



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 06:51 PM EST

PDB ID : 5LNH  
Title : Structure of full length Unliganded CodY from *Bacillus subtilis*  
Authors : Wilkinson, A.J.; Levnikov, V.M.; Blagova, E.V.  
Deposited on : 2016-08-04  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

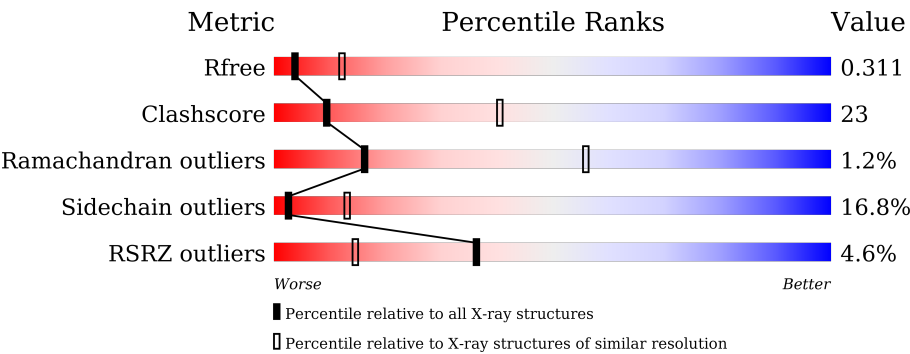
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	263	
1	B	263	
1	C	263	
1	D	263	
1	E	263	
1	F	263	

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Mol	Chain	Length	Quality of chain
1	G	263	
1	H	263	
1	I	263	
1	K	263	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	301	-	-	-	X
2	SO4	C	301	-	-	-	X
2	SO4	E	301	-	-	-	X
2	SO4	E	302	-	-	-	X
2	SO4	F	301	-	-	-	X
2	SO4	G	301	-	-	-	X
2	SO4	H	301	-	-	-	X
2	SO4	K	301	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20090 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 GTP-sensing transcriptional pleiotropic repressor CodY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	B	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	C	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	D	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	E	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	F	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	G	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	H	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	I	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	K	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

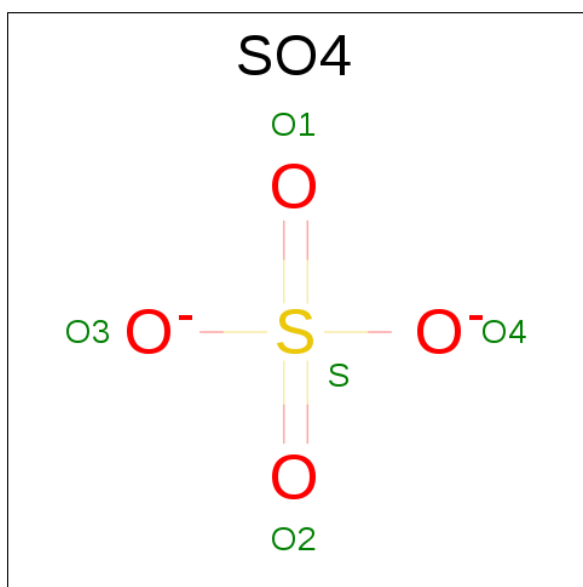
Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P39779
A	261	HIS	-	expression tag	UNP P39779
A	262	HIS	-	expression tag	UNP P39779
A	263	HIS	-	expression tag	UNP P39779
A	264	HIS	-	expression tag	UNP P39779
B	260	HIS	-	expression tag	UNP P39779
B	261	HIS	-	expression tag	UNP P39779
B	262	HIS	-	expression tag	UNP P39779
B	263	HIS	-	expression tag	UNP P39779

