



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:02 am GMT

PDB ID : 2I2X
Title : Crystal structure of methanol:cobalamin methyltransferase complex MtaBC from *Methanosarcina barkeri*
Authors : Hagemeyer, 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

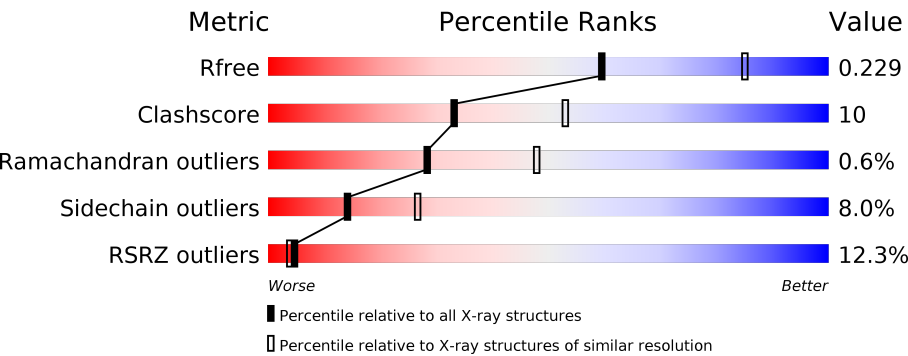
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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.











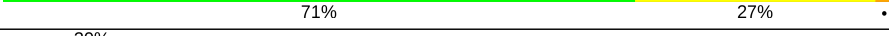

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	<div><div></div><div>82%14%•</div></div>
1	C	461	<div><div></div><div>82%15%•</div></div>
1	E	461	<div><div>6%</div><div>80%18%•</div></div>
1	G	461	<div><div>2%</div><div>79%18%•</div></div>
1	I	461	<div><div>%</div><div>84%13%•</div></div>
1	K	461	<div><div>%</div><div>82%15%•</div></div>

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Mol	Chain	Length	Quality of chain
1	M	461	
1	O	461	
2	B	258	
2	D	258	
2	F	258	
2	H	258	
2	J	258	
2	L	258	
2	N	258	
2	P	258	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K	G	514	-	-	-	X

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	P	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			

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

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

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

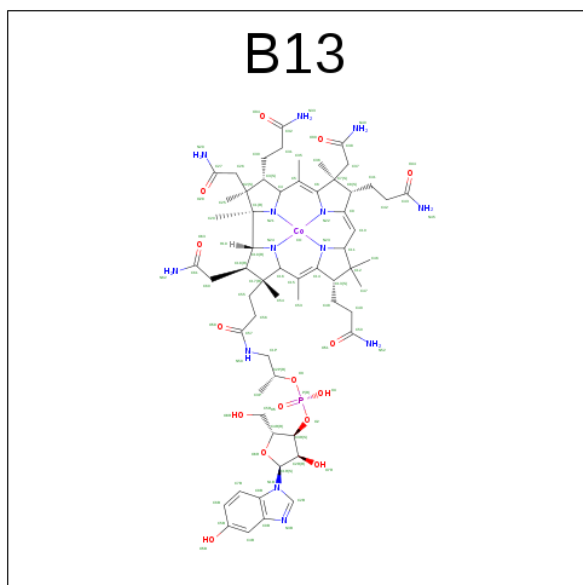
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	K	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	I	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	O	1	Total	K	0	0
			1	1		

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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 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	D	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	F	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	H	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	J	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	L	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	N	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0
5	P	1	Total 90	C 60	Co 1	N 13	O 15	P 1	0	0

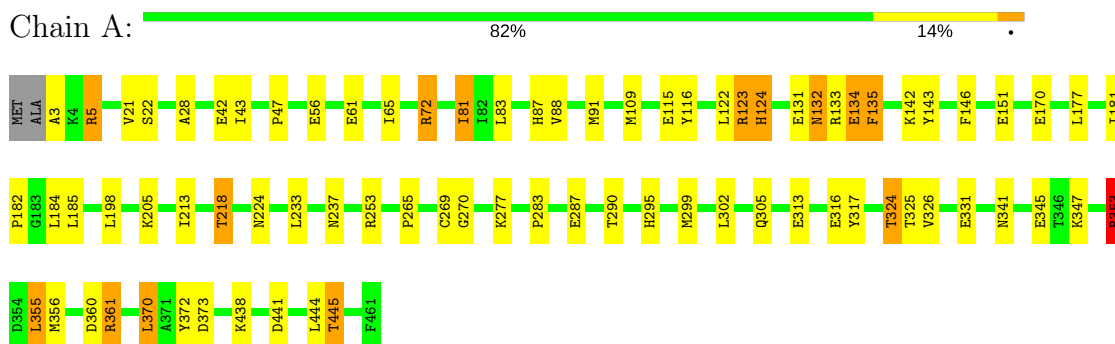
- Molecule 6 is water.

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

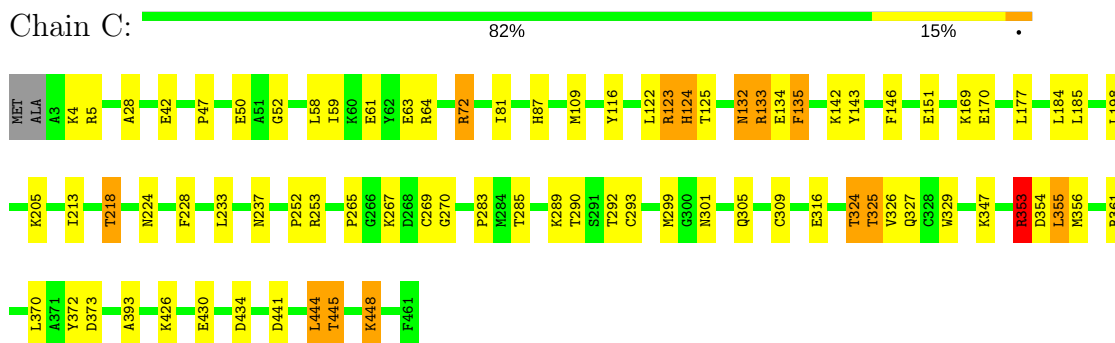
3 Residue-property plots

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

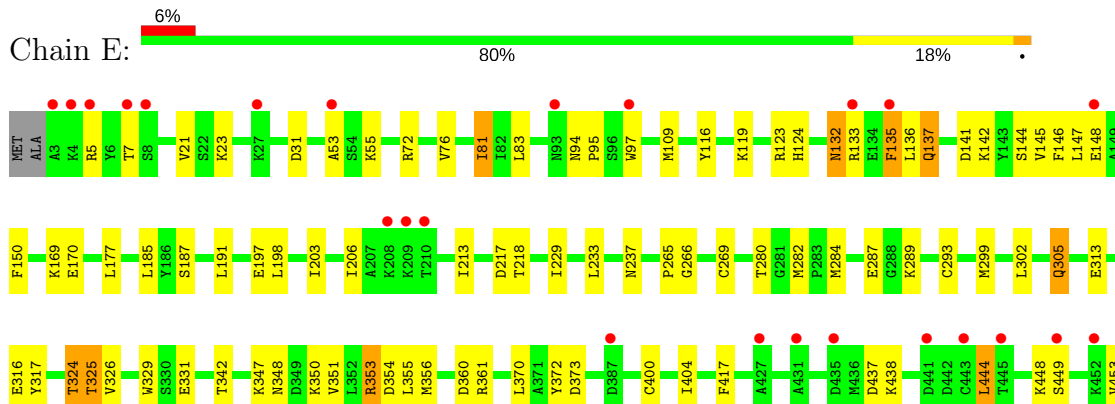
• Molecule 1: Methyltransferase 1

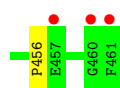


• Molecule 1: Methyltransferase 1

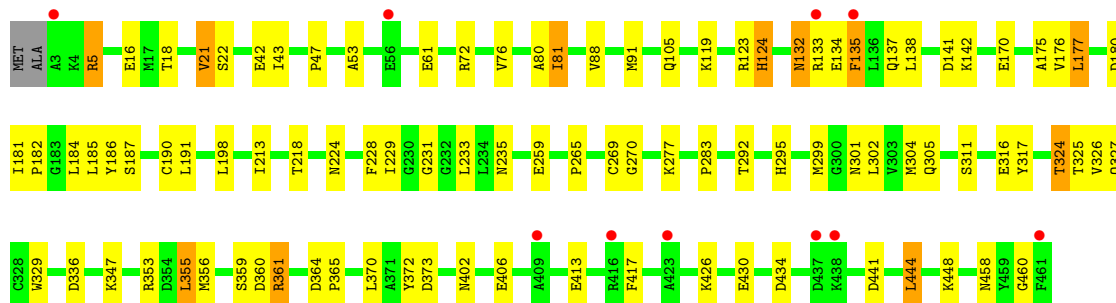
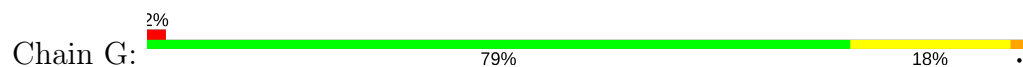


• Molecule 1: Methyltransferase 1

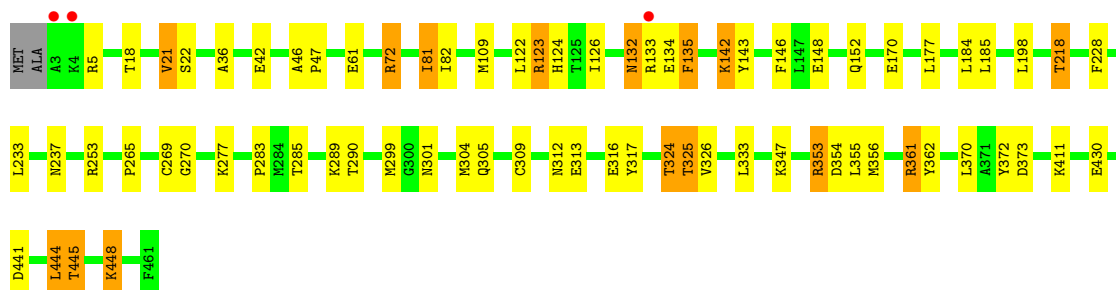
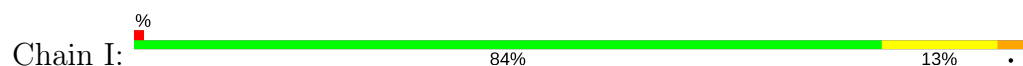




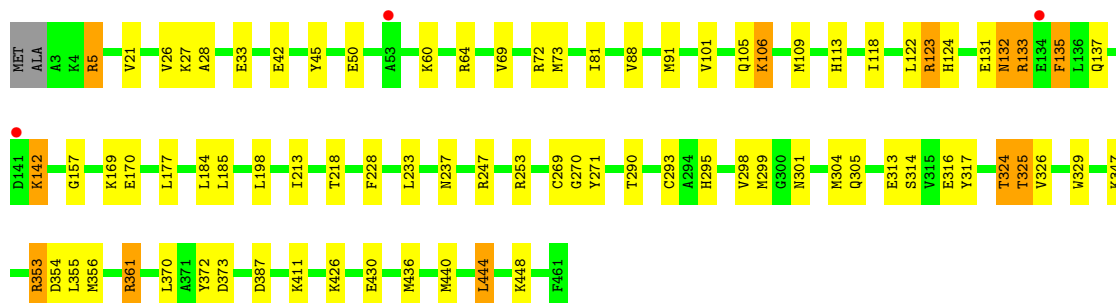
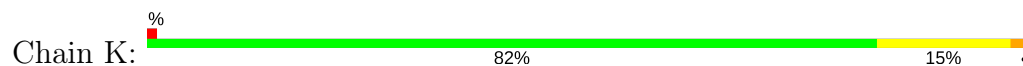
• Molecule 1: Methyltransferase 1



