	-3.70	105.73	109.75
5	P	500	B13	C60-C18-C17	3.70	120.93	114.50
5	F	500	B13	C53-C15-C14	-3.66	118.16	124.17
5	J	500	B13	C7-C37-C38	3.65	125.95	114.57
5	F	500	B13	C3-C4-C5	3.64	125.11	117.91
5	J	500	B13	C3-C4-N21	3.63	113.50	104.63
5	N	500	B13	C53-C15-C16	3.54	125.32	116.65
5	J	500	B13	C18-C60-C61	3.52	124.44	114.06
5	P	500	B13	C18-C60-C61	3.49	124.33	114.06
5	J	500	B13	C53-C15-C14	-3.48	118.44	124.17
5	D	500	B13	C15-C16-N24	3.46	123.49	111.90
5	H	500	B13	C54-C17-C55	-3.46	102.62	109.43
5	D	500	B13	C41-C42-C43	-3.46	100.96	112.60
5	B	500	B13	C8-C9-C10	-3.44	119.19	123.03
5	H	500	B13	C3-C4-N21	3.40	112.94	104.63
5	L	500	B13	C15-C16-N24	3.38	123.22	111.90
5	D	500	B13	C3-C4-N21	3.37	112.88	104.63
5	N	500	B13	C12-C11-C10	3.36	127.01	117.76
5	N	500	B13	C60-C18-C17	3.34	120.31	114.50
5	L	500	B13	C53-C15-C14	-3.32	118.72	124.17
5	J	500	B13	C15-C16-N24	3.31	122.96	111.90
5	H	500	B13	O8R-C5R-C4R	3.28	122.64	111.36
5	L	500	B13	C3-C4-N21	3.24	112.56	104.63
5	F	500	B13	C8-C9-C10	-3.24	119.42	123.03
5	J	500	B13	C5B-C4B-C9B	-3.24	116.89	119.17
5	H	500	B13	C8-C9-C10	-3.23	119.42	123.03
5	N	500	B13	C7-C37-C38	3.22	124.62	114.57
5	F	500	B13	O8R-C5R-C4R	3.21	122.41	111.36
5	D	500	B13	C60-C18-C17	3.20	120.07	114.50
5	P	500	B13	C3-C4-C5	3.20	124.23	117.91
5	L	500	B13	C3-C4-C5	3.19	124.22	117.91
5	F	500	B13	C36-C7-C6	3.19	127.01	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	C3-C4-N21	3.17	112.38	104.63
5	P	500	B13	C7B-C8B-N1B	-3.16	128.24	131.98
5	B	500	B13	C3-C4-C5	3.16	124.17	117.91
5	B	500	B13	C36-C7-C6	3.15	126.82	110.15
5	D	500	B13	C41-C8-C7	-3.15	105.22	114.28
5	B	500	B13	C15-C16-N24	3.14	122.40	111.90
5	N	500	B13	O8R-C5R-C4R	3.12	122.10	111.36
5	N	500	B13	C36-C7-C6	3.12	126.64	110.15
5	H	500	B13	C55-C17-C16	3.11	122.78	112.94
5	L	500	B13	C53-C15-C16	3.08	124.18	116.65
5	F	500	B13	C15-C16-N24	3.08	122.19	111.90
5	L	500	B13	C60-C18-C17	3.07	119.84	114.50
5	N	500	B13	C36-C7-C37	-3.07	105.92	110.86
5	D	500	B13	C36-C7-C37	-3.06	105.94	110.86
5	H	500	B13	C53-C15-C16	3.03	124.05	116.65
5	P	500	B13	C53-C15-C16	3.02	124.03	116.65
5	L	500	B13	C36-C7-C37	-3.01	106.01	110.86
5	N	500	B13	C15-C16-N24	3.01	121.97	111.90
5	N	500	B13	C55-C17-C16	3.00	122.44	112.94
5	P	500	B13	C15-C16-N24	3.00	121.93	111.90
5	P	500	B13	C36-C7-C6	2.97	125.89	110.15
5	H	500	B13	C3-C4-C5	2.92	123.69	117.91
5	B	500	B13	C17-C18-C19	2.92	103.86	100.94
5	P	500	B13	C42-C41-C8	2.89	124.43	114.85
5	N	500	B13	C3-C4-N21	2.88	111.67	104.63
5	J	500	B13	C41-C42-C43	-2.88	102.91	112.60
5	J	500	B13	C53-C15-C16	2.86	123.66	116.65