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP P39779
C	260	HIS	-	expression tag	UNP P39779
C	261	HIS	-	expression tag	UNP P39779
C	262	HIS	-	expression tag	UNP P39779
C	263	HIS	-	expression tag	UNP P39779
C	264	HIS	-	expression tag	UNP P39779
D	260	HIS	-	expression tag	UNP P39779
D	261	HIS	-	expression tag	UNP P39779
D	262	HIS	-	expression tag	UNP P39779
D	263	HIS	-	expression tag	UNP P39779
D	264	HIS	-	expression tag	UNP P39779
E	260	HIS	-	expression tag	UNP P39779
E	261	HIS	-	expression tag	UNP P39779
E	262	HIS	-	expression tag	UNP P39779
E	263	HIS	-	expression tag	UNP P39779
E	264	HIS	-	expression tag	UNP P39779
F	260	HIS	-	expression tag	UNP P39779
F	261	HIS	-	expression tag	UNP P39779
F	262	HIS	-	expression tag	UNP P39779
F	263	HIS	-	expression tag	UNP P39779
F	264	HIS	-	expression tag	UNP P39779
G	260	HIS	-	expression tag	UNP P39779
G	261	HIS	-	expression tag	UNP P39779
G	262	HIS	-	expression tag	UNP P39779
G	263	HIS	-	expression tag	UNP P39779
G	264	HIS	-	expression tag	UNP P39779
H	260	HIS	-	expression tag	UNP P39779
H	261	HIS	-	expression tag	UNP P39779
H	262	HIS	-	expression tag	UNP P39779
H	263	HIS	-	expression tag	UNP P39779
H	264	HIS	-	expression tag	UNP P39779
I	260	HIS	-	expression tag	UNP P39779
I	261	HIS	-	expression tag	UNP P39779
I	262	HIS	-	expression tag	UNP P39779
I	263	HIS	-	expression tag	UNP P39779
I	264	HIS	-	expression tag	UNP P39779
K	260	HIS	-	expression tag	UNP P39779
K	261	HIS	-	expression tag	UNP P39779
K	262	HIS	-	expression tag	UNP P39779
K	263	HIS	-	expression tag	UNP P39779
K	264	HIS	-	expression tag	UNP P39779

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

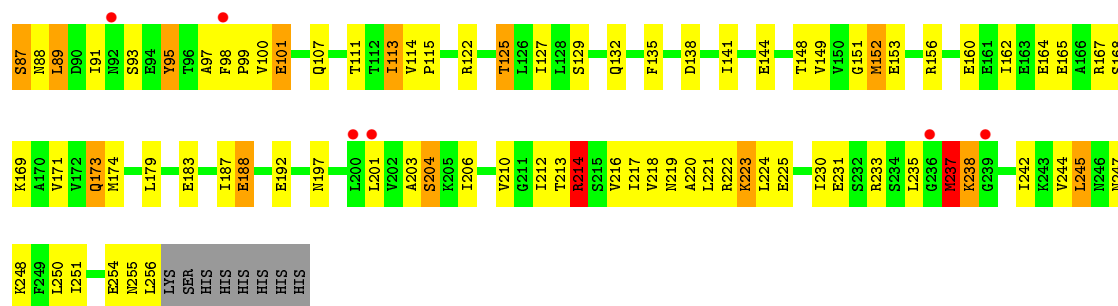


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

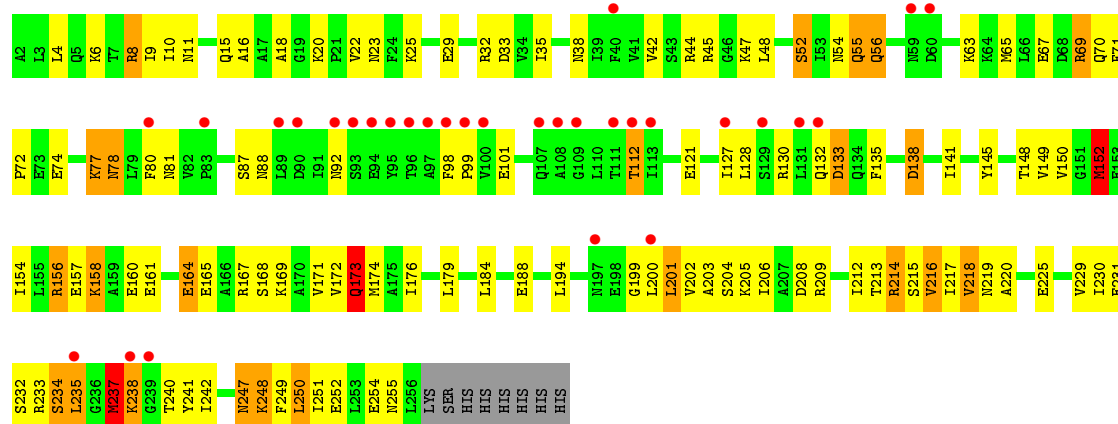
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0