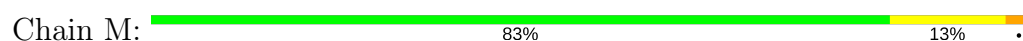
• Molecule 1: Methyltransferase 1

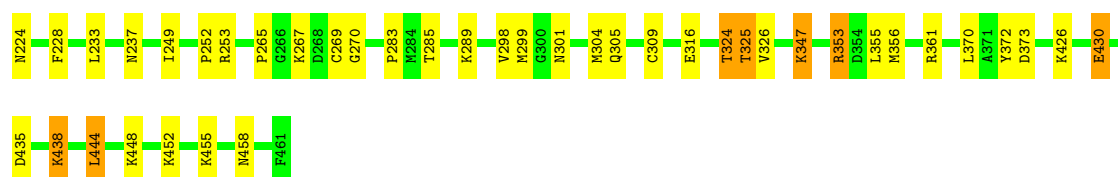


• Molecule 1: Methyltransferase 1



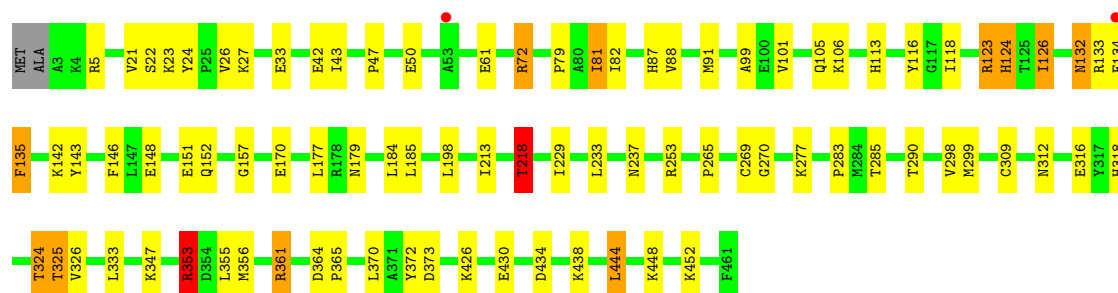
• Molecule 1: Methyltransferase 1





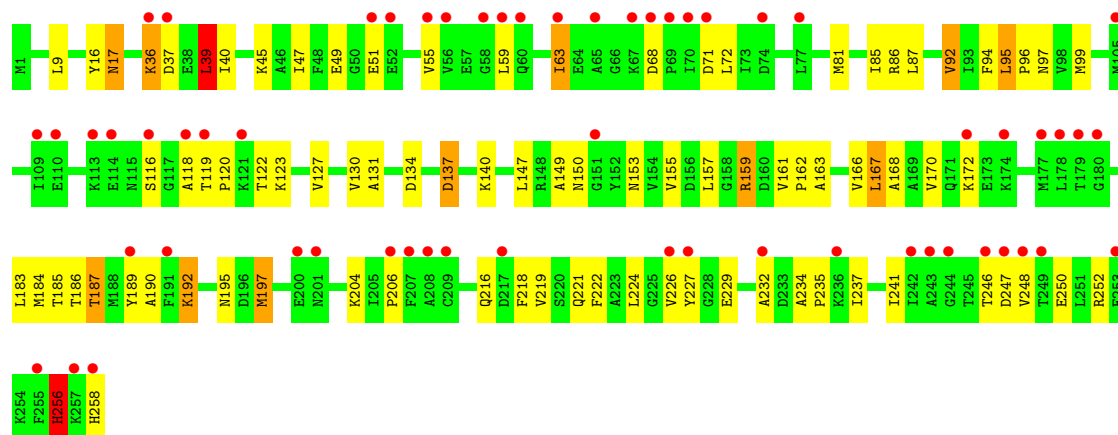
• Molecule 1: Methyltransferase 1

Chain O: 81% 16%



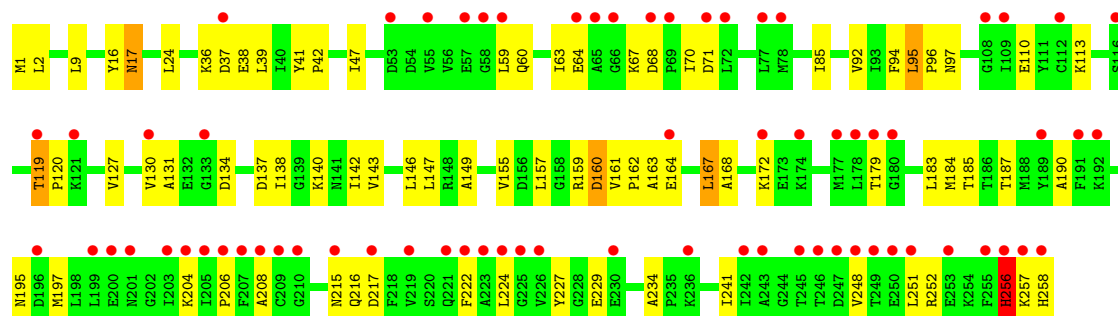
• Molecule 2: Methyltransferase 1

Chain B: 22% 66% 29%

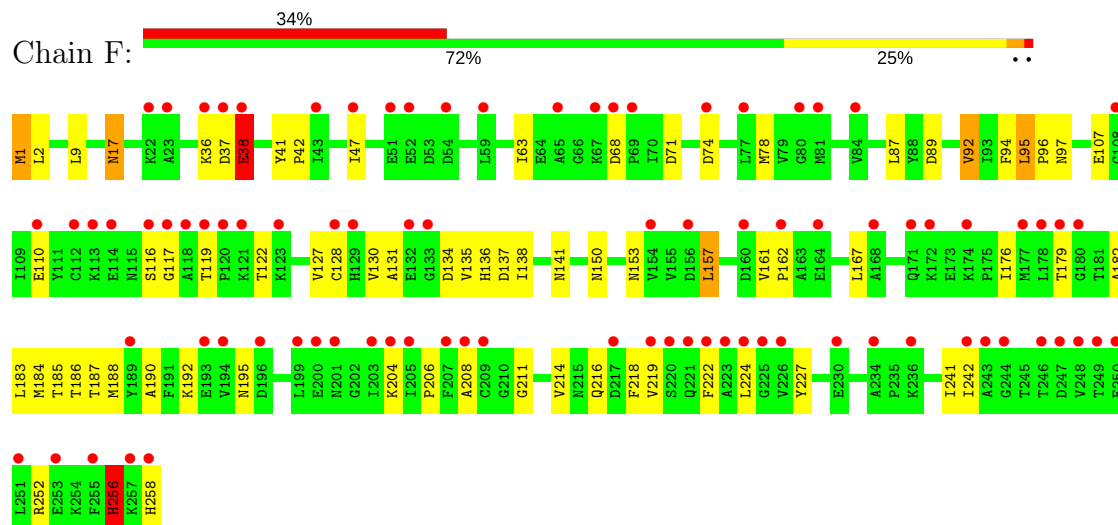


• Molecule 2: Methyltransferase 1

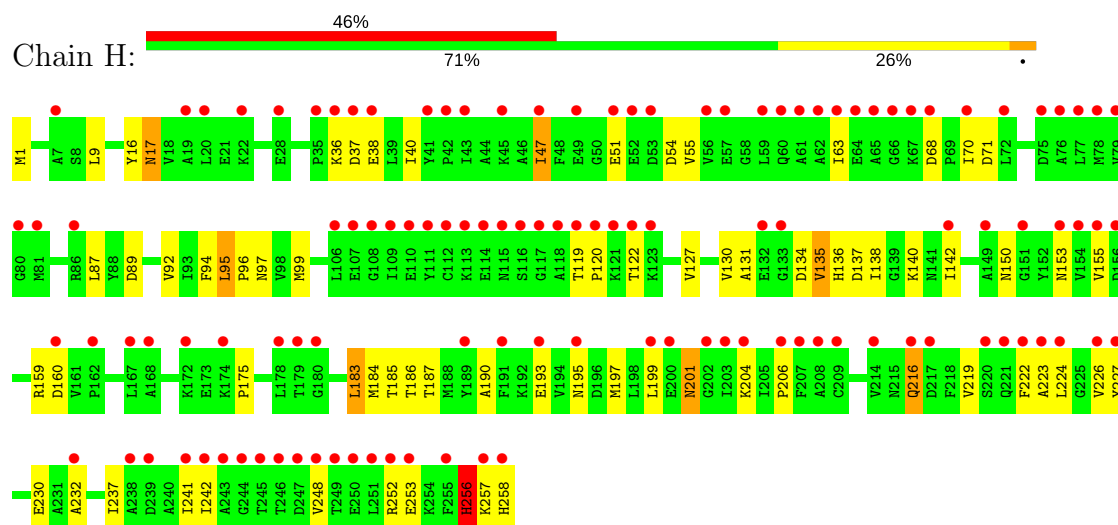
Chain D: 27% 69% 29%



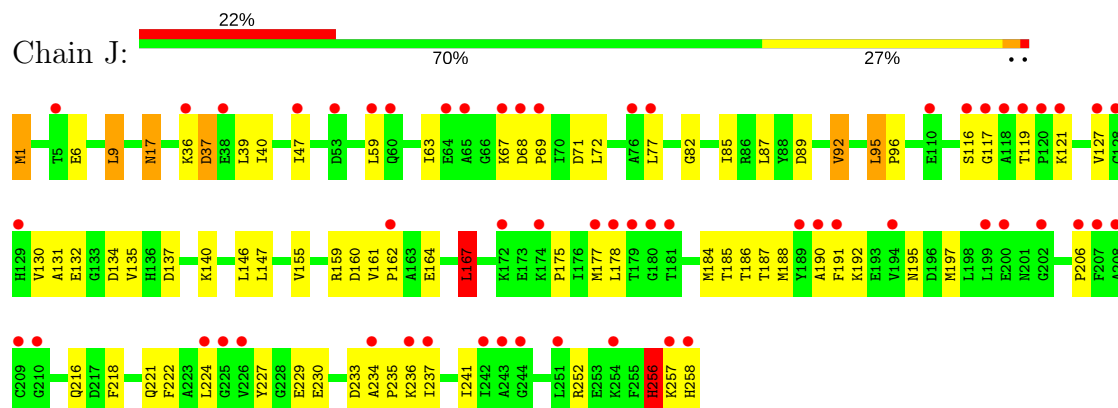
• Molecule 2: Methyltransferase 1



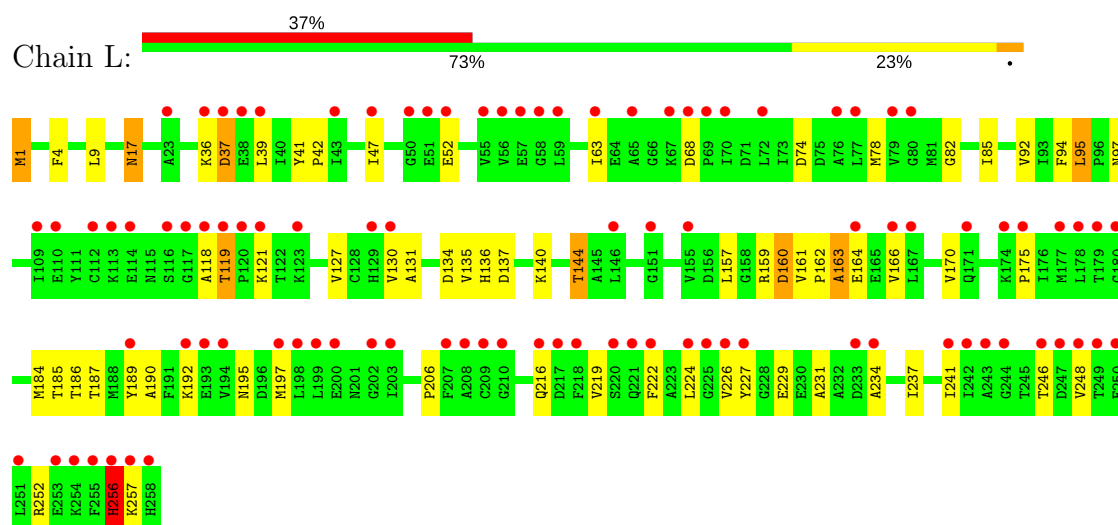
• Molecule 2: Methyltransferase 1



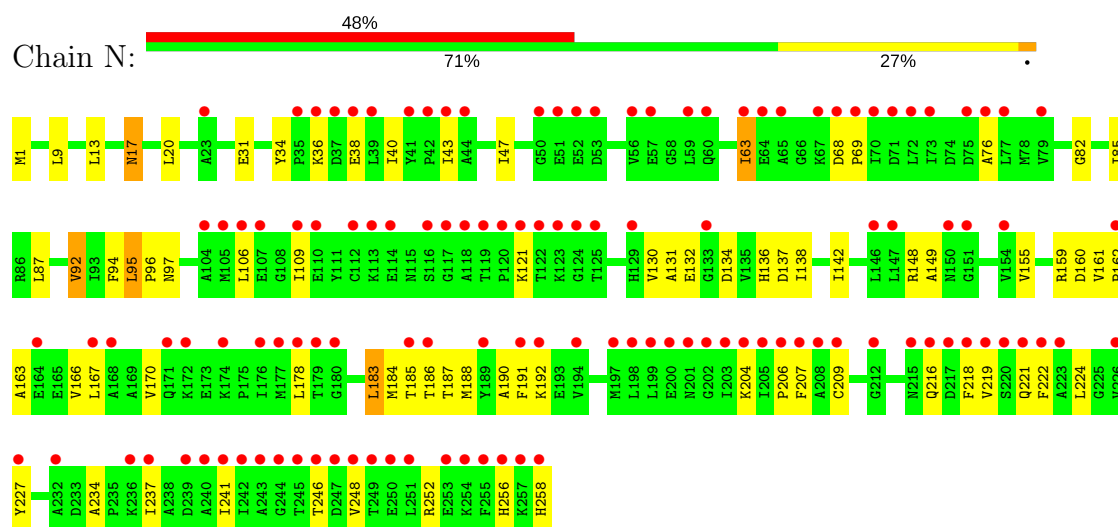
• Molecule 2: Methyltransferase 1



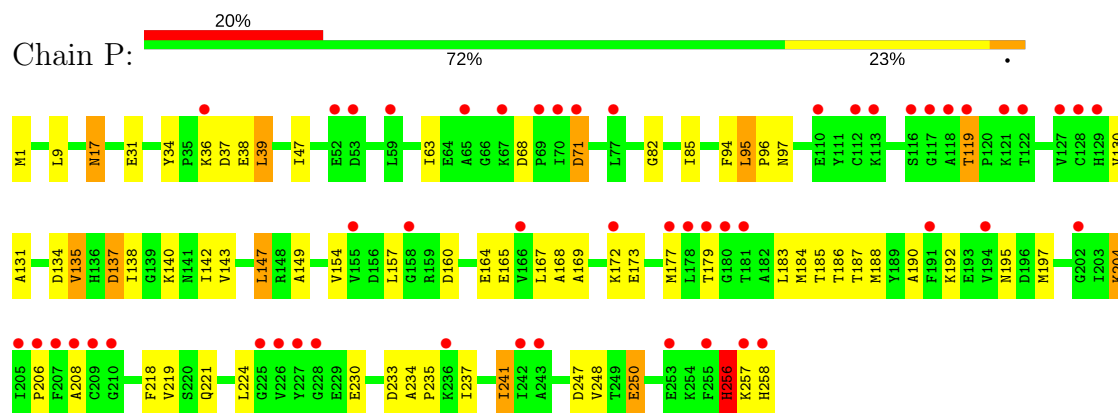
• Molecule 2: Methyltransferase 1



• Molecule 2: Methyltransferase 1



• Molecule 2: Methyltransferase 1



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 , 0.229	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)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
1	K	3534	0	3462	61	0
1	M	3534	0	3462	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	H	1	0	0	0	0
6	I	93	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (865) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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
1:A:72:ARG:NH2	6:A:681:HOH:O	2.09	0.85
2:F:184:MET:HG2	5:F:500:B13:H302	1.58	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	Interatomic distance (Å)	Clash overlap (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:C:324:THR:CG2	1:C:326:VAL:HG22	2.18	0.73
1:M:353:ARG:HA	1:M:356:MET:HE1	1.71	0.73
1:C:218:THR:HG21	1:C:269:CYS:SG	2.29	0.73
2:B:17:ASN:H	2:B:17:ASN:ND2	1.86	0.73
1:E:444:LEU:O	1:E:448:LYS:HB2	1.89	0.73
1:K:218:THR:HG21	1:K:269:CYS:SG	2.29	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:D:85:ILE:HD11	2:D:149:ALA:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:219:VAL:HG21	2:N:227:TYR:HB2	1.73	0.70
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:G:316:GLU:O	1:G:325:THR:HG21	1.91	0.69
1:K:28:ALA:HB2	1:K:213:ILE:HD12	1.74	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:B:134:ASP:OD2	2:B:187:THR:HG21	1.92	0.69
2:J:184:MET:HG2	5:J:500:B13:H302	1.73	0.69
2:B:130:VAL:HG23	2:B:140:LYS:HD3	1.74	0.69
2:P:17:ASN:H	2:P:17:ASN:HD22	1.39	0.69
2:P:134:ASP:HB2	2:P:187:THR:HG21	1.74	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:C:28:ALA:HB2	1:C:213:ILE:HD13	1.76	0.68
1:I:354:ASP:OD2	2:J:1:MET:HA	1.94	0.68
2:B:185:THR:H	5:B:500:B13:H332	1.40	0.68
1:K:26:VAL:CG1	1:K:213:ILE:HD13	2.23	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
2:F:17:ASN:H	2:F:17:ASN:HD22	1.41	0.66
1:O:132:ASN:HD22	1:O:134:GLU:H	1.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:301:ASN:HD22	1:G:304:MET:HE2	1.60	0.65
1:I:361:ARG:HH22	1:I:373:ASP:CG	2.00	0.65
1:G:417:PHE:HZ	2:H:97:ASN:HD21	1.43	0.65
2:B:192:LYS:HG2	2:B:222:PHE:HE2	1.62	0.65
1:O:43:ILE:HG22	1:O:81:ILE:HD11	1.79	0.65
2:B:206:PRO:HG2	2:B:241:ILE:HD12	1.79	0.65
1:M:353:ARG:HD3	1:M:372:TYR:CE1	2.31	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: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
1:M:353:ARG:HA	1:M:356:MET:HE2	1.79	0.64
1:C:353:ARG:HA	1:C:356:MET:HE2	1.78	0.64
2:J:17:ASN:N	2:J:17:ASN:HD22	1.94	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
1:G:302:LEU:HB2	1:G:360:ASP:HB2	1.81	0.63
5:J:500:B13:H351	5:J:500:B13:H361	1.80	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
2:B:137:ASP:HB2	5:B:500:B13:H522	1.64	0.63
5:D:500:B13:H363	5:D:500:B13:N40	2.14	0.63
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
2:N:185:THR:HG23	5:N:500:B13:H332	1.64	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:D:131:ALA:HB1	2:D:190:ALA:HB3	1.81	0.62
2:P:168:ALA:O	2:P:172:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LYS:HG2	2:B:222:PHE:CE2	2.34	0.61
2:B:195:ASN:HD21	2:B:224:LEU:H	1.47	0.61
2:D:168:ALA:O	2:D:172:LYS:HG2	2.00	0.61
2:D:215:ASN:HD22	2:D:217:ASP:H	1.48	0.61
2:P:185:THR:HG23	5:P:500:B13:H332	1.65	0.61
1:K:133:ARG:HD2	2:L:160:ASP:HB3	1.80	0.61
1:C:42:GLU:OE2	1:C:123:ARG:HD2	2.00	0.61
1:O:72:ARG:NH2	6:O:616:HOH:O	2.33	0.61
1:G:460:GLY:HA2	6:G:554:HOH:O	2.00	0.61
2:P:177:MET:CE	2:P:237:ILE:HG13	2.30	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:M:426:LYS:HE3	1:M:430:GLU:OE2	2.00	0.61
1:O:132:ASN:ND2	1:O:134:GLU:H	1.98	0.61
2:P:131:ALA:HB1	2:P:190:ALA:HB3	1.81	0.61
1:C:426:LYS:O	1:C:430:GLU:HG3	2.01	0.61
2:N:94:PHE:H	2:N:97:ASN:HD22	1.49	0.61
5:D:500:B13:H361	5:D:500:B13:H351	1.83	0.61
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:94:PHE:H	2:N:97:ASN:ND2	1.98	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:C:4:LYS:HG2	6:O:629:HOH:O	2.02	0.60
1:O:132:ASN:ND2	1:O:135:PHE:H	1.98	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: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
1:I:312:ASN:HB3	1:I:333:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:184:MET:HG2	5:P:500:B13:H302	1.85	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:N:137:ASP:HB2	5:N:500:B13:N52	2.18	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:D:94:PHE:H	2:D:97:ASN:HD22	1.51	0.58
2:H:130:VAL:HG23	2:H:140:LYS:HD3	1.86	0.58
1:K:293:CYS:HB3	1:K:329:TRP:CZ2	2.39	0.58
1:E:132:ASN:ND2	1:E:135:PHE:H	2.02	0.58
1:G:18:THR:HG23	1:G:21:VAL:HG13	1.86	0.58
1:I:444:LEU:HD22	1:I:448:LYS:HD2	1.85	0.58
2:J:185:THR:H	5:J:500:B13:H332	1.50	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
2:B:184:MET:HG2	5:B:500:B13:H302	1.84	0.57
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
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:B:36:LYS:H	2:B:36:LYS:HD3	1.69	0.57
2:H:185:THR:HG23	5:H:500:B13:H332	1.68	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
1:O:42:GLU:OE2	1:O:123:ARG:HD2	2.04	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:G:231:GLY:HA3	1:G:235:ASN:ND2	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:169:LYS:HD2	5:L:500:B13:H473	1.87	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
1:C:305:GLN:HA	1:C:356:MET:CE	2.35	0.56
2:D:17:ASN:HD22	2:D:17:ASN:N	2.02	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:B:226:VAL:HG11	2:B:237:ILE:CD1	2.31	0.56
2:D:37:ASP:O	2:D:39:LEU:N	2.29	0.56
1:G:123:ARG:NH2	1:G:265:PRO:O	2.39	0.56
2:P:188:MET:HB3	2:P:218:PHE:CZ	2.41	0.56
1:E:448:LYS:HE3	1:E:456:PRO:HG2	1.86	0.56
1:A:132:ASN:ND2	1:A:135:PHE:H	2.03	0.56
1:A:265:PRO:HA	1:A:283:PRO:O	2.06	0.56
1:E:229:ILE:HD11	2:F:138:ILE:HD13	1.88	0.56
1:K:132:ASN:ND2	1:K:135:PHE:H	2.03	0.56
1:E:353:ARG:HD3	1:E:372:TYR:CE1	2.40	0.56
2:N:131:ALA:HB1	2:N:190:ALA:HB3	1.86	0.56
1:O:444:LEU:O	1:O:448:LYS:HB2	2.06	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
1:M:87:HIS:NE2	1:M:124:HIS:HD2	2.04	0.56
2:N:216:GLN:HE22	2:N:258:HIS:H	1.54	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:B:68:ASP:HB3	2:B:71:ASP:HB2	1.88	0.55
2:F:137:ASP:HB3	2:F:141:ASN:ND2	2.21	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
1:A:47:PRO:HB3	1:A:61:GLU:HG2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:222:PHE:O	2:H:252:ARG:NH2	2.39	0.55
1:O:132:ASN:C	1:O:132:ASN:HD22	2.10	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
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
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
2:H:195:ASN:HD21	2:H:224:LEU:H	1.54	0.54
2:D:127:VAL:HG13	2:D:157:LEU:HD23	1.89	0.54
1:G:132:ASN:ND2	1:G:134:GLU:H	2.04	0.54
1:A:353:ARG:HA	1:A:356:MET:CE	2.36	0.54
2:B:127:VAL:HG13	2:B:157:LEU:HD23	1.89	0.54
2:P:164:GLU:HA	2:P:197:MET:HE1	1.89	0.54
1:G:187:SER:HA	1:G:191:LEU:HD12	1.89	0.54
2:H:51:GLU:O	2:H:55:VAL:HG23	2.08	0.54
1:I:441:ASP:O	1:I:445:THR:HG23	2.07	0.54
1:K:69:VAL:O	1:K:73:MET:HG2	2.08	0.54
1:M:224:ASN:ND2	1:M:269:CYS:HB2	2.22	0.54
1:O:143:TYR:O	1:O:146:PHE:HB3	2.07	0.54
1:O:353:ARG:HD3	1:O:372:TYR:CE1	2.43	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:K:444:LEU:O	1:K:448:LYS:HB2	2.08	0.54
1:M:43:ILE:HG22	1:M:81:ILE:HD11	1.90	0.54
1:E:354:ASP:HB3	2:F:2:LEU:HD12	1.90	0.53
2:L:134:ASP:OD1	2:L:136:HIS:ND1	2.32	0.53
2:L:166:VAL:O	2:L:170:VAL:HG23	2.08	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:F:192:LYS:HG2	2:F:222:PHE:CE2	2.42	0.53
2:D:179:THR:HG22	2:D:208:ALA:HB3	1.90	0.53
2:D:216:GLN:HE21	2:D:258:HIS:CD2	2.26	0.53
1:O:353:ARG:HA	1:O:356:MET:HE3	1.88	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
2:P:195:ASN:ND2	2:P:224:LEU:H	2.06	0.53
1:M:131:GLU:HB2	1:M:136:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:17:ASN:ND2	2:D:17:ASN:H	2.03	0.52
2:L:219:VAL:CG2	2:L:227:TYR:HB2	2.35	0.52
2:F:135:VAL:CG1	2:F:135:VAL:O	2.57	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
5:J:500:B13:H401	5:J:500:B13:H363	1.73	0.52
1:A:3:ALA:HB2	6:A:675:HOH:O	2.09	0.52
2:B:167:LEU:HB2	2:B:197:MET:CE	2.36	0.52
1:E:331:GLU:HB3	1:G:292:THR:HG21	1.90	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:K:290:THR:O	1:K:290:THR:HG22	2.10	0.52
1:O:218:THR:HG23	1:O:270:GLY:N	2.25	0.52
2:D:215:ASN:ND2	2:D:217:ASP:H	2.08	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
2:N:216:GLN:HE21	2:N:258:HIS:HD2	1.55	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:E:324:THR:CG2	1:E:326:VAL:HG22	2.40	0.52
1:G:229:ILE:HD11	2:H:138:ILE:HD13	1.90	0.52
1:M:99:ALA:HB2	1:M:152:GLN:HB3	1.92	0.52
1:M:169:LYS:HD2	5:N:500:B13:H473	1.92	0.52
2:F:128:CYS:O	2:F:157:LEU:HB2	2.10	0.51