5	D	500	B13	C17-C18-C19	2.86	103.80	100.94
5	H	500	B13	C36-C7-C6	2.86	125.26	110.15
5	H	500	B13	C15-C16-N24	2.84	121.42	111.90
5	J	500	B13	C8-C9-C10	-2.79	119.91	123.03
5	L	500	B13	C36-C7-C6	2.79	124.94	110.15
5	P	500	B13	C8-C9-C10	-2.78	119.92	123.03
5	J	500	B13	C36-C7-C6	2.78	124.87	110.15
5	F	500	B13	C36-C7-C37	-2.78	106.39	110.86
5	D	500	B13	C36-C7-C6	2.78	124.83	110.15
5	B	500	B13	C7B-C8B-N1B	-2.77	128.71	131.98
5	H	500	B13	C18-C60-C61	2.77	122.22	114.06
5	D	500	B13	O2-C3R-C4R	-2.77	99.24	110.06
5	N	500	B13	O2-C3R-C4R	-2.77	99.25	110.06
5	D	500	B13	C5-C4-N21	2.77	123.62	111.44
5	N	500	B13	P-O3-C2P	2.76	130.44	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	B13	C18-C60-C61	2.75	122.17	114.06
5	B	500	B13	C18-C60-C61	2.75	122.17	114.06
5	F	500	B13	C55-C17-C16	2.75	121.66	112.94
5	D	500	B13	C42-C41-C8	2.75	123.97	114.85
5	F	500	B13	C5-C4-N21	2.75	123.53	111.44
5	B	500	B13	C5-C4-N21	2.72	123.43	111.44
5	F	500	B13	C3-C4-N21	2.72	111.29	104.63
5	F	500	B13	C7B-C8B-N1B	-2.71	128.78	131.98
5	D	500	B13	C7-C37-C38	2.71	123.02	114.57
5	H	500	B13	C5-C4-N21	2.70	123.33	111.44
5	N	500	B13	C47-C12-C13	2.70	122.32	111.48
5	P	500	B13	C54-C17-C55	-2.70	104.13	109.43
5	D	500	B13	C8-C9-C10	-2.69	120.03	123.03
5	F	500	B13	P-O3-C2P	2.68	130.15	119.41
5	N	500	B13	C54-C17-C55	-2.67	104.17	109.43
5	J	500	B13	C5-C4-N21	2.67	123.19	111.44
5	H	500	B13	C5B-C4B-C9B	-2.67	117.29	119.17
5	J	500	B13	C54-C17-C16	-2.66	103.83	111.76
5	J	500	B13	C3-C4-C5	2.66	123.17	117.91
5	F	500	B13	C53-C15-C16	2.64	123.12	116.65
5	D	500	B13	C3-C4-C5	2.64	123.14	117.91
5	L	500	B13	C18-C60-C61	2.64	121.83	114.06
5	F	500	B13	C41-C8-C7	-2.64	106.70	114.28
5	P	500	B13	C6B-C7B-C8B	-2.63	115.02	119.34
5	L	500	B13	C5-C4-N21	2.63	123.02	111.44
5	H	500	B13	C42-C41-C8	2.62	123.53	114.85
5	L	500	B13	C54-C17-C16	-2.62	103.97	111.76
5	D	500	B13	C26-C2-C1	-2.62	105.98	110.05
5	B	500	B13	C55-C17-C16	2.59	121.15	112.94
5	B	500	B13	C36-C7-C37	-2.59	106.69	110.86
5	J	500	B13	C55-C17-C16	2.59	121.13	112.94
5	L	500	B13	C8-C9-C10	-2.58	120.16	123.03
5	N	500	B13	C5-C4-N21	2.57	122.77	111.44
5	F	500	B13	C42-C41-C8	2.57	123.37	114.85
5	H	500	B13	C48-C13-C12	-2.57	110.43	117.36
5	L	500	B13	O8R-C5R-C4R	2.57	120.20	111.36
5	L	500	B13	C31-C32-N33	2.57	124.76	116.51
5	L	500	B13	C7-C37-C38	2.57	122.58	114.57
5	P	500	B13	P-O3-C2P	2.56	129.64	119.41
5	D	500	B13	C4B-C9B-C8B	-2.51	118.53	121.10
5	L	500	B13	C31-C30-C3	-2.51	107.48	114.83
5	N	500	B13	C18-C60-C61	2.49	121.40	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	500	B13	C18-C19-N24	2.48	106.27	102.01