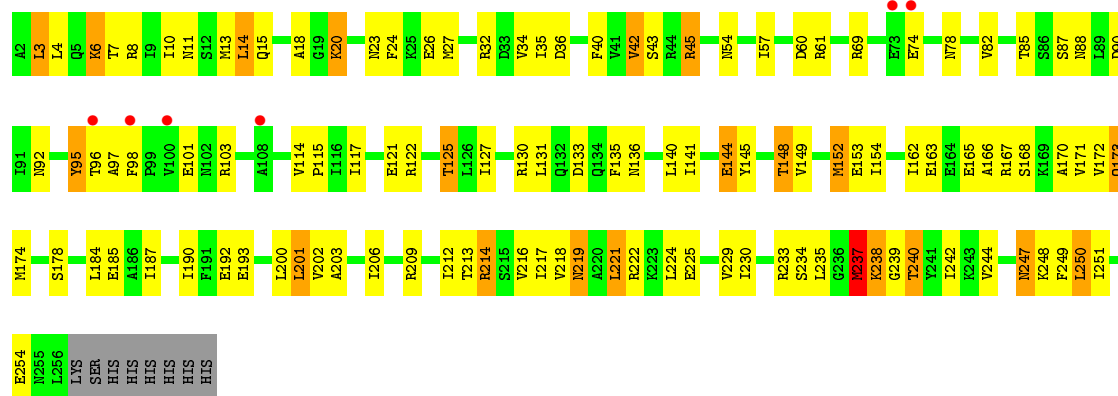




• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



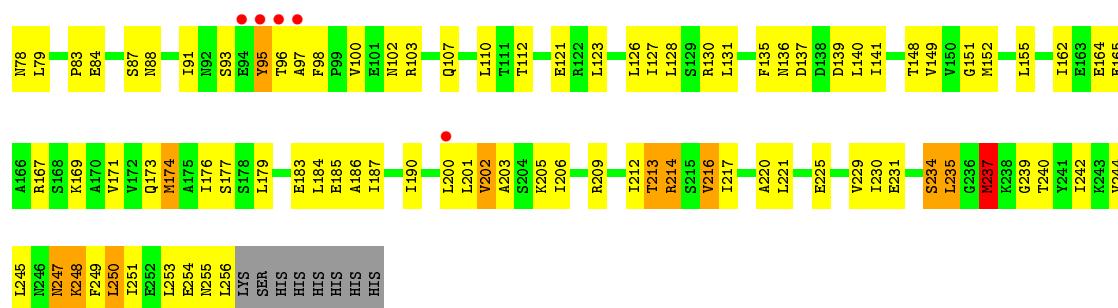
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



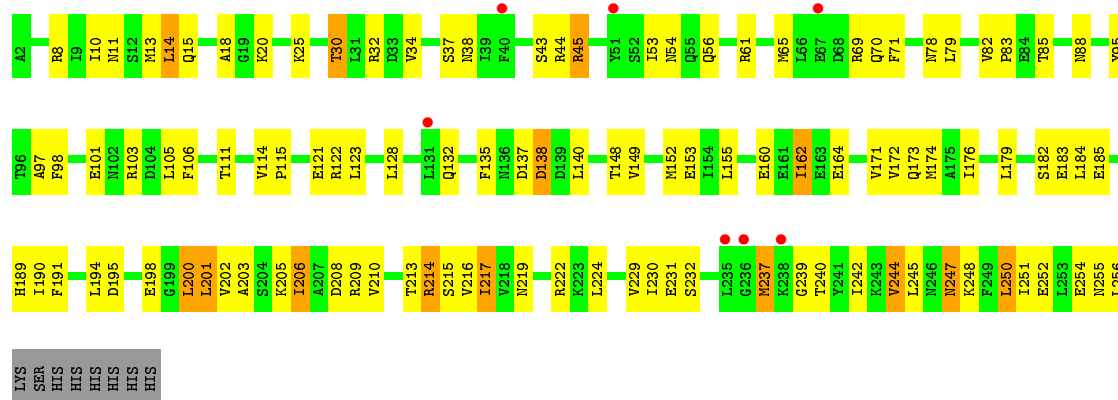
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY







- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.87Å 110.55Å 257.41Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	46.68 – 3.00 46.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.68-3.00) 72.7 (46.66-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.279 0.272 , 0.311	Depositor DCC
$R_{free}$ test set	2878 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.78	0/2015	0.88	1/2702 (0.0%)
1	B	1.37	21/2015 (1.0%)	1.16	15/2702 (0.6%)
1	C	0.70	4/2015 (0.2%)	0.77	2/2702 (0.1%)
1	D	0.96	10/2015 (0.5%)	0.83	2/2702 (0.1%)
1	E	1.00	5/2015 (0.2%)	0.85	2/2702 (0.1%)
1	F	0.98	15/2015 (0.7%)	0.79	0/2702
1	G	0.90	5/2015 (0.2%)	0.86	3/2702 (0.1%)
1	H	0.66	1/2015 (0.0%)	0.74	0/2702
1	I	0.68	0/2015	0.83	1/2702 (0.0%)
1	K	0.70	3/2015 (0.1%)	0.75	0/2702
All	All	0.90	64/20150 (0.3%)	0.85	26/27020 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	8