2:F:227:TYR:H	2:F:256:HIS:HE1	1.58	0.51
1:K:353:ARG:HA	1:K:356:MET:HE2	1.83	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:B:184:MET:HB2	2:B:187:THR:HB	1.92	0.51
2:F:184:MET:HE1	5:F:500:B13:H353	1.92	0.51
2:H:95:LEU:HB3	2:H:96:PRO:HD3	1.93	0.51
1:I:218:THR:HG23	1:I:270:GLY:N	2.26	0.51
2:J:37:ASP:C	2:J:39:LEU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:132:ASN:HD21	1:M:135:PHE:H	1.59	0.51
1:O:23:LYS:HD3	1:O:24:TYR:CZ	2.46	0.51
1:A:109:MET:HE3	1:A:122:LEU:HD13	1.91	0.51
5:B:500:B13:H252	5:B:500:B13:C61	2.41	0.51
2:J:167:LEU:HG	2:J:197:MET:HG2	1.91	0.51
1:K:27:LYS:HG2	1:K:33:GLU:HG2	1.92	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
1:C:125:THR:HG21	1:C:267:LYS:HE2	1.93	0.51
1:I:132:ASN:C	1:I:132:ASN:HD22	2.14	0.51
1:O:353:ARG:HA	1:O:356:MET:HE2	1.92	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
1:E:293:CYS:HB3	1:E:329:TRP:CE2	2.47	0.50
1:E:31:ASP:O	1:E:119:LYS:HG2	2.10	0.50
2:F:94:PHE:H	2:F:97:ASN:ND2	2.09	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:A:324:THR:CG2	1:A:326:VAL:HG22	2.42	0.50
2:B:162:PRO:O	2:B:163:ALA:HB3	2.12	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CZ2	2.46	0.50
2:F:122:THR:HG21	2:F:153:ASN:HB2	1.94	0.50
2:P:167:LEU:HB2	2:P:197:MET:HE1	1.93	0.50
2:P:167:LEU:HB2	2:P:197:MET:CE	2.41	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:B:234:ALA:HB3	2:B:235:PRO:HD3	1.93	0.50
2:F:195:ASN:ND2	2:F:224:LEU:HB2	2.27	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
2:P:230:GLU:O	2:P:233:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:353:ARG:HD3	1:K:372:TYR:CE1	2.47	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
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
2:F:135:VAL:HG12	2:F:135:VAL:O	2.12	0.49
1:G:132:ASN:ND2	1:G:134:GLU:HG2	2.28	0.49
1:K:361:ARG:NH2	1:K:373:ASP:OD1	2.45	0.49
2:H:223:ALA:O	2:H:248:VAL:HG11	2.13	0.49
1:M:353:ARG:CA	1:M:356:MET:CE	2.80	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:F:127:VAL:HG13	2:F:157:LEU:HD23	1.93	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: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:B:252:ARG:HG2	2:B:256:HIS:CE1	2.48	0.49
2:D:185:THR:HG23	5:D:500:B13:H332	1.78	0.49
1:K:42:GLU:OE2	1:K:123:ARG:HD2	2.12	0.49
1:M:218:THR:HG23	1:M:270:GLY:N	2.27	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
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:I:317:TYR:CE1	1:I:324:THR:HG21	2.44	0.49
1:E:317:TYR:HA	1:E:325:THR:CG2	2.43	0.48
1:K:60:LYS:HE3	1:K:64:ARG:HE	1.78	0.48
1:M:265:PRO:HA	1:M:283:PRO:O	2.12	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
1:E:136:LEU:HD21	1:E:169:LYS:HE3	1.96	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: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
1:C:52:GLY:HA2	1:C:58:LEU:HD13	1.96	0.48
2:D:167:LEU:HB2	2:D:197:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.95	0.48
6:C:686:HOH:O	2:D:138:ILE:HG12	2.13	0.48
1:G:132:ASN:HD21	1:G:135:PHE:H	1.61	0.48
2:J:137:ASP:HB2	5:J:500:B13:H522	1.78	0.48
1:K:317:TYR:HA	1:K:325:THR:CG2	2.44	0.48
1:M:347:LYS:HE3	6:M:616:HOH:O	2.13	0.48
1:E:354:ASP:CB	2:F:2:LEU:HD12	2.44	0.48
1:G:22:SER:HB3	1:G:277:LYS:HE3	1.96	0.48
1:G:47:PRO:HB3	1:G:61:GLU:HG2	1.95	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
5:D:500:B13:H19	5:D:500:B13:H262	1.61	0.48
1:E:350:LYS:HG2	1:E:353:ARG:NH2	2.29	0.48
1:E:305:GLN:HA	1:E:356:MET:CE	2.44	0.48
1:E:289:LYS:NZ	1:G:336:ASP:OD1	2.47	0.48
1:I:265:PRO:HA	1:I:283:PRO:O	2.14	0.48
1:I:36:ALA:HA	6:I:568:HOH:O	2.14	0.48
1:E:31:ASP:OD1	1:K:27:LYS:NZ	2.32	0.47
2:F:130:VAL:HG12	2:F:134:ASP:HB3	1.96	0.47
1:G:324:THR:HG22	1:G:327:GLN:HG3	1.96	0.47
1:K:26:VAL:HG12	1:K:213:ILE:HD13	1.95	0.47
1:M:361:ARG:HH22	1:M:373:ASP:CG	2.16	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:A:324:THR:HG23	1:A:326:VAL:HG22	1.96	0.47
1:A:331:GLU:HG2	1:C:292:THR:HG21	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: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
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
2:L:189:TYR:HD2	2:L:192:LYS:HG3	1.79	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:A:224:ASN:ND2	1:A:269:CYS:HB2	2.30	0.47
2:H:127:VAL:HG22	2:H:155:VAL:CG1	2.45	0.47
1:I:42:GLU:OE2	1:I:123:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:317:TYR:CE1	1:K:324:THR:CG2	2.97	0.47
2:L:189:TYR:O	2:L:192:LYS:HB2	2.15	0.47
2:L:37:ASP:O	2:L:39:LEU:N	2.43	0.47
1:E:83:LEU:HD13	1:E:109:MET:CE	2.45	0.47
2:H:138:ILE:O	2:H:142:ILE:HG13	2.14	0.47
2:L:227:TYR:CZ	2:L:229:GLU:HB3	2.49	0.47
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:C:218:THR:HG23	1:C:270:GLY:CA	2.45	0.47
2:F:95:LEU:HB3	2:F:96:PRO:HD3	1.97	0.47
2:J:17:ASN:H	2:J:17:ASN:ND2	2.00	0.47
1:I:228:PHE:CE2	5:J:500:B13:H543	2.49	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:O:133:ARG:HD2	2:P:160:ASP:HB3	1.97	0.47
1:A:65:ILE:HG23	1:A:326:VAL:HG11	1.97	0.47
1:E:203:ILE:O	1:E:206:ILE:HB	2.15	0.47
1:G:175:ALA:HB1	1:G:180:ASP:HB3	1.96	0.47
1:M:125:THR:HG21	1:M:267:LYS:HE2	1.96	0.47
1:O:356:MET:HE3	1:O:356:MET:HB2	1.60	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
2:B:116:SER:C	2:B:118:ALA:H	2.18	0.47
1:K:313:GLU:O	1:K:314:SER:HB2	2.15	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
2:F:216:GLN:NE2	2:F:258:HIS:H	2.13	0.46
2:H:127:VAL:HG23	2:H:175:PRO:HG3	1.96	0.46
2:H:37:ASP:HB3	2:H:40:ILE:HB	1.98	0.46
1:I:324:THR:CG2	1:I:326:VAL:HG22	2.45	0.46
2:J:137:ASP:OD2	2:J:159:ARG:HD2	2.16	0.46
1:K:353:ARG:CA	1:K:356:MET:HE1	2.45	0.46
2:N:222:PHE:O	2:N:252:ARG:NH2	2.47	0.46
1:A:88:VAL:HG22	1:A:91:MET:SD	2.56	0.46
2:B:122:THR:HG21	2:B:153:ASN:HB2	1.98	0.46
2:B:219:VAL:HG21	2:B:227:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:LEU:HD12	2:F:161:VAL:HG11	1.97	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:I:353:ARG:HD3	1:I:372:TYR:CZ	2.50	0.46
2:P:94:PHE:H	2:P:97:ASN:ND2	2.07	0.46
1:C:132:ASN:HD21	1:C:135:PHE:H	1.60	0.46
1:G:181:ILE:HB	1:G:182:PRO:HD3	1.98	0.46
1:K:293:CYS:HB3	1:K:329:TRP:CE2	2.49	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:K:317:TYR:HA	1:K:325:THR:HG21	1.98	0.46
1:O:79:PRO:HD2	6:O:595:HOH:O	2.16	0.46
2:D:159:ARG:O	2:D:161:VAL:HG23	2.15	0.46
2:J:116:SER:OG	2:J:117:GLY:N	2.49	0.46
2:L:192:LYS:HG2	2:L:222:PHE:HE2	1.80	0.46
2:L:206:PRO:HG2	2:L:241:ILE:HD12	1.96	0.46
2:H:135:VAL:O	2:H:135:VAL:HG13	2.15	0.46
5:N:500:B13:H262	5:N:500:B13:H19	1.69	0.46
2:B:185:THR:HG23	5:B:500:B13:H332	1.80	0.46
2:D:162:PRO:O	2:D:164:GLU:N	2.49	0.46
2:F:185:THR:HA	2:F:188:MET:HG3	1.98	0.46
1:M:133:ARG:HH11	1:M:133:ARG:HG2	1.80	0.46
1:O:237:ASN:HA	2:P:95:LEU:HB2	1.97	0.46
1:A:290:THR:HG22	1:A:290:THR:O	2.16	0.46
2:B:16:TYR:CD1	1:C:116:TYR:HB3	2.50	0.46
1:C:353:ARG:HD3	1:C:372:TYR:CE1	2.51	0.46
2:F:184:MET:HB3	2:F:186:THR:HG22	1.98	0.46
2:F:184:MET:HG2	5:F:500:B13:C30	2.38	0.46
5:H:500:B13:H411	5:H:500:B13:H362	1.75	0.46
1:K:301:ASN:HD22	1:K:304:MET:HE2	1.81	0.46
2:P:17:ASN:N	2:P:17:ASN:HD22	2.10	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
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:J:206:PRO:HG2	2:J:241:ILE:HD12	1.98	0.45
2:L:118:ALA:O	2:L:119:THR:HB	2.16	0.45
1:O:325:THR:CG2	1:O:326:VAL:N	2.79	0.45
2:D:59:LEU:O	2:D:63:ILE:HG12	2.17	0.45
2:H:252:ARG:O	2:H:256:HIS:HB2	2.17	0.45
2:N:219:VAL:HG21	2:N:227:TYR:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:HD2	6:B:534:HOH:O	1.99	0.45
1:G:186:TYR:O	1:G:190:CYS:HB2	2.16	0.45
1:I:143:TYR:O	1:I:146:PHE:HB3	2.16	0.45
1:I:290:THR:O	1:I:290:THR:HG22	2.16	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
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
1:A:116:TYR:HB3	2:D:16:TYR:CD1	2.52	0.45
1:G:292:THR:HA	1:G:295:HIS:O	2.17	0.45
5:J:500:B13:H19	5:J:500:B13:H262	1.66	0.45
1:K:356:MET:HE2	1:K:356:MET:HB2	1.56	0.45
2:L:161:VAL:HA	2:L:162:PRO:HD3	1.78	0.45
2:N:163:ALA:O	2:N:166:VAL:HB	2.16	0.45
1:G:361:ARG:NH2	1:G:373:ASP:OD1	2.49	0.45
1:I:411:LYS:HD3	2:J:6:GLU:HG2	1.98	0.45
2:J:59:LEU:O	2:J:63:ILE:HG12	2.16	0.45
1:K:137:GLN:NE2	1:K:142:LYS:HE2	2.31	0.45
2:F:136:HIS:CB	2:F:183:LEU:HD13	2.46	0.45
2:H:47:ILE:HD12	2:H:55:VAL:HG22	1.98	0.45
2:N:192:LYS:HG2	2:N:222:PHE:HE2	1.81	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
2:D:252:ARG:O	2:D:256:HIS:HB2	2.17	0.45
1:E:55:LYS:HG3	1:E:97:TRP:CD2	2.52	0.45
1:G:105:GLN:NE2	1:G:124:HIS:HE1	2.15	0.45
1:G:42:GLU:OE2	1:G:123:ARG:HD2	2.17	0.45
1:G:224:ASN:ND2	1:G:269:CYS:HB2	2.32	0.45
5:L:500:B13:H252	5:L:500:B13:C61	2.47	0.45
1:M:324:THR:CG2	1:M:326:VAL:HG22	2.47	0.45
1:O:318:HIS:O	1:O:325:THR:HB	2.17	0.45
1:O:87:HIS:NE2	1:O:124:HIS:CD2	2.85	0.45
1:A:356:MET:HB2	1:A:356:MET:HE3	1.80	0.44
1:C:237:ASN:HA	2:D:95:LEU:HB2	1.99	0.44
2:F:222:PHE:O	2:F:252:ARG:NH2	2.50	0.44
1:I:126:ILE:N	1:I:126:ILE:HD12	2.32	0.44
2:D:248:VAL:HA	2:D:251:LEU:HD12	1.98	0.44
1:I:325:THR:CG2	1:I:326:VAL:N	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:LYS:NZ	1:I:301:ASN:HD21	2.15	0.44
2:J:63:ILE:HG23	2:J:72:LEU:HD12	1.99	0.44
1:M:224:ASN:O	1:M:228:PHE:HD2	2.01	0.44
2:D:227:TYR:CE2	2:D:229:GLU:HB3	2.52	0.44
1:G:325:THR:O	1:G:329:TRP:HD1	2.01	0.44
2:H:95:LEU:HD22	2:H:99:MET:HG2	2.00	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
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:L:130:VAL:HG23	2:L:140:LYS:HD3	1.99	0.44
2:L:234:ALA:O	2:L:237:ILE:HG22	2.18	0.44
1:M:133:ARG:CG	1:M:133:ARG:NH1	2.80	0.44
2:P:204:LYS:HZ1	2:P:248:VAL:H	1.66	0.44
1:A:317:TYR:HE1	1:A:324:THR:HG21	1.82	0.44
2:B:59:LEU:HD23	2:B:72:LEU:HD13	2.00	0.44
1:K:228:PHE:HE1	1:K:295:HIS:HB2	1.82	0.44