5	D	500	B13	O8R-C5R-C4R	2.48	119.90	111.36
5	F	500	B13	C5B-C4B-C9B	-2.47	117.43	119.17
5	F	500	B13	C54-C17-C16	-2.45	104.46	111.76
5	P	500	B13	C31-C32-N33	2.45	124.37	116.51
5	J	500	B13	O8R-C5R-C4R	2.44	119.77	111.36
5	L	500	B13	C42-C41-C8	2.44	122.95	114.85
5	D	500	B13	C18-C60-C61	2.43	121.21	114.06
5	D	500	B13	C47-C12-C13	2.42	121.19	111.48
5	H	500	B13	C31-C32-N33	2.41	124.27	116.51
5	B	500	B13	C60-C18-C17	2.42	118.70	114.50
5	L	500	B13	C18-C19-N24	2.41	106.14	102.01
5	D	500	B13	C2P-C1P-N59	-2.41	109.16	112.98
5	D	500	B13	C55-C17-C16	2.41	120.56	112.94
5	P	500	B13	C20-C1-N21	-2.39	104.31	111.20
5	P	500	B13	C5-C4-N21	2.39	121.95	111.44
5	F	500	B13	C1-C19-C18	-2.39	117.98	121.76
5	D	500	B13	O6R-C1R-C2R	2.39	110.43	106.77
5	D	500	B13	C31-C32-N33	2.38	124.14	116.51
5	P	500	B13	C17-C18-C19	2.37	103.31	100.94
5	L	500	B13	O2-C3R-C4R	-2.37	100.81	110.06
5	L	500	B13	C55-C17-C16	2.34	120.36	112.94
5	N	500	B13	C5B-C4B-C9B	-2.33	117.53	119.17
5	L	500	B13	C26-C2-C1	-2.32	106.44	110.05
5	F	500	B13	C41-C42-C43	-2.32	104.80	112.60
5	F	500	B13	C25-C2-C3	2.32	116.42	111.83
5	H	500	B13	O2-C3R-C4R	-2.32	101.01	110.06
5	L	500	B13	C47-C12-C13	2.31	120.77	111.48
5	P	500	B13	C36-C7-C37	-2.31	107.14	110.86
5	B	500	B13	C5B-C4B-C9B	-2.30	117.55	119.17
5	J	500	B13	C60-C18-C17	2.30	118.51	114.50
5	L	500	B13	C5B-C4B-C9B	-2.30	117.55	119.17
5	P	500	B13	C35-C5-C6	2.30	126.61	123.68
5	L	500	B13	O6R-C1R-C2R	2.29	110.29	106.77
5	L	500	B13	C25-C2-C1	2.29	117.26	113.82
5	P	500	B13	C3P-C2P-C1P	-2.29	106.34	111.28
5	P	500	B13	O8R-C5R-C4R	2.28	119.21	111.36
5	L	500	B13	C12-C11-C10	2.28	124.02	117.76
5	J	500	B13	C3P-C2P-C1P	-2.27	106.37	111.28
5	L	500	B13	P-O3-C2P	2.26	128.47	119.41
5	D	500	B13	C12-C11-C10	2.26	123.97	117.76
5	B	500	B13	C12-C13-C14	2.25	105.61	100.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	500	B13	C55-C17-C16	2.25	120.06	112.94
5	F	500	B13	C7-C37-C38	2.25	121.58	114.57
5	P	500	B13	C12-C11-C10	2.24	123.93	117.76
5	F	500	B13	O2-C3R-C4R	-2.24	101.33	110.06
5	F	500	B13	C31-C32-N33	2.23	123.67	116.51
5	N	500	B13	C54-C17-C16	-2.23	105.13	111.76
5	D	500	B13	C54-C17-C16	-2.21	105.17	111.76
5	N	500	B13	C31-C32-N33	2.21	123.62	116.51
5	L	500	B13	C41-C42-C43	-2.20	105.18	112.60
5	D	500	B13	O3-P-O2	-2.20	98.05	104.37
5	L	500	B13	C2-C26-C27	2.20	121.72	115.21
5	B	500	B13	C20-C1-N21	-2.20	104.87	111.20
5	B	500	B13	C6B-C7B-C8B	-2.19	115.74	119.34
5	B	500	B13	C31-C32-N33	2.19	123.55	116.51
5	P	500	B13	O7R-C2R-C1R	2.19	117.84	111.23
5	N	500	B13	C42-C41-C8	2.18	122.08	114.85
5	J	500	B13	C47-C12-C13	2.18	120.24	111.48