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	LYS	CD-CE	25.69	2.15	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ASP	CG-OD1	19.59	1.70	1.25
1	E	173	GLN	CD-NE2	17.84	1.77	1.32
1	D	234	SER	CB-OG	17.26	1.64	1.42
1	E	144	GLU	CD-OE2	16.55	1.43	1.25
1	G	101	GLU	CD-OE2	16.18	1.43	1.25
1	B	209	ARG	CZ-NH1	15.03	1.52	1.33
1	E	144	GLU	CD-OE1	13.71	1.40	1.25
1	K	198	GLU	CG-CD	12.69	1.71	1.51
1	D	56	GLN	CD-NE2	12.40	1.63	1.32
1	D	173	GLN	CD-OE1	11.85	1.50	1.24
1	F	182	SER	CB-OG	11.69	1.57	1.42
1	B	208	ASP	CG-OD2	11.55	1.51	1.25
1	B	214	ARG	CZ-NH1	11.38	1.47	1.33
1	F	181	TYR	CE1-CZ	10.91	1.52	1.38
1	F	231	GLU	CD-OE1	10.33	1.37	1.25
1	B	238	LYS	CE-NZ	10.09	1.74	1.49
1	D	158	LYS	CD-CE	9.97	1.76	1.51
1	H	243	LYS	CE-NZ	9.65	1.73	1.49
1	E	178	SER	CB-OG	9.61	1.54	1.42
1	B	193	GLU	CG-CD	9.56	1.66	1.51
1	E	20	LYS	CB-CG	9.39	1.77	1.52
1	F	243	LYS	CD-CE	9.30	1.74	1.51
1	G	241	TYR	CE2-CZ	9.09	1.50	1.38
1	G	101	GLU	CD-OE1	8.98	1.35	1.25
1	F	181	TYR	CG-CD2	8.65	1.50	1.39
1	B	233	ARG	CZ-NH2	8.60	1.44	1.33
1	B	209	ARG	CZ-NH2	8.55	1.44	1.33
1	D	55	GLN	CD-NE2	8.53	1.54	1.32
1	C	223	LYS	CE-NZ	8.28	1.69	1.49
1	F	231	GLU	CD-OE2	8.22	1.34	1.25
1	F	134	GLN	CD-OE1	8.15	1.41	1.24
1	F	243	LYS	CE-NZ	8.02	1.69	1.49
1	D	233	ARG	CZ-NH2	8.00	1.43	1.33
1	B	195	ASP	CG-OD2	7.97	1.43	1.25
1	F	198	GLU	CG-CD	7.91	1.63	1.51
1	B	241	TYR	CD1-CE1	7.55	1.50	1.39
1	F	180	SER	CB-OG	7.42	1.51	1.42
1	D	55	GLN	CD-OE1	7.21	1.39	1.24
1	F	183	GLU	CG-CD	7.21	1.62	1.51
1	F	134	GLN	CD-NE2	7.07	1.50	1.32
1	B	193	GLU	CB-CG	7.01	1.65	1.52
1	B	209	ARG	CD-NE	6.94	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	ARG	NE-CZ	6.75	1.41	1.33
1	C	173	GLN	CG-CD	6.63	1.66	1.51
1	F	241	TYR	CE2-CZ	6.54	1.47	1.38
1	D	56	GLN	CD-OE1	6.50	1.38	1.24
1	B	214	ARG	CZ-NH2	6.46	1.41	1.33
1	K	198	GLU	CD-OE2	6.38	1.32	1.25
1	K	198	GLU	CB-CG	6.26	1.64	1.52
1	B	209	ARG	NE-CZ	6.25	1.41	1.33
1	B	195	ASP	CG-OD1	6.04	1.39	1.25
1	B	238	LYS	CD-CE	6.03	1.66	1.51
1	B	241	TYR	CE2-CZ	-6.01	1.30	1.38
1	C	214	ARG	NE-CZ	5.97	1.40	1.33
1	G	181	TYR	CE1-CZ	5.55	1.45	1.38
1	B	204	SER	CB-OG	5.51	1.49	1.42
1	D	92	ASN	CG-OD1	5.49	1.36	1.24
1	F	181	TYR	CG-CD1	5.46	1.46	1.39
1	G	243	LYS	CE-NZ	5.45	1.62	1.49
1	F	183	GLU	CB-CG	5.22	1.62	1.52
1	D	233	ARG	NE-CZ	5.08	1.39	1.33
1	B	198	GLU	CD-OE1	-5.07	1.20	1.25
1	C	214	ARG	CZ-NH1	5.02	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	B	214	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	D	233	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	B	214	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	B	233	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	B	241	TYR	CZ-CE2-CD2	8.98	127.89	119.80
1	B	208	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	B	233	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	C	152	MSE	CB-CG-SE	-7.97	88.80	112.70
1	I	44	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	E	172	VAL	CG1-CB-CG2	-7.13	99.50	110.90
1	B	152	MSE	CB-CA-C	-6.39	97.62	110.40
1	B	241	TYR	CB-CG-CD1	6.36	124.82	121.00
1	B	152	MSE	CB-CG-SE	-6.11	94.36	112.70
1	G	155	LEU	CA-CB-CG	-6.08	101.33	115.30
1	B	241	TYR	CD1-CE1-CZ	5.97	125.17	119.80
1	G	241	TYR	CG-CD2-CE2	-5.91	116.57	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	221	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	214	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	G	241	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	B	209	ARG	CD-NE-CZ	-5.43	115.99	123.60
1	E	172	VAL	CA-CB-CG2	-5.40	102.81	110.90
1	B	209	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	209	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	D	152	MSE	CB-CG-SE	-5.00	97.70	112.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ASP	Sidechain
1	B	237	MSE	Peptide
1	C	237	MSE	Peptide
1	D	237	MSE	Peptide
1	E	237	MSE	Peptide
1	G	237	MSE	Peptide
1	H	237	MSE	Peptide
1	I	237	MSE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2002	0	2041	103	0
1	B	2002	0	2041	116	0
1	C	2002	0	2041	80	0
1	D	2002	0	2041	106	0
1	E	2002	0	2041	92	0
1	F	2002	0	2041	82	0
1	G	2002	0	2041	90	0
1	H	2002	0	2041	117	0
1	I	2002	0	2041	101	0
1	K	2002	0	2041	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	K	5	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
All	All	20090	0	20410	914	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 23.