2:N:162:PRO:O	2:N:163:ALA:HB3	2.18	0.44
2:P:82:GLY:HA2	2:P:85:ILE:HD12	2.00	0.44
1:A:132:ASN:HD22	1:A:134:GLU:H	1.66	0.44
1:C:218:THR:HG23	1:C:270:GLY:N	2.33	0.44
1:C:441:ASP:O	1:C:445:THR:HG23	2.18	0.44
1:M:132:ASN:ND2	1:M:135:PHE:H	2.14	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
5:P:500:B13:H363	5:P:500:B13:H401	1.83	0.44
1:C:356:MET:HE3	1:C:356:MET:HB2	1.82	0.44
1:C:237:ASN:O	2:D:96:PRO:HD3	2.18	0.44
2:F:188:MET:HB3	2:F:218:PHE:CZ	2.52	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: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
2:J:130:VAL:HG23	2:J:140:LYS:HD3	2.00	0.44
1:K:105:GLN:O	1:K:109:MET:HG3	2.18	0.44
2:B:51:GLU:O	2:B:55:VAL:HG23	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:L:219:VAL:HG21	2:L:227:TYR:CB	2.38	0.43
1:M:356:MET:HE2	1:M:356:MET:HB2	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:138:ILE:O	2:N:142:ILE:HG13	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
2:B:131:ALA:HB1	2:B:190:ALA:HB3	1.99	0.43
1:C:373:ASP:N	1:C:373:ASP:OD1	2.50	0.43
1:C:47:PRO:HB3	1:C:61:GLU:HG2	2.00	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
2:L:94:PHE:H	2:L:97:ASN:HD22	1.66	0.43
2:N:95:LEU:HB3	2:N:96:PRO:HD3	1.99	0.43
2:B:17:ASN:ND2	2:B:17:ASN:N	2.57	0.43
1:E:145:VAL:HA	1:E:148:GLU:OE1	2.18	0.43
2:H:68:ASP:HB3	2:H:71:ASP:HB2	2.00	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
5:N:500:B13:H252	5:N:500:B13:C61	2.48	0.43
1:A:43:ILE:HG22	1:A:81:ILE:HD11	2.01	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:D:127:VAL:HG22	2:D:155:VAL:HG13	2.00	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
2:B:37:ASP:HB3	2:B:40:ILE:HB	2.01	0.43
2:D:95:LEU:HB3	2:D:96:PRO:HD3	2.01	0.43
1:G:132:ASN:ND2	1:G:135:PHE:H	2.15	0.43
2:N:87:LEU:HD22	2:N:92:VAL:HG21	2.01	0.43
2:F:87:LEU:HB3	2:F:92:VAL:HG22	1.99	0.43
2:H:216:GLN:HE21	2:H:258:HIS:HB2	1.83	0.43
2:J:127:VAL:HG22	2:J:155:VAL:CG1	2.49	0.43
1:K:218:THR:HG23	1:K:270:GLY:N	2.33	0.43
1:O:106:LYS:NZ	1:O:157:GLY:O	2.51	0.43
2:J:82:GLY:HA2	2:J:85:ILE:HD12	2.01	0.43
2:B:229:GLU:O	5:B:500:B13:H2R	2.19	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
1:A:361:ARG:NH2	1:A:373:ASP:OD1	2.51	0.43
1:E:132:ASN:HD21	1:E:135:PHE:H	1.65	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
2:L:206:PRO:HG2	2:L:241:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:82:GLY:HA2	2:N:85:ILE:HD12	2.00	0.43
1:O:105:GLN:NE2	1:O:124:HIS:HE1	2.17	0.43
1:O:26:VAL:CG1	1:O:213:ILE:HD13	2.49	0.43
1:A:287:GLU:OE1	1:A:313:GLU:OE2	2.36	0.42
5:D:500:B13:H411	5:D:500:B13:H362	1.73	0.42
1:G:402:ASN:O	1:G:406:GLU:HG3	2.18	0.42
2:J:17:ASN:N	2:J:17:ASN:ND2	2.62	0.42
1:O:364:ASP:CG	1:O:365:PRO:HD2	2.38	0.42
2:B:224:LEU:HA	2:B:248:VAL:HG21	2.00	0.42
1:E:317:TYR:HA	1:E:325:THR:HG22	2.01	0.42
2:H:242:ILE:HG22	2:H:242:ILE:O	2.19	0.42
1:I:285:THR:OG1	1:I:309:CYS:HB2	2.19	0.42
2:J:161:VAL:HA	2:J:162:PRO:HD3	1.95	0.42
2:J:233:ASP:O	2:J:237:ILE:HG22	2.19	0.42
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.93	0.42
2:D:95:LEU:HD11	2:D:142:ILE:HG12	2.01	0.42
1:E:417:PHE:HZ	2:F:97:ASN:HD21	1.67	0.42
1:G:305:GLN:HA	1:G:356:MET:HE1	2.02	0.42
1:G:43:ILE:HG22	1:G:81:ILE:HD11	2.01	0.42
2:H:224:LEU:HA	2:H:248:VAL:HG21	2.01	0.42
1:I:81:ILE:HD13	1:I:82:ILE:N	2.34	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:K:324:THR:CG2	1:K:326:VAL:HG22	2.49	0.42
1:O:47:PRO:HB3	1:O:61:GLU:HG2	2.01	0.42
1:A:441:ASP:O	1:A:445:THR:HG23	2.19	0.42
2:B:130:VAL:HG12	2:B:134:ASP:HB3	2.01	0.42
1:C:224:ASN:HB3	1:C:228:PHE:HE2	1.85	0.42
2:D:161:VAL:HA	2:D:162:PRO:HD3	1.70	0.42
1:G:119:LYS:HE3	6:G:561:HOH:O	2.18	0.42
2:H:256:HIS:HB3	2:H:257:LYS:H	1.59	0.42
2:J:188:MET:O	2:J:191:PHE:HB2	2.18	0.42
2:J:67:LYS:HB3	2:J:68:ASP:H	1.65	0.42
1:K:436:MET:O	1:K:440:MET:HG2	2.19	0.42
5:N:500:B13:H401	5:N:500:B13:H8	1.84	0.42
1:O:426:LYS:O	1:O:430:GLU:HG3	2.19	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:G:76:VAL:O	1:G:76:VAL:HG12	2.19	0.42
1:G:88:VAL:HG22	1:G:91:MET:SD	2.59	0.42
1:I:18:THR:HG23	1:I:21:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:THR:HG23	1:K:270:GLY:CA	2.50	0.42
1:M:128:ASP:HA	1:M:146:PHE:HE1	1.84	0.42
2:B:37:ASP:O	2:B:39:LEU:N	2.49	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
2:F:136:HIS:HB2	2:F:183:LEU:HD13	2.02	0.42
1:K:106:LYS:NZ	1:K:157:GLY:O	2.53	0.42
2:L:192:LYS:HG2	2:L:222:PHE:CE2	2.54	0.42
5:L:500:B13:H351	5:L:500:B13:H361	2.01	0.42
1:M:353:ARG:HD3	1:M:372:TYR:CZ	2.55	0.42
2:N:132:GLU:HB3	2:N:161:VAL:O	2.20	0.42
1:O:22:SER:HB3	1:O:277:LYS:HE3	2.02	0.42
1:A:132:ASN:C	1:A:132:ASN:HD22	2.23	0.42
1:A:22:SER:HB3	1:A:277:LYS:HE3	2.02	0.42
1:I:132:ASN:HD21	1:I:135:PHE:H	1.66	0.42
1:K:101:VAL:O	1:K:105:GLN:HG3	2.20	0.42
1:M:249:ILE:O	1:M:252:PRO:HD2	2.19	0.42
2:D:67:LYS:HB3	2:D:68:ASP:H	1.56	0.42
5:F:500:B13:H362	5:F:500:B13:H411	1.67	0.42
2:L:17:ASN:HD22	2:L:17:ASN:N	2.15	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:126:ILE:N	1:O:126:ILE:HD12	2.34	0.42
1:O:285:THR:OG1	1:O:309:CYS:HB2	2.20	0.42
2:D:110:GLU:HA	2:D:113:LYS:HB2	2.02	0.42
2:D:134:ASP:OD2	2:D:187:THR:HG21	2.20	0.42
1:E:187:SER:HA	1:E:191:LEU:HD12	2.01	0.42
1:E:203:ILE:HA	1:E:206:ILE:HD12	2.02	0.42
2:F:41:TYR:HB3	2:F:42:PRO:HD3	2.02	0.42
1:G:132:ASN:OD1	1:G:137:GLN:NE2	2.51	0.42
1:G:218:THR:HG23	1:G:270:GLY:N	2.35	0.42
2:L:135:VAL:HG13	2:L:135:VAL:O	2.19	0.42
2:N:130:VAL:HG12	2:N:134:ASP:HB3	2.02	0.42
2:N:43:ILE:HG21	2:N:76:ALA:HB1	2.01	0.42
1:E:132:ASN:OD1	1:E:137:GLN:NE2	2.53	0.41
2:D:130:VAL:HG23	2:D:140:LYS:HD3	2.02	0.41
2:N:161:VAL:HA	2:N:162:PRO:HD3	1.78	0.41
1:O:452:LYS:HA	1:O:452:LYS:HD3	1.95	0.41
1:A:87:HIS:NE2	1:A:124:HIS:CD2	2.89	0.41
2:F:216:GLN:HE21	2:F:258:HIS:HD2	1.68	0.41
2:J:135:VAL:HB	5:J:500:B13:H421	2.02	0.41
2:J:159:ARG:O	2:J:161:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:234:ALA:HB3	2:J:235:PRO:HD3	2.01	0.41
5:J:500:B13:N40	5:J:500:B13:H363	2.35	0.41
5:B:500:B13:H411	5:B:500:B13:H362	1.80	0.41
2:D:195:ASN:HD22	2:D:224:LEU:HB2	1.86	0.41
2:D:70:ILE:HD11	2:D:120:PRO:HG3	2.01	0.41
1:E:266:GLY:HA3	1:E:284:MET:SD	2.60	0.41
1:G:356:MET:HB2	1:G:356:MET:HE3	1.83	0.41
1:K:106:LYS:HD3	1:K:106:LYS:HA	1.76	0.41
2:L:226:VAL:HG11	2:L:237:ILE:HD11	2.02	0.41
2:L:74:ASP:HA	2:L:78:MET:HB2	2.02	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:B:216:GLN:NE2	2:B:258:HIS:H	2.15	0.41
2:B:95:LEU:HB3	2:B:96:PRO:HD3	2.03	0.41
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:E:287:GLU:OE1	1:E:313:GLU:OE2	2.38	0.41
1:I:317:TYR:HE1	1:I:324:THR:CG2	2.30	0.41
2:L:185:THR:HG23	5:L:500:B13:H332	1.86	0.41
1:M:452:LYS:HD3	1:M:452:LYS:HA	1.78	0.41
5:P:500:B13:H411	5:P:500:B13:H362	1.74	0.41
2:B:195:ASN:HD22	2:B:224:LEU:HB2	1.84	0.41
1:E:146:PHE:CZ	1:E:150:PHE:HE2	2.39	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
2:L:256:HIS:HB3	2:L:257:LYS:H	1.57	0.41
2:N:159:ARG:O	2:N:161:VAL:N	2.52	0.41
1:C:109:MET:HE1	1:C:122:LEU:HD13	2.01	0.41
2:D:60:GLN:O	2:D:64:GLU:HG3	2.21	0.41
2:F:214:VAL:HG12	2:F:227:TYR:CE1	2.55	0.41
5:H:500:B13:H472	5:H:500:B13:H481	1.88	0.41
2:J:252:ARG:O	2:J:256:HIS:HB2	2.21	0.41
2:N:136:HIS:CB	2:N:183:LEU:HD13	2.51	0.41
1:O:126:ILE:N	1:O:126:ILE:CD1	2.84	0.41
1:A:131:GLU:OE2	2:B:159:ARG:NH2	2.52	0.41
1:A:218:THR:HG23	1:A:270:GLY:CA	2.50	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
1:I:301:ASN:HD22	1:I:304:MET:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:135:VAL:HB	5:P:500:B13:C43	2.50	0.41
1:A:123:ARG:NH2	1:A:265:PRO:O	2.53	0.41
1:I:47:PRO:HB3	1:I:61:GLU:HG2	2.02	0.41
2:J:159:ARG:HB3	2:J:160:ASP:H	1.63	0.41
2:L:135:VAL:O	2:L:135:VAL:CG1	2.68	0.41
1:M:87:HIS:NE2	1:M:124:HIS:CD2	2.87	0.41
1:O:132:ASN:ND2	1:O:134:GLU:HG2	2.36	0.41
2:P:143:VAL:HG21	5:P:500:B13:C9B	2.50	0.41
2:P:169:ALA:O	2:P:173:GLU:HG2	2.21	0.41
2:P:256:HIS:HB3	2:P:257:LYS:H	1.76	0.41
2:P:95:LEU:HB3	2:P:96:PRO:HD3	2.02	0.41
1:E:116:TYR:HB3	2:H:16:TYR:CD1	2.55	0.41
2:H:193:GLU:O	2:H:197:MET:HB3	2.20	0.41
1:I:317:TYR:CE1	1:I:324:THR:CG2	3.04	0.41
1:K:247:ARG:CZ	1:K:271:TYR:HB2	2.50	0.41
1:O:101:VAL:O	1:O:105:GLN:HG3	2.21	0.41
2:P:37:ASP:O	2:P:37:ASP:OD2	2.39	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:B:247:ASP:HB3	2:B:250:GLU:HB2	2.01	0.41
1:C:305:GLN:HA	1:C:356:MET:HE1	2.03	0.41
1:C:50:GLU:H	1:C:50:GLU:CD	2.24	0.41
2:D:119:THR:HA	2:D:120:PRO:HD3	1.90	0.41
2:F:182:ALA:O	2:F:211:GLY:HA3	2.21	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
1:E:94:ASN:HB2	1:E:97:TRP:CD1	2.56	0.40
2:J:132:GLU:HB3	2:J:161:VAL:O	2.21	0.40
1:M:325:THR:CG2	1:M:326:VAL:N	2.83	0.40
2:N:63:ILE:H	2:N:63:ILE:HG12	1.74	0.40
1:O:88:VAL:HG22	1:O:91:MET:SD	2.62	0.40
2:B:218:PHE:O	2:B:221:GLN:HG2	2.21	0.40
1:C:224:ASN:HB3	1:C:228:PHE:CE2	2.56	0.40
1:E:76:VAL:O	1:E:76:VAL:HG12	2.22	0.40
2:F:206:PRO:HG2	2:F:241:ILE:CD1	2.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:THR:OG1	1:M:309:CYS:HB2	2.22	0.40
1:O:290:THR:O	1:O:290:THR:HG22	2.22	0.40
2:D:143:VAL:HG13	2:D:234:ALA:CB	2.52	0.40
1:E:94:ASN:O	1:E:95:PRO:C	2.59	0.40
1:G:265:PRO:HA	1:G:283:PRO:O	2.21	0.40
2:H:226:VAL:HG11	2:H:237:ILE:HG12	2.04	0.40
1:I:228:PHE:CE2	5:J:500:B13:C54	3.05	0.40
2:J:134:ASP:HB2	2:J:187:THR:HG21	2.03	0.40
2:J:229:GLU:HG3	2:J:230:GLU:H	1.86	0.40
1:O:179:ASN:HA	6:O:526:HOH:O	2.20	0.40
1:C:252:PRO:HG3	1:C:393:ALA:HA	2.04	0.40
1:C:285:THR:OG1	1:C:309:CYS:HB2	2.20	0.40
2:D:138:ILE:HG13	5:D:500:B13:C50	2.52	0.40
1:E:123:ARG:NH2	1:E:265:PRO:O	2.54	0.40
1:E:348:ASN:O	1:E:351:VAL:HG12	2.20	0.40
1:I:362:TYR:HB2	2:J:9:LEU:HD21	2.03	0.40
1:K:353:ARG:CA	1:K:356:MET:CE	2.83	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