5	H	500	B13	C8-C9-N22	2.16	114.50	110.68
5	D	500	B13	C53-C15-C16	2.14	121.89	116.65
5	H	500	B13	C37-C7-C8	-2.14	102.11	108.05
5	J	500	B13	C7B-C8B-N1B	-2.14	129.46	131.98
5	J	500	B13	C31-C32-N33	2.13	123.36	116.51
5	N	500	B13	C17-C18-C19	2.13	103.07	100.94
5	F	500	B13	C3P-C2P-C1P	-2.12	106.69	111.28
5	L	500	B13	C6B-C7B-C8B	-2.12	115.86	119.34
5	D	500	B13	C7B-C8B-N1B	-2.12	129.48	131.98
5	J	500	B13	C41-C8-C9	-2.11	106.63	111.05
5	F	500	B13	C8-C9-N22	2.10	114.39	110.68
5	P	500	B13	C37-C38-N40	2.09	123.95	116.58
5	N	500	B13	C46-C12-C47	-2.09	102.67	108.69
5	P	500	B13	C25-C2-C3	2.08	115.95	111.83
5	H	500	B13	C47-C12-C13	2.07	119.80	111.48
5	H	500	B13	P-O3-C2P	2.07	127.69	119.41
5	H	500	B13	C10-C11-N23	2.07	124.38	113.28
5	F	500	B13	C48-C13-C12	-2.07	111.78	117.36
5	B	500	B13	C7-C37-C38	2.07	121.02	114.57
5	J	500	B13	P-O3-C2P	2.06	127.67	119.41
5	L	500	B13	C7B-C8B-N1B	-2.06	129.55	131.98
5	N	500	B13	O6R-C1R-C2R	2.05	109.92	106.77
5	F	500	B13	C18-C19-N24	2.05	105.53	102.01
5	B	500	B13	C47-C12-C13	2.05	119.70	111.48
5	N	500	B13	O7R-C2R-C1R	2.04	117.41	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	B13	C47-C12-C13	2.04	119.68	111.48
5	N	500	B13	C47-C12-C11	2.04	117.21	111.53
5	B	500	B13	C12-C11-N23	2.04	113.99	103.83
5	F	500	B13	C31-C30-C3	-2.04	108.87	114.83
5	P	500	B13	C41-C8-C7	-2.03	108.44	114.28
5	N	500	B13	C13-C12-C11	-2.03	97.32	102.58
5	B	500	B13	C25-C2-C3	2.03	115.85	111.83
5	L	500	B13	C6-N22-C9	2.03	109.75	107.71
5	J	500	B13	C10-C11-N23	2.01	124.07	113.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	459/461 (99%)	-0.58	0 100 100	3, 11, 26, 38	0
1	C	459/461 (99%)	-0.61	0 100 100	3, 10, 23, 39	0
1	E	459/461 (99%)	0.11	14 (3%) 47 48	25, 33, 42, 49	0
1	G	459/461 (99%)	-0.21	6 (1%) 74 76	18, 29, 40, 49	0
1	I	459/461 (99%)	-0.47	3 (0%) 84 86	9, 20, 34, 50	0
1	K	459/461 (99%)	-0.47	3 (0%) 84 86	12, 20, 33, 46	0
1	M	459/461 (99%)	-0.47	2 (0%) 90 92	10, 20, 34, 48	0
1	O	459/461 (99%)	-0.50	1 (0%) 93 94	7, 18, 32, 45	0
2	B	258/258 (100%)	0.92	44 (17%) 2 2	4, 67, 100, 107	0
2	D	258/258 (100%)	1.00	51 (19%) 2 1	5, 66, 100, 110	0
2	F	258/258 (100%)	1.30	67 (25%) 1 1	18, 72, 102, 112	0
2	H	258/258 (100%)	1.63	82 (31%) 1 1	28, 73, 104, 110	0
2	J	258/258 (100%)	0.90	37 (14%) 3 3	17, 64, 97, 107	0
2	L	258/258 (100%)	1.23	63 (24%) 1 1	12, 71, 102, 113	0
2	N	258/258 (100%)	1.73	109 (42%) 1 0	12, 73, 103, 110	0
2	P	258/258 (100%)	0.96	39 (15%) 3 3	17, 67, 98, 108	0
All	All	5736/5752 (99%)	0.18	521 (9%) 10 8	3, 29, 92, 113	0

All (521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	258	HIS	7.6