All (914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:LYS:CE	1:F:243:LYS:CD	1.74	1.63
1:E:20:LYS:CB	1:E:20:LYS:CG	1.77	1.58
1:D:158:LYS:CD	1:D:158:LYS:CE	1.76	1.58
1:F:243:LYS:NZ	1:F:243:LYS:CE	1.69	1.55
1:C:223:LYS:CE	1:C:223:LYS:NZ	1.69	1.54
1:H:243:LYS:CE	1:H:243:LYS:NZ	1.73	1.52
1:B:238:LYS:CE	1:B:238:LYS:NZ	1.74	1.49
1:D:234:SER:OG	1:D:234:SER:CB	1.64	1.45
1:E:173:GLN:CD	1:E:173:GLN:NE2	1.77	1.38
1:B:208:ASP:CG	1:B:208:ASP:OD1	1.70	1.29
1:E:174:MSE:HE3	1:F:174:MSE:SE	1.82	1.29
1:B:205:LYS:CD	1:B:205:LYS:CE	2.15	1.23
1:D:250:LEU:H	1:D:250:LEU:HD23	1.09	1.08
1:B:214:ARG:HD3	1:B:214:ARG:H	1.19	1.08
1:E:174:MSE:CE	1:F:174:MSE:SE	2.53	1.07
1:B:247:ASN:HD22	1:B:247:ASN:N	1.48	1.05
1:D:201:LEU:HG	1:D:206:ILE:HD11	1.38	1.02
1:B:46:GLY:HA3	1:B:76:THR:CG2	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:ND2	1:B:247:ASN:H	1.53	1.01
1:G:174:MSE:HE1	1:H:170:ALA:HB3	1.44	0.99
1:D:247:ASN:H	1:D:247:ASN:ND2	1.48	0.97
1:F:214:ARG:H	1:F:214:ARG:HD3	1.28	0.96
1:E:214:ARG:H	1:E:214:ARG:HD3	1.29	0.95
1:D:247:ASN:N	1:D:247:ASN:HD22	1.65	0.94
1:D:29:GLU:HG2	1:D:52:SER:OG	1.67	0.94
1:I:3:LEU:HA	1:I:6:LYS:HD2	1.47	0.94
1:G:12:SER:HA	1:G:15:GLN:HG3	1.48	0.94
1:A:88:ASN:HD21	1:A:135:PHE:H	0.95	0.93
1:B:88:ASN:HD21	1:B:135:PHE:H	1.17	0.92
1:K:213:THR:HG23	1:K:214:ARG:NH1	1.83	0.92
1:C:88:ASN:HD21	1:C:135:PHE:H	1.17	0.92
1:B:214:ARG:H	1:B:214:ARG:CD	1.83	0.92
1:I:58:GLU:HA	1:I:58:GLU:OE2	1.68	0.91
1:G:201:LEU:HD23	1:G:206:ILE:HD11	1.53	0.91
1:B:24:PHE:HD1	1:B:27:MSE:HE2	1.35	0.90
1:C:173:GLN:HE21	1:E:166:ALA:HA	1.35	0.90
1:E:174:MSE:HB2	1:F:174:MSE:HE1	1.52	0.89
1:E:247:ASN:H	1:E:247:ASN:ND2	1.66	0.88
1:E:136:ASN:O	1:E:140:LEU:HD12	1.72	0.88
1:A:95:TYR:HE2	1:A:97:ALA:HB3	1.37	0.87
1:E:90:ASP:OD2	1:E:92:ASN:HB2	1.75	0.87
1:K:250:LEU:H	1:K:250:LEU:HD23	1.40	0.87
1:B:95:TYR:CE2	1:B:97:ALA:HB3	2.09	0.86
1:A:88:ASN:ND2	1:A:135:PHE:H	1.71	0.85
1:A:247:ASN:H	1:A:247:ASN:HD22	1.20	0.85
1:D:174:MSE:HG3	1:E:174:MSE:HE1	1.56	0.85
1:K:213:THR:HG23	1:K:214:ARG:HH12	1.36	0.85