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%)	25	43
1	G	457/461 (99%)	434 (95%)	22 (5%)	1 (0%)	51	73
1	I	457/461 (99%)	439 (96%)	17 (4%)	1 (0%)	51	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	19
2	D	256/258 (99%)	224 (88%)	28 (11%)	4 (2%)	11	19
2	F	256/258 (99%)	227 (89%)	26 (10%)	3 (1%)	15	27
2	H	256/258 (99%)	235 (92%)	18 (7%)	3 (1%)	15	27
2	J	256/258 (99%)	237 (93%)	14 (6%)	5 (2%)	9	14
2	L	256/258 (99%)	235 (92%)	15 (6%)	6 (2%)	7	11
2	N	256/258 (99%)	229 (90%)	23 (9%)	4 (2%)	11	19
2	P	256/258 (99%)	240 (94%)	13 (5%)	3 (1%)	15	27
All	All	5704/5752 (99%)	5371 (94%)	296 (5%)	37 (1%)	28	48

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
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

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Mol	Chain	Res	Type
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%)	15	28
1	C	373/374 (100%)	344 (92%)	29 (8%)	15	28
1	E	373/374 (100%)	339 (91%)	34 (9%)	11	21
1	G	373/374 (100%)	346 (93%)	27 (7%)	17	31
1	I	373/374 (100%)	345 (92%)	28 (8%)	16	29
1	K	373/374 (100%)	348 (93%)	25 (7%)	19	35
1	M	373/374 (100%)	344 (92%)	29 (8%)	15	28
1	O	373/374 (100%)	343 (92%)	30 (8%)	14	27
2	B	206/206 (100%)	183 (89%)	23 (11%)	7	13
2	D	206/206 (100%)	192 (93%)	14 (7%)	18	34
2	F	206/206 (100%)	189 (92%)	17 (8%)	13	25
2	H	206/206 (100%)	190 (92%)	16 (8%)	15	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	206/206 (100%)	190 (92%)	16 (8%)	15	28
2	L	206/206 (100%)	190 (92%)	16 (8%)	15	28
2	N	206/206 (100%)	189 (92%)	17 (8%)	13	25
2	P	206/206 (100%)	184 (89%)	22 (11%)	8	15
All	All	4632/4640 (100%)	4260 (92%)	372 (8%)	14	27

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	80,100,100	2.04	18 (22%)	98,164,164	1.88	21 (21%)
5	B13	D	500	2	80,100,100	2.10	21 (26%)	98,164,164	1.95	26 (26%)
5	B13	F	500	2	80,100,100	2.05	17 (21%)	98,164,164	1.92	26 (26%)
5	B13	H	500	2	80,100,100	2.07	17 (21%)	98,164,164	1.91	21 (21%)
5	B13	J	500	2,6	80,100,100	2.03	15 (18%)	98,164,164	1.89	20 (20%)
5	B13	L	500	2,6	80,100,100	2.07	17 (21%)	98,164,164	1.88	26 (26%)
5	B13	N	500	2	80,100,100	2.07	18 (22%)	98,164,164	1.91	21 (21%)
5	B13	P	500	2	80,100,100	2.00	17 (21%)	98,164,164	2.04	27 (27%)

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	-	0/52/223/223	0/3/11/11
5	B13	D	500	2	-	0/52/223/223	0/3/11/11
5	B13	F	500	2	-	0/52/223/223	0/3/11/11
5	B13	H	500	2	-	0/52/223/223	0/3/11/11
5	B13	J	500	2,6	-	0/52/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	B13	L	500	2,6	-	0/52/223/223	0/3/11/11
5	B13	N	500	2	-	0/52/223/223	0/3/11/11
5	B13	P	500	2	-	0/52/223/223	0/3/11/11

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	B13	C5R-C4R	-8.77	1.21	1.51
5	D	500	B13	C5R-C4R	-8.74	1.22	1.51
5	P	500	B13	C5R-C4R	-8.63	1.22	1.51
5	J	500	B13	C5R-C4R	-8.62	1.22	1.51
5	L	500	B13	C5R-C4R	-8.62	1.22	1.51
5	H	500	B13	C5R-C4R	-8.54	1.22	1.51
5	F	500	B13	C5R-C4R	-8.53	1.22	1.51
5	N	500	B13	C5R-C4R	-8.49	1.22	1.51
5	J	500	B13	C11-C10	-5.34	1.36	1.49
5	B	500	B13	C11-C10	-5.34	1.36	1.49
5	H	500	B13	C11-C10	-5.32	1.37	1.49
5	F	500	B13	C11-C10	-5.23	1.37	1.49
5	L	500	B13	C11-C10	-5.05	1.37	1.49
5	D	500	B13	C11-C10	-5.02	1.37	1.49
5	P	500	B13	C11-C10	-5.02	1.37	1.49
5	N	500	B13	C11-C10	-4.96	1.37	1.49
5	D	500	B13	C2R-C3R	-2.66	1.47	1.53
5	L	500	B13	C2R-C3R	-2.55	1.47	1.53
5	D	500	B13	C60-C61	-2.51	1.45	1.51
5	J	500	B13	C2R-C3R	-2.32	1.47	1.53
5	P	500	B13	C8B-N1B	-2.27	1.35	1.38
5	H	500	B13	C2R-C3R	-2.24	1.48	1.53
5	N	500	B13	C2R-C3R	-2.24	1.48	1.53
5	D	500	B13	C8B-N1B	-2.10	1.36	1.38
5	D	500	B13	O7R-C2R	-2.08	1.38	1.43
5	B	500	B13	C2R-C3R	-2.07	1.48	1.53
5	B	500	B13	C8B-N1B	-2.04	1.36	1.38
5	F	500	B13	C2R-C3R	-2.03	1.48	1.53
5	J	500	B13	C60-C61	-2.03	1.46	1.51
5	N	500	B13	C60-C61	-2.01	1.46	1.51
5	N	500	B13	P-O4	-2.00	1.45	1.55
5	H	500	B13	C60-C61	-2.00	1.46	1.51
5	P	500	B13	C7-C6	2.02	1.59	1.54
5	B	500	B13	C14-N23	2.02	1.39	1.32
5	N	500	B13	C2-C1	2.06	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	500	B13	C13-C14	2.08	1.56	1.52
5	P	500	B13	C2-C1	2.09	1.60	1.53
5	P	500	B13	C14-N23	2.13	1.39	1.32
5	H	500	B13	C14-N23	2.13	1.39	1.32
5	B	500	B13	C30-C3	2.13	1.57	1.53
5	B	500	B13	C2-C1	2.15	1.60	1.53
5	L	500	B13	C2-C1	2.16	1.60	1.53
5	D	500	B13	C53-C15	2.17	1.54	1.50
5	B	500	B13	C4B-C5B	2.18	1.41	1.37
5	L	500	B13	C13-C14	2.21	1.56	1.52
5	D	500	B13	O6R-C1R	2.21	1.44	1.41
5	D	500	B13	C2-C1	2.22	1.60	1.53
5	F	500	B13	C4B-C5B	2.23	1.41	1.37
5	P	500	B13	C48-C13	2.23	1.59	1.54
5	F	500	B13	C13-C14	2.23	1.56	1.52
5	F	500	B13	C14-N23	2.24	1.40	1.32
5	N	500	B13	C14-N23	2.24	1.40	1.32
5	L	500	B13	C7-C6	2.29	1.59	1.54
5	J	500	B13	C14-N23	2.31	1.40	1.32
5	H	500	B13	C7-C6	2.32	1.59	1.54
5	D	500	B13	C7-C6	2.33	1.59	1.54
5	B	500	B13	O6R-C1R	2.34	1.44	1.41
5	B	500	B13	C36-C7	2.34	1.58	1.54
5	D	500	B13	C4B-C5B	2.35	1.41	1.37
5	H	500	B13	C25-C2	2.36	1.59	1.54
5	L	500	B13	C25-C2	2.41	1.59	1.54
5	L	500	B13	C14-N23	2.46	1.40	1.32
5	N	500	B13	C25-C2	2.55	1.59	1.54
5	D	500	B13	C14-N23	2.55	1.41	1.32
5	P	500	B13	C36-C7	2.57	1.59	1.54
5	L	500	B13	C36-C7	2.61	1.59	1.54
5	P	500	B13	O6R-C1R	2.62	1.44	1.41
5	D	500	B13	C36-C7	2.62	1.59	1.54
5	F	500	B13	C25-C2	2.68	1.59	1.54
5	B	500	B13	C25-C2	2.68	1.59	1.54
5	F	500	B13	C55-C17	2.71	1.59	1.55
5	D	500	B13	C55-C17	2.73	1.59	1.55
5	N	500	B13	C7-C6	2.74	1.60	1.54
5	P	500	B13	C25-C2	2.75	1.59	1.54
5	J	500	B13	C55-C17	2.78	1.59	1.55
5	F	500	B13	C7-C6	2.78	1.60	1.54
5	J	500	B13	O6R-C1R	2.78	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	500	B13	C55-C17	2.85	1.59	1.55
5	N	500	B13	C55-C17	2.89	1.59	1.55
5	N	500	B13	O6R-C1R	2.89	1.45	1.41
5	J	500	B13	C36-C7	2.92	1.59	1.54
5	N	500	B13	C36-C7	2.93	1.59	1.54
5	P	500	B13	C55-C17	2.96	1.59	1.55
5	F	500	B13	C36-C7	2.97	1.59	1.54
5	L	500	B13	C55-C17	2.99	1.59	1.55
5	J	500	B13	C25-C2	3.05	1.60	1.54
5	D	500	B13	C20-C1	3.10	1.60	1.52
5	F	500	B13	C35-C5	3.11	1.55	1.50
5	P	500	B13	C35-C5	3.12	1.55	1.50
5	H	500	B13	O6R-C1R	3.17	1.45	1.41
5	L	500	B13	O6R-C1R	3.19	1.45	1.41
5	H	500	B13	C36-C7	3.21	1.60	1.54
5	H	500	B13	C35-C5	3.21	1.55	1.50
5	D	500	B13	C25-C2	3.22	1.60	1.54
5	B	500	B13	C55-C17	3.22	1.60	1.55
5	N	500	B13	C35-C5	3.30	1.56	1.50
5	F	500	B13	O6R-C1R	3.32	1.45	1.41
5	P	500	B13	C6B-C5B	3.34	1.45	1.38
5	B	500	B13	C35-C5	3.41	1.56	1.50
5	B	500	B13	O8R-C5R	3.42	1.56	1.42
5	P	500	B13	O8R-C5R	3.43	1.56	1.42
5	L	500	B13	O8R-C5R	3.43	1.56	1.42
5	D	500	B13	O8R-C5R	3.44	1.56	1.42
5	L	500	B13	C20-C1	3.44	1.61	1.52
5	N	500	B13	O8R-C5R	3.49	1.57	1.42
5	F	500	B13	O8R-C5R	3.49	1.57	1.42
5	H	500	B13	C20-C1	3.50	1.61	1.52
5	N	500	B13	C20-C1	3.54	1.61	1.52
5	H	500	B13	O8R-C5R	3.54	1.57	1.42
5	J	500	B13	C35-C5	3.55	1.56	1.50
5	P	500	B13	C20-C1	3.57	1.61	1.52
5	J	500	B13	O8R-C5R	3.57	1.57	1.42
5	J	500	B13	C20-C1	3.59	1.61	1.52
5	B	500	B13	C6B-C5B	3.60	1.46	1.38
5	F	500	B13	C20-C1	3.64	1.61	1.52
5	L	500	B13	C35-C5	3.64	1.56	1.50
5	J	500	B13	C6B-C5B	3.67	1.46	1.38
5	B	500	B13	C20-C1	3.72	1.61	1.52
5	D	500	B13	C35-C5	3.73	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	500	B13	C6B-C5B	3.81	1.46	1.38
5	L	500	B13	C6B-C5B	3.83	1.46	1.38
5	D	500	B13	C6B-C5B	3.84	1.46	1.38
5	N	500	B13	C6B-C5B	3.86	1.46	1.38
5	H	500	B13	C6B-C5B	4.13	1.47	1.38
5	B	500	B13	C6-N22	5.35	1.41	1.35
5	P	500	B13	O5B-C5B	5.39	1.49	1.37
5	J	500	B13	O5B-C5B	5.47	1.49	1.37
5	D	500	B13	O5B-C5B	5.75	1.50	1.37
5	P	500	B13	C6-N22	5.87	1.42	1.35
5	F	500	B13	O5B-C5B	5.93	1.50	1.37
5	N	500	B13	O5B-C5B	5.97	1.51	1.37
5	H	500	B13	O5B-C5B	6.04	1.51	1.37
5	L	500	B13	O5B-C5B	6.05	1.51	1.37
5	J	500	B13	C6-N22	6.07	1.42	1.35
5	F	500	B13	C6-N22	6.18	1.43	1.35
5	B	500	B13	O5B-C5B	6.19	1.51	1.37
5	L	500	B13	C6-N22	6.22	1.43	1.35
5	H	500	B13	C6-N22	6.40	1.43	1.35
5	N	500	B13	C6-N22	6.59	1.43	1.35
5	D	500	B13	C6-N22	6.65	1.43	1.35