2	J	207	PHE	7.2
2	P	207	PHE	7.1
2	J	178	LEU	7.1
2	H	207	PHE	7.0

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Mol	Chain	Res	Type	RSRZ
2	L	207	PHE	7.0
2	L	118	ALA	6.9
2	H	65	ALA	6.7
2	F	257	LYS	6.6
2	F	207	PHE	6.6
2	N	258	HIS	6.6
2	P	208	ALA	6.5
2	N	118	ALA	6.3
2	L	257	LYS	6.3
2	J	180	GLY	6.2
2	N	117	GLY	6.2
2	N	257	LYS	6.1
2	F	223	ALA	6.1
2	H	258	HIS	5.8
2	N	70	ILE	5.8
2	H	123	LYS	5.8
2	L	119	THR	5.8
2	N	255	PHE	5.6
2	D	65	ALA	5.6
2	P	118	ALA	5.6
2	N	221	GLN	5.6
2	P	209	CYS	5.6
2	D	258	HIS	5.5
2	L	189	TYR	5.5
2	N	199	LEU	5.4
2	J	209	CYS	5.4
2	N	113	LYS	5.4
2	H	253	GLU	5.4
2	J	179	THR	5.3
2	F	208	ALA	5.3
2	H	178	LEU	5.3
2	B	119	THR	5.3
2	J	208	ALA	5.3
2	L	117	GLY	5.3
2	J	258	HIS	5.2
2	L	65	ALA	5.2
2	N	207	PHE	5.2
2	P	119	THR	5.2
2	N	72	LEU	5.2
2	P	121	LYS	5.1
2	L	258	HIS	5.1
2	N	151	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	H	119	THR	5.0
2	H	77	LEU	5.0
2	D	199	LEU	5.0
2	H	248	VAL	5.0
2	N	121	LYS	5.0
2	F	178	LEU	4.9
2	H	208	ALA	4.9
2	N	227	TYR	4.9
2	L	179	THR	4.9
2	P	178	LEU	4.9
2	N	176	ILE	4.9
2	F	200	GLU	4.8
2	D	59	LEU	4.8
2	N	247	ASP	4.8
2	H	243	ALA	4.8
2	N	243	ALA	4.7
2	H	242	ILE	4.7
2	N	179	THR	4.7
2	F	67	LYS	4.7
2	F	179	THR	4.7
2	N	178	LEU	4.7
2	H	61	ALA	4.7
2	N	123	LYS	4.6
2	H	151	GLY	4.6
2	H	70	ILE	4.6
2	P	179	THR	4.6
2	H	245	THR	4.6
2	F	123	LYS	4.6
2	N	119	THR	4.6
2	H	118	ALA	4.6
2	N	68	ASP	4.5
2	N	36	LYS	4.5
2	L	243	ALA	4.5
2	N	240	ALA	4.5
2	N	246	THR	4.5
2	H	110	GLU	4.4
2	H	79	VAL	4.3
2	L	208	ALA	4.3
2	N	114	GLU	4.3
2	F	204	LYS	4.2
2	J	119	THR	4.2
2	F	249	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	222	PHE	4.2
2	N	204	LYS	4.2
2	F	119	THR	4.2
2	N	37	ASP	4.2
2	H	257	LYS	4.2
2	N	112	CYS	4.2
2	H	113	LYS	4.2
2	P	67	LYS	4.2
2	D	246	THR	4.2
2	H	133	GLY	4.2
2	N	69	PRO	4.2
2	D	249	THR	4.1
2	F	68	ASP	4.1
2	H	36	LYS	4.1
2	N	150	ASN	4.1
2	D	68	ASP	4.1
2	N	189	TYR	4.1
2	N	249	THR	4.1
2	N	59	LEU	4.1
2	N	242	ILE	4.1
2	H	121	LYS	4.0
2	D	77	LEU	4.0
2	B	68	ASP	4.0
2	B	178	LEU	4.0
2	D	243	ALA	4.0
2	N	174	LYS	4.0
2	H	247	ASP	4.0
2	F	189	TYR	4.0
2	B	65	ALA	4.0
2	N	77	LEU	3.9
1	E	3	ALA	3.9
2	H	209	CYS	3.9
2	L	242	ILE	3.9
2	D	226	VAL	3.9
2	H	216	GLN	3.9
2	F	243	ALA	3.9
2	N	56	VAL	3.9
2	L	120	PRO	3.9
2	F	244	GLY	3.9
2	D	189	TYR	3.9
2	D	207	PHE	3.9
2	L	253	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	203	ILE	3.9
2	H	67	LYS	3.9
2	N	67	LYS	3.9
2	D	178	LEU	3.8
2	F	77	LEU	3.8
2	J	191	PHE	3.8
2	F	180	GLY	3.8
2	N	116	SER	3.8
2	D	257	LYS	3.8
2	F	117	GLY	3.8
2	H	180	GLY	3.8
2	H	115	ASN	3.8
2	B	208	ALA	3.8
2	J	194	VAL	3.8