1:H:247:ASN:H	1:H:247:ASN:HD22	1.24	0.84
1:H:88:ASN:HD21	1:H:135:PHE:H	1.24	0.84
1:F:88:ASN:HD21	1:F:135:PHE:H	1.23	0.84
1:C:188:GLU:O	1:C:192:GLU:HG3	1.78	0.84
1:C:23:ASN:ND2	1:C:26:GLU:HG2	1.93	0.83
1:I:91:ILE:HD12	1:I:107:GLN:HA	1.60	0.83
1:G:201:LEU:HG	1:G:202:VAL:H	1.42	0.82
1:B:213:THR:HB	1:B:216:VAL:HG13	1.61	0.82
1:A:167:ARG:O	1:A:171:VAL:HG12	1.80	0.82
1:C:173:GLN:NE2	1:E:166:ALA:HA	1.94	0.82
1:G:14:LEU:HD13	1:G:149:VAL:HG13	1.62	0.82
1:H:145:TYR:O	1:H:149:VAL:HG23	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:ASN:HD22	1:F:247:ASN:H	1.26	0.82
1:D:250:LEU:N	1:D:250:LEU:HD23	1.94	0.81
1:H:88:ASN:HD22	1:H:110:LEU:HD13	1.45	0.81
1:I:78:ASN:HB3	1:I:98:PHE:CZ	2.15	0.81
1:G:85:THR:HG23	1:G:114:VAL:HG22	1.61	0.81
1:A:95:TYR:CE2	1:A:97:ALA:HB3	2.16	0.81
1:A:115:PRO:HB3	1:A:122:ARG:NH1	1.95	0.81
1:D:250:LEU:H	1:D:250:LEU:CD2	1.88	0.81
1:D:145:TYR:O	1:D:149:VAL:HG23	1.80	0.81
1:H:24:PHE:HA	1:H:27:MSE:HE3	1.62	0.80
1:B:198:GLU:HG2	1:B:243:LYS:HG3	1.64	0.80
1:E:250:LEU:HD23	1:E:250:LEU:H	1.44	0.80
1:C:213:THR:HB	1:C:216:VAL:HG13	1.63	0.80
1:F:214:ARG:CD	1:F:214:ARG:H	1.93	0.80
1:A:46:GLY:HA3	1:A:76:THR:HG23	1.62	0.80
1:D:158:LYS:CG	1:D:158:LYS:CE	2.60	0.79
1:E:32:ARG:HD2	1:E:54:ASN:HB3	1.63	0.79
1:B:247:ASN:HD22	1:B:247:ASN:H	0.81	0.79
1:D:70:GLN:HE21	1:D:71:PHE:H	1.31	0.79
1:D:247:ASN:H	1:D:247:ASN:HD22	0.82	0.79
1:G:251:ILE:O	1:G:254:GLU:HB2	1.82	0.79
1:D:88:ASN:HD21	1:D:135:PHE:H	1.31	0.78
1:K:213:THR:HB	1:K:216:VAL:HG12	1.65	0.78
1:F:243:LYS:CG	1:F:243:LYS:CE	2.61	0.78
1:I:237:MSE:HE1	1:I:240:THR:HG22	1.64	0.78
1:K:201:LEU:HD13	1:K:202:VAL:H	1.47	0.78
1:E:201:LEU:HD13	1:E:202:VAL:H	1.48	0.78
1:G:174:MSE:HE2	1:H:174:MSE:HE1	1.65	0.78
1:I:171:VAL:HA	1:I:174:MSE:HE2	1.65	0.78
1:K:247:ASN:HD22	1:K:247:ASN:N	1.80	0.78
1:D:218:VAL:HG12	1:D:219:ASN:N	1.99	0.77
1:K:78:ASN:HB3	1:K:98:PHE:CE2	2.19	0.77
1:A:88:ASN:HD21	1:A:135:PHE:N	1.77	0.77
1:H:172:VAL:HG12	1:H:176:ILE:HD11	1.66	0.77
1:I:95:TYR:HE2	1:I:97:ALA:HB3	1.49	0.77