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	C4R-O6R-C1R	-6.41	102.95	109.77
5	J	500	B13	C4R-O6R-C1R	-5.70	103.70	109.77
5	L	500	B13	C4R-O6R-C1R	-5.67	103.73	109.77
5	P	500	B13	C4R-O6R-C1R	-5.65	103.75	109.77
5	D	500	B13	C4R-O6R-C1R	-5.57	103.84	109.77
5	N	500	B13	C4R-O6R-C1R	-4.74	104.73	109.77
5	H	500	B13	O34-C32-C31	-4.54	107.80	121.06
5	F	500	B13	C4R-O6R-C1R	-4.40	105.08	109.77
5	F	500	B13	O34-C32-C31	-4.36	108.33	121.06
5	N	500	B13	C53-C15-C14	-4.33	117.02	124.08
5	D	500	B13	O34-C32-C31	-4.18	108.87	121.06
5	P	500	B13	C5B-C4B-C9B	-4.16	116.41	119.17
5	B	500	B13	O34-C32-C31	-4.15	108.95	121.06
5	L	500	B13	O34-C32-C31	-4.14	108.98	121.06
5	P	500	B13	O34-C32-C31	-4.09	109.11	121.06
5	H	500	B13	C53-C15-C14	-4.09	117.40	124.08
5	N	500	B13	O34-C32-C31	-4.00	109.38	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	500	B13	O34-C32-C31	-3.89	109.69	121.06
5	H	500	B13	C4R-O6R-C1R	-3.80	105.73	109.77
5	P	500	B13	C53-C15-C14	-3.76	117.95	124.08
5	F	500	B13	C53-C15-C14	-3.63	118.16	124.08
5	D	500	B13	C41-C42-C43	-3.55	100.96	112.65
5	H	500	B13	C54-C17-C55	-3.51	102.62	109.38
5	J	500	B13	C53-C15-C14	-3.45	118.44	124.08
5	P	500	B13	C7B-C8B-N1B	-3.43	128.24	131.92
5	J	500	B13	C5B-C4B-C9B	-3.43	116.89	119.17
5	L	500	B13	C53-C15-C14	-3.28	118.72	124.08
5	D	500	B13	C41-C8-C7	-3.28	105.22	114.21
5	B	500	B13	C7B-C8B-N1B	-3.00	128.71	131.92
5	N	500	B13	C36-C7-C37	-3.00	105.92	110.77
5	D	500	B13	C36-C7-C37	-2.98	105.94	110.77
5	J	500	B13	C41-C42-C43	-2.96	102.91	112.65
5	L	500	B13	C36-C7-C37	-2.94	106.01	110.77
5	F	500	B13	C7B-C8B-N1B	-2.93	128.78	131.92
5	D	500	B13	O2-C3R-C4R	-2.88	99.24	110.04
5	N	500	B13	O2-C3R-C4R	-2.87	99.25	110.04
5	H	500	B13	C5B-C4B-C9B	-2.82	117.29	119.17
5	P	500	B13	C6B-C7B-C8B	-2.80	115.02	119.62
5	F	500	B13	C41-C8-C7	-2.74	106.70	114.21
5	P	500	B13	C54-C17-C55	-2.73	104.13	109.38
5	L	500	B13	C31-C30-C3	-2.71	107.48	114.49
5	F	500	B13	C36-C7-C37	-2.71	106.39	110.77
5	N	500	B13	C54-C17-C55	-2.70	104.17	109.38
5	D	500	B13	C26-C2-C1	-2.66	105.98	110.04
5	D	500	B13	C2P-C1P-N59	-2.64	109.16	112.96
5	F	500	B13	C5B-C4B-C9B	-2.61	117.43	119.17
5	P	500	B13	C3P-C2P-C1P	-2.53	106.34	111.40
5	B	500	B13	C36-C7-C37	-2.52	106.69	110.77
5	D	500	B13	C4B-C9B-C8B	-2.51	118.53	121.10
5	J	500	B13	C3P-C2P-C1P	-2.51	106.37	111.40
5	N	500	B13	C5B-C4B-C9B	-2.47	117.53	119.17
5	L	500	B13	O2-C3R-C4R	-2.46	100.81	110.04
5	B	500	B13	C5B-C4B-C9B	-2.44	117.55	119.17
5	L	500	B13	C5B-C4B-C9B	-2.43	117.55	119.17
5	H	500	B13	O2-C3R-C4R	-2.40	101.01	110.04
5	F	500	B13	C41-C42-C43	-2.39	104.80	112.65
5	L	500	B13	C26-C2-C1	-2.36	106.44	110.04
5	B	500	B13	C6B-C7B-C8B	-2.36	115.74	119.62
5	F	500	B13	C3P-C2P-C1P	-2.35	106.69	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	B13	O2-C3R-C4R	-2.32	101.33	110.04
5	J	500	B13	C7B-C8B-N1B	-2.30	129.46	131.92
5	H	500	B13	C37-C7-C8	-2.29	102.11	108.31
5	L	500	B13	C6B-C7B-C8B	-2.29	115.86	119.62
5	D	500	B13	C7B-C8B-N1B	-2.28	129.48	131.92
5	L	500	B13	C41-C42-C43	-2.27	105.18	112.65
5	P	500	B13	C36-C7-C37	-2.24	107.14	110.77
5	N	500	B13	C46-C12-C47	-2.22	102.67	108.54
5	L	500	B13	C7B-C8B-N1B	-2.22	129.55	131.92
5	F	500	B13	C31-C30-C3	-2.18	108.87	114.49
5	P	500	B13	C1P-N59-C57	-2.17	117.73	122.73
5	D	500	B13	C3P-C2P-C1P	-2.16	107.07	111.40
5	J	500	B13	C6B-C7B-C8B	-2.16	116.08	119.62
5	F	500	B13	C6B-C7B-C8B	-2.12	116.13	119.62
5	H	500	B13	C6B-C7B-C8B	-2.11	116.16	119.62
5	P	500	B13	C41-C8-C7	-2.10	108.44	114.21
5	D	500	B13	C5B-C4B-C9B	-2.08	117.78	119.17
5	L	500	B13	C46-C12-C13	-2.05	104.69	111.75
5	P	500	B13	C41-C42-C43	-2.05	105.92	112.65
5	B	500	B13	O2-C3R-C4R	-2.04	102.39	110.04
5	B	500	B13	C41-C8-C7	-2.03	108.64	114.21
5	D	500	B13	C1P-N59-C57	-2.01	118.09	122.73
5	L	500	B13	C11-N23-C14	-2.00	108.43	111.81
5	F	500	B13	O34-C32-N33	2.01	128.00	122.47
5	D	500	B13	C7B-C8B-C9B	2.03	124.64	121.33
5	N	500	B13	C47-C12-C11	2.04	117.21	111.53
5	P	500	B13	C47-C12-C13	2.05	118.83	111.75
5	B	500	B13	C25-C2-C3	2.08	115.85	111.81
5	J	500	B13	C42-C41-C8	2.10	120.98	114.78
5	J	500	B13	C31-C32-N33	2.12	123.36	116.55
5	P	500	B13	C7B-C8B-C9B	2.12	124.79	121.33
5	P	500	B13	C25-C2-C3	2.13	115.95	111.81
5	B	500	B13	C31-C32-N33	2.18	123.55	116.55
5	B	500	B13	C42-C41-C8	2.19	121.24	114.78
5	B	500	B13	C7-C37-C38	2.19	121.02	114.29
5	N	500	B13	C31-C32-N33	2.20	123.62	116.55
5	H	500	B13	C12-C13-C14	2.22	105.00	100.81
5	F	500	B13	C31-C32-N33	2.22	123.67	116.55
5	J	500	B13	C60-C18-C17	2.25	118.51	114.56
5	P	500	B13	C37-C38-N40	2.26	123.95	116.55
5	L	500	B13	C2-C26-C27	2.28	121.72	115.29
5	F	500	B13	C47-C12-C13	2.30	119.68	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	C47-C12-C13	2.31	119.70	111.75
5	H	500	B13	C47-C12-C13	2.33	119.80	111.75
5	P	500	B13	O8R-C5R-C4R	2.34	119.21	111.34
5	B	500	B13	C60-C18-C17	2.36	118.70	114.56
5	D	500	B13	C31-C32-N33	2.36	124.14	116.55
5	F	500	B13	C25-C2-C3	2.37	116.42	111.81
5	F	500	B13	C7-C37-C38	2.38	121.58	114.29
5	H	500	B13	C31-C32-N33	2.40	124.27	116.55
5	P	500	B13	C31-C32-N33	2.43	124.37	116.55
5	J	500	B13	C47-C12-C13	2.46	120.24	111.75
5	N	500	B13	C42-C41-C8	2.47	122.08	114.78
5	J	500	B13	O8R-C5R-C4R	2.50	119.77	111.34
5	B	500	B13	C12-C13-C14	2.54	105.61	100.81
5	D	500	B13	O8R-C5R-C4R	2.54	119.90	111.34
5	L	500	B13	C31-C32-N33	2.55	124.76	116.55
5	L	500	B13	C47-C12-C13	2.62	120.77	111.75
5	L	500	B13	O8R-C5R-C4R	2.63	120.20	111.34
5	B	500	B13	C16-N24-C19	2.65	110.20	100.41
5	F	500	B13	C16-N24-C19	2.67	110.29	100.41
5	L	500	B13	C7-C37-C38	2.70	122.58	114.29
5	D	500	B13	C16-N24-C19	2.70	110.41	100.41
5	P	500	B13	C16-N24-C19	2.71	110.43	100.41
5	D	500	B13	C47-C12-C13	2.74	121.19	111.75
5	L	500	B13	C42-C41-C8	2.77	122.95	114.78
5	D	500	B13	C18-C60-C61	2.78	121.21	113.98
5	D	500	B13	C36-C7-C6	2.78	124.83	110.26
5	J	500	B13	C36-C7-C6	2.79	124.87	110.26
5	L	500	B13	C36-C7-C6	2.80	124.94	110.26
5	H	500	B13	C16-N24-C19	2.81	110.80	100.41
5	N	500	B13	C16-N24-C19	2.81	110.81	100.41
5	J	500	B13	C16-N24-C19	2.83	110.87	100.41
5	D	500	B13	C7-C37-C38	2.85	123.02	114.29
5	N	500	B13	C18-C60-C61	2.85	121.40	113.98
5	H	500	B13	C36-C7-C6	2.87	125.26	110.26
5	F	500	B13	C42-C41-C8	2.91	123.37	114.78
5	H	500	B13	C42-C41-C8	2.96	123.53	114.78
5	P	500	B13	C36-C7-C6	2.99	125.89	110.26
5	L	500	B13	C16-N24-C19	2.99	111.47	100.41
5	L	500	B13	C60-C18-C17	3.01	119.84	114.56
5	L	500	B13	C18-C60-C61	3.02	121.83	113.98
5	N	500	B13	C47-C12-C13	3.07	122.32	111.75
5	D	500	B13	C42-C41-C8	3.11	123.97	114.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	500	B13	C36-C7-C6	3.13	126.64	110.26
5	D	500	B13	C60-C18-C17	3.14	120.07	114.56
5	B	500	B13	C18-C60-C61	3.15	122.17	113.98
5	F	500	B13	C18-C60-C61	3.15	122.17	113.98
5	B	500	B13	C36-C7-C6	3.16	126.82	110.26
5	H	500	B13	C18-C60-C61	3.17	122.22	113.98
5	N	500	B13	O8R-C5R-C4R	3.20	122.10	111.34
5	F	500	B13	C36-C7-C6	3.20	127.01	110.26
5	P	500	B13	C42-C41-C8	3.27	124.43	114.78
5	N	500	B13	C60-C18-C17	3.27	120.31	114.56
5	F	500	B13	O8R-C5R-C4R	3.29	122.41	111.34
5	H	500	B13	O8R-C5R-C4R	3.36	122.64	111.34
5	N	500	B13	C7-C37-C38	3.37	124.62	114.29
5	P	500	B13	C60-C18-C17	3.63	120.93	114.56
5	F	500	B13	C60-C18-C17	3.65	120.98	114.56
5	J	500	B13	C7-C37-C38	3.80	125.95	114.29
5	H	500	B13	C7-C37-C38	3.88	126.19	114.29
5	D	500	B13	O7R-C2R-C3R	3.89	122.25	111.18
5	P	500	B13	C18-C60-C61	3.98	124.33	113.98
5	J	500	B13	C18-C60-C61	4.02	124.44	113.98
5	L	500	B13	O7R-C2R-C3R	4.10	122.83	111.18
5	P	500	B13	C7-C37-C38	4.11	126.89	114.29
5	J	500	B13	O7R-C2R-C3R	4.14	122.94	111.18
5	F	500	B13	O7R-C2R-C3R	4.20	123.12	111.18
5	N	500	B13	C5R-C4R-C3R	4.47	129.47	114.89
5	H	500	B13	O7R-C2R-C3R	4.50	123.99	111.18
5	B	500	B13	C5R-C4R-C3R	4.60	129.92	114.89
5	D	500	B13	C5R-C4R-C3R	4.61	129.93	114.89
5	P	500	B13	O7R-C2R-C3R	4.61	124.30	111.18
5	N	500	B13	O7R-C2R-C3R	4.63	124.36	111.18
5	H	500	B13	C60-C18-C17	4.66	122.74	114.56
5	B	500	B13	O7R-C2R-C3R	4.82	124.90	111.18
5	F	500	B13	C5R-C4R-C3R	4.88	130.81	114.89
5	P	500	B13	C5R-C4R-C3R	4.91	130.92	114.89
5	L	500	B13	C5R-C4R-C3R	4.91	130.92	114.89
5	J	500	B13	C5R-C4R-C3R	5.17	131.76	114.89
5	H	500	B13	C5R-C4R-C3R	5.25	132.03	114.89
5	H	500	B13	O6R-C4R-C5R	7.30	124.78	109.16
5	D	500	B13	O6R-C4R-C5R	7.56	125.33	109.16
5	L	500	B13	O6R-C4R-C5R	7.57	125.36	109.16
5	P	500	B13	O6R-C4R-C5R	7.63	125.48	109.16
5	J	500	B13	O6R-C4R-C5R	7.67	125.58	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	O6R-C4R-C5R	8.01	126.29	109.16
5	N	500	B13	O6R-C4R-C5R	8.05	126.38	109.16
5	F	500	B13	O6R-C4R-C5R	8.06	126.41	109.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	500	B13	9	0
5	D	500	B13	13	0
5	F	500	B13	7	0
5	H	500	B13	10	0
5	J	500	B13	13	0
5	L	500	B13	10	0
5	N	500	B13	11	0
5	P	500	B13	9	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.26	0 100 100	3, 11, 26, 38	0
1	C	459/461 (99%)	-0.25	0 100 100	3, 10, 23, 39	0
1	E	459/461 (99%)	0.33	27 (5%) 23 24	25, 33, 42, 49	0
1	G	459/461 (99%)	0.02	10 (2%) 62 64	18, 29, 40, 49	0
1	I	459/461 (99%)	-0.17	3 (0%) 87 88	9, 20, 34, 50	0
1	K	459/461 (99%)	-0.16	3 (0%) 87 88	12, 20, 33, 46	0
1	M	459/461 (99%)	-0.20	1 (0%) 94 95	10, 20, 34, 48	0
1	O	459/461 (99%)	-0.21	2 (0%) 92 92	7, 18, 32, 45	0
2	B	258/258 (100%)	1.22	58 (22%) 1 1	4, 67, 100, 107	0
2	D	258/258 (100%)	1.31	70 (27%) 1 0	5, 66, 100, 110	0
2	F	258/258 (100%)	1.67	87 (33%) 0 0	18, 72, 102, 112	0
2	H	258/258 (100%)	2.09	118 (45%) 0 0	28, 73, 104, 110	0
2	J	258/258 (100%)	1.21	57 (22%) 1 1	17, 64, 97, 107	0
2	L	258/258 (100%)	1.62	95 (36%) 0 0	12, 71, 102, 113	0
2	N	258/258 (100%)	2.11	123 (47%) 0 0	12, 73, 103, 110	0
2	P	258/258 (100%)	1.24	51 (19%) 1 1	17, 67, 98, 108	0
All	All	5736/5752 (99%)	0.49	705 (12%) 5 4	3, 29, 92, 113	0