2	L	246	THR	3.8
2	L	36	LYS	3.8
2	D	236	LYS	3.8
2	B	207	PHE	3.8
2	D	253	GLU	3.8
2	N	250	GLU	3.7
2	P	36	LYS	3.7
2	F	242	ILE	3.7
2	H	179	THR	3.7
2	H	217	ASP	3.7
2	B	253	GLU	3.7
1	E	97	TRP	3.7
2	L	255	PHE	3.6
2	F	209	CYS	3.6
2	J	257	LYS	3.6
2	P	65	ALA	3.6
2	N	201	ASN	3.6
2	H	244	GLY	3.6
2	L	174	LYS	3.6
2	D	255	PHE	3.5
2	J	117	GLY	3.5
2	J	226	VAL	3.5
2	F	255	PHE	3.5
2	N	222	PHE	3.5
2	F	225	GLY	3.5
2	N	223	ALA	3.5
2	P	180	GLY	3.5
2	L	178	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	445	THR	3.5
2	H	122	THR	3.5
2	L	249	THR	3.5
2	B	77	LEU	3.4
2	D	121	LYS	3.4
2	L	200	GLU	3.4
2	P	77	LEU	3.4
2	D	208	ALA	3.4
2	N	208	ALA	3.4
2	N	253	GLU	3.4
2	N	106	LEU	3.4
2	H	63	ILE	3.4
2	J	67	LYS	3.4
2	D	225	GLY	3.4
2	N	35	PRO	3.4
2	B	56	VAL	3.4
2	N	215	ASN	3.3
2	H	223	ALA	3.3
2	B	110	GLU	3.3
2	H	255	PHE	3.3
2	N	202	GLY	3.3
2	D	223	ALA	3.3
2	H	52	GLU	3.3
2	H	250	GLU	3.3
2	P	226	VAL	3.3
2	J	110	GLU	3.3
2	B	258	HIS	3.3
2	H	57	GLU	3.3
2	H	172	LYS	3.3
2	N	124	GLY	3.3
2	B	226	VAL	3.3
2	D	224	LEU	3.3
2	B	179	THR	3.3
2	N	71	ASP	3.2
2	N	60	GLN	3.2
2	H	120	PRO	3.2
2	L	110	GLU	3.2
2	F	133	GLY	3.2
2	N	254	LYS	3.2
2	B	71	ASP	3.2
2	F	247	ASP	3.2
2	N	168	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	106	LEU	3.2
2	P	191	PHE	3.2
2	H	189	TYR	3.2
2	D	200	GLU	3.2
2	N	110	GLU	3.2
2	H	249	THR	3.2
2	D	112	CYS	3.1
2	H	117	GLY	3.1
2	B	70	ILE	3.1
2	H	241	ILE	3.1
2	N	217	ASP	3.1
2	P	258	HIS	3.1
2	P	117	GLY	3.1
2	B	255	PHE	3.1
2	N	164	GLU	3.1
2	B	69	PRO	3.1
2	H	204	LYS	3.1
2	P	113	LYS	3.1
2	N	51	GLU	3.1
2	B	109	ILE	3.1
2	B	236	LYS	3.1
2	D	172	LYS	3.1
2	L	76	ALA	3.1
2	D	133	GLY	3.1
2	F	59	LEU	3.1
2	B	242	ILE	3.1
2	N	206	PRO	3.1
2	H	116	SER	3.0
2	L	177	MET	3.0
2	N	107	GLU	3.0
2	H	174	LYS	3.0
2	P	177	MET	3.0
2	N	226	VAL	3.0
2	N	248	VAL	3.0
2	J	237	ILE	3.0
2	F	250	GLU	3.0
2	H	199	LEU	3.0
2	J	59	LEU	3.0
2	J	118	ALA	3.0
2	H	64	GLU	3.0
2	D	69	PRO	3.0
2	H	51	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	177	MET	3.0
2	D	180	GLY	3.0
2	P	69	PRO	3.0
2	B	227	TYR	3.0
2	N	192	LYS	3.0
2	B	244	GLY	3.0
2	F	217	ASP	3.0
2	P	243	ALA	2.9
2	N	154	VAL	2.9
2	N	53	ASP	2.9
2	B	189	TYR	2.9
2	F	222	PHE	2.9
2	N	76	ALA	2.9
2	L	225	GLY	2.9
1	E	4	LYS	2.9
2	H	226	VAL	2.9
2	F	246	THR	2.9
1	G	56	GLU	2.9
2	J	128	CYS	2.9
2	N	200	GLU	2.9
1	E	8	SER	2.9
2	F	84	VAL	2.9
2	P	110	GLU	2.8
2	L	221	GLN	2.8
1	E	53	ALA	2.8
2	F	116	SER	2.8
2	L	77	LEU	2.8
2	L	121	LYS	2.8
2	L	69	PRO	2.8
2	L	171	GLN	2.8
2	H	41	TYR	2.8
2	P	257	LYS	2.8
2	L	226	VAL	2.8
2	N	194	VAL	2.8
2	H	108	GLY	2.7
2	N	162	PRO	2.7
2	F	193	GLU	2.7
2	F	112	CYS	2.7
2	B	60	GLN	2.7
2	F	253	GLU	2.7
2	L	59	LEU	2.7