1:H:11:ASN:O	1:H:15:GLN:HG2	1.83	0.77
1:I:51:TYR:HE1	1:I:53:ILE:HD11	1.49	0.76
1:A:99:PRO:HB2	1:A:101:GLU:OE2	1.84	0.76
1:G:174:MSE:HE1	1:H:170:ALA:CB	2.15	0.76
1:D:203:ALA:HB3	1:D:237:MSE:HE1	1.66	0.76
1:K:205:LYS:HE2	1:K:209:ARG:NH2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:THR:HG23	1:H:114:VAL:HG22	1.68	0.75
1:B:46:GLY:HA3	1:B:76:THR:HG23	1.68	0.75
1:G:214:ARG:CD	1:G:214:ARG:H	1.99	0.75
1:B:201:LEU:HD12	1:B:202:VAL:H	1.50	0.75
1:D:167:ARG:O	1:D:171:VAL:HG13	1.87	0.74
1:I:95:TYR:CE2	1:I:97:ALA:HB3	2.22	0.74
1:B:121:GLU:HG3	1:H:212:ILE:HG12	1.68	0.74
1:I:247:ASN:H	1:I:247:ASN:HD22	1.36	0.74
1:B:179:LEU:HD22	1:B:183:GLU:HB3	1.69	0.74
1:D:138:ASP:HA	1:D:141:ILE:HD12	1.70	0.74
1:A:150:VAL:HG12	1:A:154:ILE:HD11	1.70	0.74
1:I:212:ILE:HG12	1:K:121:GLU:HG3	1.69	0.74
1:A:214:ARG:HH11	1:A:214:ARG:H	1.35	0.73
1:H:149:VAL:HG13	1:H:152:MSE:HE3	1.69	0.73
1:I:78:ASN:HB3	1:I:98:PHE:CE2	2.24	0.73
1:E:213:THR:HB	1:E:216:VAL:HG13	1.71	0.73
1:B:24:PHE:CD1	1:B:27:MSE:HE2	2.21	0.73
1:C:156:ARG:O	1:C:160:GLU:HG2	1.89	0.73
1:D:169:LYS:HB3	1:F:173:GLN:HE21	1.52	0.73
1:E:203:ALA:HB3	1:E:237:MSE:SE	2.38	0.73
1:G:250:LEU:HD23	1:G:250:LEU:H	1.54	0.73
1:H:138:ASP:HA	1:H:141:ILE:HD12	1.69	0.73
1:B:95:TYR:OH	1:B:98:PHE:HD1	1.70	0.73
1:B:32:ARG:HD2	1:B:54:ASN:HB3	1.69	0.73
1:D:121:GLU:HG3	1:F:212:ILE:HG12	1.68	0.73
1:D:247:ASN:ND2	1:D:247:ASN:N	2.28	0.72
1:I:149:VAL:HA	1:I:152:MSE:HE3	1.71	0.72
1:E:20:LYS:CB	1:E:20:LYS:CD	2.67	0.72
1:H:214:ARG:NH2	1:H:215:SER:OG	2.23	0.72
1:K:219:ASN:HA	1:K:222:ARG:HG3	1.70	0.72
1:A:2:ALA:HA	1:A:5:GLN:NE2	2.05	0.72
1:G:11:ASN:O	1:G:15:GLN:HG2	1.90	0.71
1:F:23:ASN:HB3	1:F:26:GLU:HG3	1.72	0.71
1:F:156:ARG:HD3	1:F:160:GLU:OE2	1.89	0.71
1:G:45:ARG:H	1:G:45:ARG:HD3	1.54	0.71
1:E:20:LYS:CA	1:E:20:LYS:CG	2.68	0.70
1:A:54:ASN:OD1	1:A:55:GLN:HG2	1.91	0.70
1:H:193:GLU:OE2	1:H:209:ARG:NH1	2.25	0.70
1:K:247:ASN:H	1:K:247:ASN:HD22	1.39	0.70
1:D:4:LEU:HD11	1:D:8:ARG:HH11	1.55	0.70
1:F:6:LYS:HA	1:F:9:ILE:HD12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:MSE:HE2	1:H:174:MSE:CE	2.22	0.70