All (705) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	207	PHE	8.7
2	L	118	ALA	8.6
2	J	178	LEU	8.4
2	P	207	PHE	8.2
2	H	207	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
2	F	207	PHE	8.0
2	P	208	ALA	7.9
2	N	255	PHE	7.6
2	L	119	THR	7.6
2	J	180	GLY	7.5
2	F	258	HIS	7.4
2	L	258	HIS	7.3
2	H	65	ALA	7.2
2	L	257	LYS	7.1
2	J	208	ALA	7.1
2	L	207	PHE	7.0
2	N	258	HIS	6.9
2	F	208	ALA	6.9
2	H	178	LEU	6.9
2	N	118	ALA	6.8
2	N	70	ILE	6.7
2	L	117	GLY	6.7
2	N	178	LEU	6.7
2	F	223	ALA	6.7
2	P	118	ALA	6.6
2	H	119	THR	6.5
2	B	119	THR	6.5
2	H	151	GLY	6.5
2	H	253	GLU	6.4
2	H	61	ALA	6.4
2	N	72	LEU	6.4
2	N	117	GLY	6.4
2	H	258	HIS	6.4
2	P	178	LEU	6.3
2	F	178	LEU	6.3
2	H	208	ALA	6.2
2	J	209	CYS	6.2
2	N	257	LYS	6.2
2	L	179	THR	6.1
2	P	119	THR	6.1
2	H	245	THR	6.1
2	D	226	VAL	6.0
2	N	179	THR	6.0
2	D	199	LEU	6.0
2	H	123	LYS	6.0
2	P	179	THR	5.9
2	P	209	CYS	5.9