2	N	220	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	53	ALA	2.7
2	N	232	ALA	2.7
2	H	200	GLU	2.7
2	N	52	GLU	2.7
2	N	43	ILE	2.7
2	L	114	GLU	2.7
2	B	59	LEU	2.7
2	N	244	GLY	2.7
2	N	63	ILE	2.7
2	N	73	ILE	2.7
2	F	36	LYS	2.7
2	H	221	GLN	2.7
2	L	67	LYS	2.7
2	N	236	LYS	2.7
1	E	135	PHE	2.7
2	J	177	MET	2.7
2	P	194	VAL	2.7
2	D	179	THR	2.7
2	J	200	GLU	2.7
2	B	118	ALA	2.7
2	B	209	CYS	2.6
2	L	216	GLN	2.6
2	F	156	ASP	2.6
2	N	239	ASP	2.6
2	P	172	LYS	2.6
2	P	206	PRO	2.6
2	H	49	GLU	2.6
2	B	121	LYS	2.6
2	D	251	LEU	2.6
2	F	113	LYS	2.6
2	H	167	LEU	2.6
2	N	209	CYS	2.6
2	L	227	TYR	2.6
2	H	38	GLU	2.6
2	L	56	VAL	2.6
2	L	248	VAL	2.6
2	L	146	LEU	2.6
1	E	460	GLY	2.6
2	J	225	GLY	2.6
2	B	63	ILE	2.6
2	J	254	LYS	2.6
2	L	109	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	201	ASN	2.6
2	P	116	SER	2.6
2	H	227	TYR	2.6
1	K	134	GLU	2.6
2	D	58	GLY	2.6
2	D	250	GLU	2.6
2	B	243	ALA	2.5
2	H	66	GLY	2.5
2	F	199	LEU	2.5
2	J	251	LEU	2.5
2	N	167	LEU	2.5
2	H	153	ASN	2.5
2	P	155	VAL	2.5
1	I	133	ARG	2.5
2	N	133	GLY	2.5
2	F	132	GLU	2.5
1	E	431	ALA	2.5
2	H	193	GLU	2.5
2	J	243	ALA	2.5
2	P	52	GLU	2.5
2	B	257	LYS	2.5
2	D	192	LYS	2.5
2	L	113	LYS	2.5
2	N	172	LYS	2.5
2	B	249	THR	2.5
1	E	133	ARG	2.5
2	L	123	LYS	2.5
1	I	3	ALA	2.5
2	F	69	PRO	2.5
2	N	197	MET	2.5
2	L	244	GLY	2.5
2	D	204	LYS	2.5
2	F	236	LYS	2.5
2	J	53	ASP	2.5
2	D	191	PHE	2.5
2	N	196	ASP	2.5
2	N	64	GLU	2.5
2	D	174	LYS	2.5
2	H	109	ILE	2.5
2	J	68	ASP	2.4
2	L	52	GLU	2.4
2	L	234	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	116	SER	2.4
2	F	22	LYS	2.4
2	N	125	THR	2.4
2	F	51	GLU	2.4
2	L	43	ILE	2.4
2	D	119	THR	2.4
2	J	116	SER	2.4
2	N	38	GLU	2.4
2	N	65	ALA	2.4
2	J	65	ALA	2.4
2	N	186	THR	2.4
2	N	171	GLN	2.4
2	F	162	PRO	2.4
2	J	236	LYS	2.4
2	P	59	LEU	2.4
1	K	141	ASP	2.4
1	E	93	ASN	2.3
2	B	114	GLU	2.3
2	N	122	THR	2.3
2	H	78	MET	2.3
2	L	70	ILE	2.3
2	N	241	ILE	2.3
2	H	162	PRO	2.3
2	F	219	VAL	2.3
2	N	256	HIS	2.3
2	N	218	PHE	2.3
2	D	109	ILE	2.3
2	H	7	ALA	2.3
2	N	120	PRO	2.3
2	L	233	ASP	2.3
2	L	192	LYS	2.3
2	N	224	LEU	2.3
2	F	23	ALA	2.3
2	J	60	GLN	2.3
2	F	160	ASP	2.3
2	P	129	HIS	2.3
2	B	200	GLU	2.3
2	D	205	ILE	2.3
2	H	203	ILE	2.3
2	N	205	ILE	2.3
2	F	37	ASP	2.3
2	L	193	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	248	VAL	2.3
2	L	209	CYS	2.3
2	F	194	VAL	2.3
1	M	134	GLU	2.2
2	B	67	LYS	2.2
1	K	53	ALA	2.2
2	J	234	ALA	2.2
2	L	58	GLY	2.2
2	D	247	ASP	2.2
2	H	53	ASP	2.2
2	H	107	GLU	2.2
2	J	69	PRO	2.2
2	J	162	PRO	2.2
2	L	151	GLY	2.2
2	H	86	ARG	2.2
2	H	114	GLU	2.2
2	P	253	GLU	2.2
2	L	202	GLY	2.2
2	P	210	GLY	2.2
2	B	191	PHE	2.2
2	H	154	VAL	2.2
2	N	153	ASN	2.2