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Mol	Chain	Res	Type	RSRZ
2	L	189	TYR	5.9
2	D	65	ALA	5.8
2	J	179	THR	5.7
2	H	118	ALA	5.7
2	N	250	GLU	5.7
2	H	242	ILE	5.7
2	D	59	LEU	5.7
2	H	117	GLY	5.7
2	J	119	THR	5.7
2	F	249	THR	5.6
2	D	258	HIS	5.6
2	F	179	THR	5.6
2	N	121	LYS	5.6
2	N	227	TYR	5.6
2	N	113	LYS	5.6
2	N	207	PHE	5.5
2	D	243	ALA	5.5
2	N	151	GLY	5.5
2	H	77	LEU	5.4
2	L	243	ALA	5.4
2	N	59	LEU	5.4
2	F	119	THR	5.4
2	H	113	LYS	5.4
2	H	250	GLU	5.4
2	N	56	VAL	5.4
2	H	79	VAL	5.3
2	N	199	LEU	5.3
2	N	36	LYS	5.3
2	F	244	GLY	5.3
2	N	243	ALA	5.3
2	D	77	LEU	5.2
2	N	119	THR	5.2
2	F	189	TYR	5.2
2	L	208	ALA	5.2
2	D	207	PHE	5.2
2	F	117	GLY	5.1
2	B	178	LEU	5.1
2	N	246	THR	5.1
2	B	77	LEU	5.1
2	H	115	ASN	5.1
2	N	221	GLN	5.1
2	N	226	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
2	H	116	SER	5.1
2	F	123	LYS	5.0
2	L	65	ALA	5.0
2	H	243	ALA	5.0
2	F	243	ALA	5.0
2	B	208	ALA	4.9
2	N	76	ALA	4.9
2	P	36	LYS	4.9
2	H	57	GLU	4.9
2	N	240	ALA	4.9
2	N	114	GLU	4.9
2	N	189	TYR	4.9
2	D	249	THR	4.9
2	F	247	ASP	4.9
2	H	133	GLY	4.9
2	P	121	LYS	4.9
2	B	65	ALA	4.9
2	H	257	LYS	4.8
2	L	174	LYS	4.8
2	B	207	PHE	4.8
2	H	121	LYS	4.8
2	F	67	LYS	4.8
2	J	226	VAL	4.8
2	D	68	ASP	4.8
2	D	253	GLU	4.8
2	N	168	ALA	4.8
2	N	77	LEU	4.8
2	P	77	LEU	4.8
2	F	200	GLU	4.8
1	E	97	TRP	4.8
2	F	257	LYS	4.8
2	B	253	GLU	4.8
2	L	242	ILE	4.8
2	H	244	GLY	4.7
2	H	179	THR	4.7
2	J	191	PHE	4.7
2	P	67	LYS	4.7
2	D	178	LEU	4.7
2	N	242	ILE	4.7
2	N	204	LYS	4.7
2	D	208	ALA	4.7
2	P	226	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	J	258	HIS	4.6
2	H	180	GLY	4.6
2	L	120	PRO	4.6
2	F	77	LEU	4.6
2	N	208	ALA	4.6
2	F	180	GLY	4.6
2	H	122	THR	4.6
2	B	226	VAL	4.6
2	H	209	CYS	4.6
2	N	112	CYS	4.6
2	P	243	ALA	4.5
2	N	220	SER	4.5
2	B	244	GLY	4.5
2	N	247	ASP	4.5
2	D	223	ALA	4.5
2	L	76	ALA	4.5
2	F	219	VAL	4.5
2	N	176	ILE	4.4
2	L	246	THR	4.4
1	E	3	ALA	4.4
2	N	123	LYS	4.4
2	N	69	PRO	4.4
2	D	255	PHE	4.4
2	B	68	ASP	4.4
2	N	200	GLU	4.4
1	E	445	THR	4.4
2	N	249	THR	4.4
2	H	216	GLN	4.4
2	P	180	GLY	4.4
2	B	258	HIS	4.4
2	H	110	GLU	4.3
2	B	179	THR	4.3
2	N	37	ASP	4.3
2	N	68	ASP	4.3
2	F	204	LYS	4.3
2	H	199	LEU	4.3
2	N	209	CYS	4.3
2	H	62	ALA	4.3
2	L	253	GLU	4.3
2	H	217	ASP	4.3
2	F	177	MET	4.3
2	H	70	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	67	LYS	4.2
2	B	249	THR	4.2
2	F	246	THR	4.2
2	N	71	ASP	4.2
2	L	177	MET	4.2
2	L	249	THR	4.2
2	H	36	LYS	4.2
2	P	117	GLY	4.1
2	B	242	ILE	4.1
2	N	236	LYS	4.1
2	F	68	ASP	4.1
2	P	65	ALA	4.1
2	L	178	LEU	4.1
2	B	110	GLU	4.1
2	D	219	VAL	4.1
2	D	224	LEU	4.1
2	B	118	ALA	4.1
2	D	172	LYS	4.1
2	F	225	GLY	4.1
2	N	248	VAL	4.1
2	L	110	GLU	4.1
2	H	255	PHE	4.1
2	H	112	CYS	4.0
2	N	116	SER	4.0
2	N	120	PRO	4.0
2	N	203	ILE	4.0
2	L	222	PHE	3.9
2	H	172	LYS	3.9
2	L	43	ILE	3.9
2	F	193	GLU	3.9
2	N	106	LEU	3.9
2	H	226	VAL	3.9
2	D	112	CYS	3.9
2	D	179	THR	3.9
2	H	64	GLU	3.9
2	J	59	LEU	3.9
2	D	180	GLY	3.9
2	P	258	HIS	3.9
2	D	189	TYR	3.9
2	B	63	ILE	3.8
2	J	67	LYS	3.8
2	F	220	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	N	217	ASP	3.8
2	L	221	GLN	3.8
2	N	202	GLY	3.8
2	F	59	LEU	3.8
2	L	200	GLU	3.8
2	P	191	PHE	3.8
2	J	117	GLY	3.8
2	B	209	CYS	3.8
2	J	110	GLU	3.8
2	P	177	MET	3.7
2	N	150	ASN	3.7
2	N	186	THR	3.7
2	J	177	MET	3.7
2	H	51	GLU	3.7
2	P	69	PRO	3.7
2	L	59	LEU	3.7
2	L	151	GLY	3.7
2	N	154	VAL	3.7
2	B	109	ILE	3.6
2	N	256	HIS	3.6
2	L	36	LYS	3.6
2	P	110	GLU	3.6
2	H	248	VAL	3.6
2	N	232	ALA	3.6
2	B	243	ALA	3.6
2	D	119	THR	3.6
2	F	84	VAL	3.6
2	N	124	GLY	3.6
2	F	222	PHE	3.6
2	F	116	SER	3.6
2	D	121	LYS	3.6
2	D	236	LYS	3.6
2	N	174	LYS	3.6
2	P	257	LYS	3.6
2	H	38	GLU	3.5
2	L	202	GLY	3.5
2	N	201	ASN	3.5
2	N	194	VAL	3.5
2	D	200	GLU	3.5
2	H	200	GLU	3.5
2	N	110	GLU	3.5
2	N	206	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	209	CYS	3.5
2	N	218	PHE	3.5
2	H	204	LYS	3.5
1	G	56	GLU	3.5
2	F	251	LEU	3.5
2	J	118	ALA	3.5
1	E	8	SER	3.5
2	H	53	ASP	3.5
2	L	171	GLN	3.5
1	K	53	ALA	3.5
2	F	253	GLU	3.5
2	L	226	VAL	3.5
2	N	253	GLU	3.5
2	N	53	ASP	3.5
2	F	133	GLY	3.5
2	N	215	ASN	3.5
2	F	242	ILE	3.4
2	J	194	VAL	3.4
2	H	52	GLU	3.4
2	N	43	ILE	3.4
2	H	174	LYS	3.4
2	F	255	PHE	3.4
2	N	44	ALA	3.4
2	L	69	PRO	3.4
2	B	151	GLY	3.4
2	J	257	LYS	3.4
2	D	250	GLU	3.4
2	J	225	GLY	3.4
2	D	246	THR	3.4
2	N	192	LYS	3.4
2	F	162	PRO	3.4
2	N	239	ASP	3.4
2	H	241	ILE	3.3
2	H	247	ASP	3.3
2	N	164	GLU	3.3
2	H	107	GLU	3.3
2	P	116	SER	3.3
2	B	69	PRO	3.3
2	P	122	THR	3.3
1	K	134	GLU	3.3
2	N	64	GLU	3.3
2	B	71	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	114	GLU	3.3
2	L	180	GLY	3.3
2	H	189	TYR	3.3
2	J	53	ASP	3.3
2	H	120	PRO	3.3
2	N	35	PRO	3.3
2	L	77	LEU	3.3
2	H	249	THR	3.3
2	L	241	ILE	3.3
2	B	180	GLY	3.3
2	H	66	GLY	3.3
1	E	4	LYS	3.3
2	N	67	LYS	3.3
1	E	460	GLY	3.2
2	L	209	CYS	3.2
2	F	196	ASP	3.2
2	J	237	ILE	3.2
2	N	42	PRO	3.2
2	N	65	ALA	3.2
2	H	68	ASP	3.2
2	J	128	CYS	3.2
2	L	199	LEU	3.2
2	N	122	THR	3.2
2	L	192	LYS	3.2
2	B	247	ASP	3.2
2	D	58	GLY	3.2
2	N	219	VAL	3.2
2	B	236	LYS	3.2
2	N	198	LEU	3.2
2	P	155	VAL	3.2
2	F	112	CYS	3.1
2	L	112	CYS	3.1
2	F	226	VAL	3.1
2	H	7	ALA	3.1
2	F	156	ASP	3.1
2	H	49	GLU	3.1
2	B	59	LEU	3.1
2	L	166	VAL	3.1
2	F	47	ILE	3.1
2	P	172	LYS	3.1
2	H	75	ASP	3.1
2	B	200	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	194	VAL	3.1
2	P	194	VAL	3.1
2	N	222	PHE	3.1
2	F	65	ALA	3.1
2	F	38	GLU	3.0
2	L	255	PHE	3.0
2	L	248	VAL	3.0
2	D	109	ILE	3.0
2	P	112	CYS	3.0
2	N	38	GLU	3.0
1	E	53	ALA	3.0
2	H	59	LEU	3.0
2	N	63	ILE	3.0
1	E	93	ASN	3.0
2	H	108	GLY	3.0
2	N	52	GLU	3.0
1	O	53	ALA	3.0
2	H	162	PRO	3.0
2	F	23	ALA	3.0
2	N	172	LYS	3.0
1	E	135	PHE	3.0
2	D	191	PHE	3.0
2	D	242	ILE	3.0
2	B	37	ASP	3.0
2	L	227	TYR	3.0
2	P	242	ILE	3.0
2	N	107	GLU	3.0
2	F	22	LYS	3.0
2	H	41	TYR	3.0
2	L	113	LYS	3.0
2	D	251	LEU	3.0
2	D	225	GLY	3.0
2	B	56	VAL	2.9
2	J	68	ASP	2.9
2	F	113	LYS	2.9
2	J	116	SER	2.9
2	B	227	TYR	2.9
2	H	251	LEU	2.9
2	H	223	ALA	2.9
2	L	39	LEU	2.9
2	H	153	ASN	2.9
2	J	251	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	194	VAL	2.9
2	B	60	GLN	2.9
2	H	78	MET	2.9
2	F	118	ALA	2.9
2	H	227	TYR	2.9
2	N	60	GLN	2.9
2	F	248	VAL	2.9
2	H	155	VAL	2.9
2	D	222	PHE	2.9
2	N	205	ILE	2.9
1	I	3	ALA	2.9
2	P	253	GLU	2.9
2	F	201	ASN	2.9
2	B	246	THR	2.9
2	D	201	ASN	2.8
2	H	80	GLY	2.8
2	L	217	ASP	2.8
2	B	121	LYS	2.8
2	D	174	LYS	2.8
2	H	63	ILE	2.8
2	H	191	PHE	2.8
2	L	129	HIS	2.8
2	F	160	ASP	2.8
2	P	210	GLY	2.8
2	J	254	LYS	2.8
2	N	254	LYS	2.8
1	E	431	ALA	2.8
2	N	223	ALA	2.8
2	J	200	GLU	2.8
2	H	156	ASP	2.8
2	F	174	LYS	2.8
2	F	132	GLU	2.8
2	N	129	HIS	2.8
2	B	191	PHE	2.8
2	D	116	SER	2.8
2	D	248	VAL	2.8
2	J	69	PRO	2.8
2	H	86	ARG	2.8
2	B	255	PHE	2.8
2	F	164	GLU	2.8
2	L	193	GLU	2.8
2	F	36	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	162	PRO	2.8
2	F	199	LEU	2.8
2	J	172	LYS	2.8
2	F	221	GLN	2.7
2	H	232	ALA	2.7
2	N	241	ILE	2.7
1	E	133	ARG	2.7
2	H	252	ARG	2.7
2	B	67	LYS	2.7
2	D	204	LYS	2.7
2	L	67	LYS	2.7
2	N	41	TYR	2.7
2	N	104	ALA	2.7
2	F	217	ASP	2.7
2	P	206	PRO	2.7
2	N	133	GLY	2.7
2	D	205	ILE	2.7
2	N	125	THR	2.7
2	B	217	ASP	2.7
2	D	37	ASP	2.7
2	F	171	GLN	2.7
2	F	37	ASP	2.7
2	H	45	LYS	2.7
2	P	129	HIS	2.7
2	D	206	PRO	2.7
2	P	236	LYS	2.7
2	J	234	ALA	2.7
2	P	70	ILE	2.7
2	F	129	HIS	2.7
1	I	133	ARG	2.7
2	B	51	GLU	2.7
2	D	192	LYS	2.7
2	D	257	LYS	2.7
2	L	254	LYS	2.7
2	L	56	VAL	2.7
2	H	222	PHE	2.7
2	P	59	LEU	2.7
2	N	177	MET	2.7
2	D	209	CYS	2.6
1	E	208	LYS	2.6
2	L	70	ILE	2.6
2	N	237	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	132	GLU	2.6
2	F	250	GLU	2.6
2	H	114	GLU	2.6
2	J	244	GLY	2.6
2	P	52	GLU	2.6
2	H	56	VAL	2.6
2	N	50	GLY	2.6
2	N	245	THR	2.6
1	E	452	LYS	2.6
2	P	53	ASP	2.6
2	H	47	ILE	2.6
2	F	110	GLU	2.6
2	B	257	LYS	2.6
2	J	199	LEU	2.6
2	H	43	ILE	2.6
2	L	63	ILE	2.6
2	D	66	GLY	2.6
2	P	225	GLY	2.6
2	L	155	VAL	2.6
2	L	198	LEU	2.6
2	N	167	LEU	2.6
2	N	73	ILE	2.6
2	B	58	GLY	2.6
2	B	114	GLU	2.6
2	H	106	LEU	2.5
2	N	162	PRO	2.5
2	B	116	SER	2.5
2	N	244	GLY	2.5
2	L	52	GLU	2.5
2	N	51	GLU	2.5
2	B	189	TYR	2.5
1	G	3	ALA	2.5
2	P	181	THR	2.5
2	H	60	GLN	2.5
1	E	148	GLU	2.5
2	D	247	ASP	2.5
2	L	225	GLY	2.5
2	J	181	THR	2.5
2	F	51	GLU	2.5
2	L	251	LEU	2.5
2	H	202	GLY	2.5
2	L	244	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	105	MET	2.5
2	J	60	GLN	2.5
2	J	65	ALA	2.5
2	N	75	ASP	2.5
2	D	69	PRO	2.5
2	J	206	PRO	2.5
2	L	80	GLY	2.5
2	N	147	LEU	2.5
2	H	76	ALA	2.5
2	D	256	HIS	2.5
2	H	203	ILE	2.5
2	L	109	ILE	2.5
2	N	105	MET	2.5
2	F	120	PRO	2.5
2	H	149	ALA	2.5
2	J	243	ALA	2.5
2	J	64	GLU	2.5
2	N	251	LEU	2.4
1	I	4	LYS	2.4
1	E	449	SER	2.4
1	G	461	PHE	2.4
1	G	437	ASP	2.4
2	D	64	GLU	2.4
2	D	164	GLU	2.4
2	F	224	LEU	2.4
2	J	127	VAL	2.4
2	P	166	VAL	2.4
2	J	189	TYR	2.4
2	F	69	PRO	2.4
2	F	108	GLY	2.4
2	J	202	GLY	2.4
2	L	234	ALA	2.4
2	H	167	LEU	2.4
2	H	160	ASP	2.4
2	N	191	PHE	2.4
2	H	42	PRO	2.4
2	L	23	ALA	2.4
2	N	23	ALA	2.4
1	E	457	GLU	2.4
2	L	250	GLU	2.4
2	D	196	ASP	2.4
2	B	70	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	141	ASP	2.4
2	D	133	GLY	2.4
2	N	197	MET	2.4
2	J	129	HIS	2.4
2	L	37	ASP	2.4
2	N	216	GLN	2.4
2	D	215	ASN	2.4
2	F	205	ILE	2.4
2	J	242	ILE	2.4
2	L	233	ASP	2.4
2	D	221	GLN	2.4
1	E	443	CYS	2.4
2	L	146	LEU	2.4
2	J	210	GLY	2.3
2	L	58	GLY	2.3
2	P	158	GLY	2.3
2	H	214	VAL	2.3
2	H	109	ILE	2.3
2	P	227	TYR	2.3
2	H	239	ASP	2.3
2	D	177	MET	2.3
2	D	203	ILE	2.3
2	L	218	PHE	2.3
2	H	168	ALA	2.3
2	H	20	LEU	2.3
2	L	72	LEU	2.3
2	D	217	ASP	2.3
2	L	38	GLU	2.3
2	B	177	MET	2.3
2	H	81	MET	2.3
2	N	180	GLY	2.3
2	P	202	GLY	2.3
1	E	5	ARG	2.3
2	F	114	GLU	2.3
2	F	54	ASP	2.3
2	F	203	ILE	2.3
2	B	232	ALA	2.3
2	D	230	GLU	2.3
2	F	80	GLY	2.3
2	P	127	VAL	2.3
1	G	133	ARG	2.3
1	E	210	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	185	THR	2.3
2	L	57	GLU	2.3
2	L	130	VAL	2.3
2	L	123	LYS	2.3
2	L	216	GLN	2.3
2	J	120	PRO	2.2
2	D	78	MET	2.2
2	L	210	GLY	2.2
1	E	435	ASP	2.2
2	B	52	GLU	2.2
1	E	27	LYS	2.2
2	B	206	PRO	2.2
1	E	441	ASP	2.2
2	D	71	ASP	2.2
2	F	81	MET	2.2
2	H	154	VAL	2.2
2	L	79	VAL	2.2
2	N	57	GLU	2.2
2	H	111	TYR	2.2
2	F	172	LYS	2.2
2	J	121	LYS	2.2
2	F	43	ILE	2.2
2	H	206	PRO	2.2
2	H	224	LEU	2.2
2	J	77	LEU	2.2
2	L	164	GLU	2.2
2	B	74	ASP	2.2
2	N	212	GLY	2.2
2	B	36	LYS	2.2
2	F	154	VAL	2.2
1	E	427	ALA	2.2
2	N	109	ILE	2.2
2	F	74	ASP	2.2
2	B	55	VAL	2.2
2	L	197	MET	2.2
2	J	38	GLU	2.2
1	E	7	THR	2.2
2	L	203	ILE	2.2
2	H	37	ASP	2.2
2	H	195	ASN	2.2
2	P	71	ASP	2.2
2	P	255	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	72	LEU	2.2
2	L	167	LEU	2.2
2	N	146	LEU	2.2
2	D	57	GLU	2.2
2	L	256	HIS	2.2
2	J	236	LYS	2.2
2	L	121	LYS	2.2
1	G	135	PHE	2.2
2	L	50	GLY	2.2
2	F	128	CYS	2.2
1	G	438	LYS	2.1
2	F	121	LYS	2.1
2	D	53	ASP	2.1
1	E	209	LYS	2.1
2	J	174	LYS	2.1
2	P	113	LYS	2.1
2	L	68	ASP	2.1
2	D	210	GLY	2.1
2	H	193	GLU	2.1
2	J	5	THR	2.1
2	B	113	LYS	2.1
2	L	224	LEU	2.1
2	L	247	ASP	2.1
2	F	230	GLU	2.1
1	G	423	ALA	2.1
2	F	236	LYS	2.1
2	H	19	ALA	2.1
2	J	76	ALA	2.1
2	D	245	THR	2.1
2	D	72	LEU	2.1
2	J	224	LEU	2.1
2	F	52	GLU	2.1
1	G	409	ALA	2.1
2	N	171	GLN	2.1
2	L	175	PRO	2.1
2	N	39	LEU	2.1
2	L	116	SER	2.1
2	L	220	SER	2.1
2	L	55	VAL	2.1
2	J	36	LYS	2.1
2	B	201	ASN	2.1
1	M	134	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	28	GLU	2.1
2	B	248	VAL	2.1
2	D	130	VAL	2.1
2	H	35	PRO	2.0
2	J	190	ALA	2.0
2	D	55	VAL	2.0
2	N	79	VAL	2.0
2	J	47	ILE	2.0
1	E	461	PHE	2.0
2	D	108	GLY	2.0
2	P	228	GLY	2.0
2	B	172	LYS	2.0
1	G	416	ARG	2.0
1	E	387	ASP	2.0
2	H	246	THR	2.0
2	H	142	ILE	2.0
2	L	47	ILE	2.0
2	L	51	GLU	2.0
2	B	174	LYS	2.0
2	F	168	ALA	2.0
2	F	234	ALA	2.0
2	H	22	LYS	2.0
2	H	221	GLN	2.0
2	H	238	ALA	2.0
2	P	128	CYS	2.0
2	H	220	SER	2.0
2	P	205	ILE	2.0
1	O	134	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	K	G	514	1/1	0.83	0.19	2.91	39,39,39,39	1
4	K	C	512	1/1	0.95	0.15	1.57	22,22,22,22	1
5	B13	N	500	90/90	0.92	0.22	0.19	60,66,72,73	0
5	B13	L	500	90/90	0.94	0.21	0.09	41,47,58,59	0
5	B13	F	500	90/90	0.92	0.21	0.08	53,63,71,72	0
4	K	O	518	1/1	0.92	0.12	0.07	35,35,35,35	1
3	ZN	A	501	1/1	0.98	0.11	0.04	20,20,20,20	0
3	ZN	M	507	1/1	0.99	0.13	0.00	33,33,33,33	0
3	ZN	C	502	1/1	0.99	0.11	-0.02	19,19,19,19	0
5	B13	D	500	90/90	0.96	0.17	-0.23	20,30,40,42	0
5	B13	H	500	90/90	0.94	0.18	-0.28	45,58,68,69	0
5	B13	P	500	90/90	0.94	0.18	-0.29	31,40,45,52	0
5	B13	J	500	90/90	0.96	0.17	-0.33	32,37,50,57	0
5	B13	B	500	90/90	0.97	0.14	-0.50	9,24,48,49	0
3	ZN	M	523	1/1	0.99	0.10	-0.77	21,21,21,21	0
3	ZN	K	506	1/1	0.99	0.11	-0.83	33,33,33,33	0
4	K	A	511	1/1	0.97	0.09	-1.06	23,23,23,23	1
3	ZN	I	505	1/1	0.98	0.09	-1.15	30,30,30,30	0
4	K	I	515	1/1	0.93	0.08	-1.35	28,28,28,28	1
3	ZN	I	521	1/1	0.99	0.08	-1.63	16,16,16,16	0
3	ZN	E	503	1/1	0.92	0.11	-1.64	36,36,36,36	1
3	ZN	O	508	1/1	0.96	0.07	-1.66	33,33,33,33	0
3	ZN	A	524	1/1	1.00	0.09	-1.67	9,9,9,9	0
3	ZN	E	522	1/1	0.99	0.08	-1.90	37,37,37,37	0
4	K	K	516	1/1	0.99	0.07	-2.21	31,31,31,31	1
3	ZN	G	504	1/1	0.97	0.10	-2.34	33,33,33,33	1
4	K	M	517	1/1	0.95	0.11	-	33,33,33,33	1
4	K	E	513	1/1	0.91	0.12	-	33,33,33,33	1

6.5 Other polymers ⓘ

There are no such residues in this entry.