2	H	202	GLY	2.2
2	L	39	LEU	2.2
2	F	221	GLN	2.2
2	H	222	PHE	2.2
2	F	108	GLY	2.2
2	P	237	ILE	2.2
2	N	41	TYR	2.2
2	B	174	LYS	2.2
2	H	112	CYS	2.2
2	D	177	MET	2.2
2	F	129	HIS	2.2
2	H	80	GLY	2.2
2	L	180	GLY	2.2
2	P	181	THR	2.2
2	L	224	LEU	2.1
1	E	5	ARG	2.1
2	D	256	HIS	2.1
2	B	58	GLY	2.1
2	B	151	GLY	2.1
2	L	116	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	50	GLY	2.1
1	G	135	PHE	2.1
2	J	129	HIS	2.1
2	D	66	GLY	2.1
2	D	215	ASN	2.1
2	P	225	GLY	2.1
2	L	254	LYS	2.1
2	P	255	PHE	2.1
2	N	146	LEU	2.1
2	J	172	LYS	2.1
2	D	242	ILE	2.1
2	F	81	MET	2.1
2	L	129	HIS	2.1
2	N	129	HIS	2.1
2	F	205	ILE	2.1
2	L	203	ILE	2.1
2	D	201	ASN	2.1
2	F	224	LEU	2.1
1	G	133	ARG	2.1
2	B	105	MET	2.1
2	F	203	ILE	2.1
2	F	38	GLU	2.1
2	F	220	SER	2.1
2	N	177	MET	2.1
2	D	36	LYS	2.1
2	D	37	ASP	2.1
2	B	206	PRO	2.1
2	J	127	VAL	2.1
1	E	461	PHE	2.1
1	G	228	PHE	2.1
1	G	3	ALA	2.1
2	N	44	ALA	2.1
2	B	51	GLU	2.1
1	E	449	SER	2.1
1	M	141	ASP	2.1
2	P	56	VAL	2.0
2	D	221	GLN	2.0
2	F	164	GLU	2.0
2	F	118	ALA	2.0
2	P	112	CYS	2.0
2	D	116	SER	2.0
2	F	47	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	251	LEU	2.0
2	B	217	ASP	2.0
2	D	67	LYS	2.0
2	H	246	THR	2.0
2	H	111	TYR	2.0
2	N	23	ALA	2.0
2	F	251	LEU	2.0
2	N	233	ASP	2.0
2	L	250	GLU	2.0
2	H	168	ALA	2.0
1	G	461	PHE	2.0
1	I	4	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	K	K	516	1/1	0.14	1.88	31,31,31,31	1
4	K	I	515	1/1	0.12	1.12	28,28,28,28	1
4	K	G	514	1/1	0.13	0.79	39,39,39,39	1
4	K	O	518	1/1	0.10	0.17	35,35,35,35	1
5	B13	N	500	90/90	0.18	0.11	60,66,72,73	0
5	B13	L	500	90/90	0.15	-0.23	41,47,58,59	0
5	B13	F	500	90/90	0.17	-0.26	53,63,71,72	0
5	B13	P	500	90/90	0.14	-0.41	31,40,45,52	0
5	B13	D	500	90/90	0.13	-0.44	20,30,40,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	B13	H	500	90/90	0.14	-0.50	45,58,68,69	0
5	B13	J	500	90/90	0.13	-0.55	32,37,50,57	0
5	B13	B	500	90/90	0.11	-0.60	9,24,48,49	0
4	K	C	512	1/1	0.07	-0.92	22,22,22,22	1
3	ZN	I	521	1/1	0.04	-1.98	16,16,16,16	0
3	ZN	O	508	1/1	0.05	-1.99	33,33,33,33	0
3	ZN	E	522	1/1	0.05	-2.11	37,37,37,37	0
4	K	A	511	1/1	0.04	-2.39	23,23,23,23	1
3	ZN	A	524	1/1	0.04	-2.39	9,9,9,9	0
3	ZN	G	504	1/1	0.07	-2.49	33,33,33,33	1
3	ZN	I	505	1/1	0.04	-2.54	30,30,30,30	0
3	ZN	K	506	1/1	0.04	-2.70	33,33,33,33	0
3	ZN	M	523	1/1	0.03	-2.84	21,21,21,21	0
4	K	M	517	1/1	0.07	-3.05	33,33,33,33	1
3	ZN	A	501	1/1	0.03	-3.09	20,20,20,20	0
4	K	E	513	1/1	0.10	-3.14	33,33,33,33	1
3	ZN	C	502	1/1	0.03	-3.28	19,19,19,19	0
3	ZN	M	507	1/1	0.03	-4.18	33,33,33,33	0
3	ZN	E	503	1/1	0.05	-6.12	36,36,36,36	1

6.5 Other polymers ⓘ

There are no such residues in this entry.