1:I:231:GLU:HB2	1:I:245:LEU:HD11	1.71	0.70
1:C:88:ASN:ND2	1:C:135:PHE:H	1.90	0.70
1:B:8:ARG:O	1:B:11:ASN:HB2	1.93	0.69
1:G:146:GLY:O	1:G:150:VAL:HG23	1.92	0.69
1:K:252:GLU:HA	1:K:255:ASN:HD22	1.55	0.69
1:I:205:LYS:HG2	1:I:209:ARG:HH12	1.58	0.69
1:B:95:TYR:HE2	1:B:97:ALA:HB3	1.54	0.69
1:C:99:PRO:HB2	1:C:101:GLU:OE2	1.93	0.69
1:H:78:ASN:HB3	1:H:98:PHE:CE2	2.29	0.69
1:I:8:ARG:HA	1:I:11:ASN:HD22	1.56	0.69
1:K:88:ASN:HD21	1:K:135:PHE:H	1.41	0.69
1:D:22:VAL:HG21	1:D:157:GLU:HB2	1.76	0.68
1:A:30:THR:O	1:A:34:VAL:HG23	1.93	0.68
1:E:95:TYR:CE2	1:E:97:ALA:HB3	2.28	0.68
1:I:203:ALA:H	1:I:237:MSE:HE1	1.59	0.68
1:K:38:ASN:HD22	1:K:53:ILE:HG12	1.59	0.68
1:I:250:LEU:H	1:I:250:LEU:HD23	1.57	0.68
1:C:32:ARG:HD2	1:C:54:ASN:HB3	1.75	0.68
1:B:15:GLN:OE1	1:G:117:ILE:HG22	1.93	0.67
1:F:203:ALA:HB3	1:F:237:MSE:HE1	1.75	0.67
1:G:214:ARG:H	1:G:214:ARG:HD3	1.59	0.67
1:H:213:THR:HG22	1:H:215:SER:H	1.59	0.67
1:A:213:THR:O	1:A:217:ILE:HG13	1.92	0.67
1:C:95:TYR:OH	1:C:98:PHE:HB2	1.94	0.67
1:E:174:MSE:HE2	1:F:174:MSE:SE	2.45	0.67
1:E:214:ARG:CD	1:E:214:ARG:H	1.99	0.67
1:G:201:LEU:HD23	1:G:206:ILE:CD1	2.25	0.67
1:H:6:LYS:HA	1:H:9:ILE:HD12	1.77	0.67
1:I:202:VAL:HA	1:I:237:MSE:HE2	1.77	0.66
1:G:22:VAL:HG13	1:G:27:MSE:HE2	1.77	0.66
1:C:78:ASN:HB3	1:C:98:PHE:CE2	2.29	0.66
1:G:88:ASN:HD21	1:G:135:PHE:H	1.43	0.66
1:G:137:ASP:HA	1:G:140:LEU:HD12	1.78	0.66
1:A:170:ALA:CB	1:B:174:MSE:HE1	2.26	0.66
1:C:138:ASP:HA	1:C:141:ILE:HD12	1.78	0.66
1:C:223:LYS:CD	1:C:223:LYS:NZ	2.57	0.66
1:G:148:THR:HG22	1:G:152:MSE:HE3	1.78	0.66
1:E:95:TYR:CD1	1:E:95:TYR:C	2.68	0.66
1:H:243:LYS:CD	1:H:243:LYS:NZ	2.57	0.66
1:G:229:VAL:HG11	1:G:249:PHE:CD1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:LYS:HA	1:G:66:LEU:HD12	1.77	0.66
1:D:70:GLN:HE21	1:D:71:PHE:N	1.93	0.66
1:H:137:ASP:HA	1:H:140:LEU:HD12	1.78	0.66
1:H:231:GLU:HB2	1:H:245:LEU:HD21	1.77	0.66
1:K:176:ILE:HA	1:K:179:LEU:CD1	2.25	0.66
1:H:32:ARG:HD2	1:H:54:ASN:HB3	1.78	0.66
1:I:214:ARG:HA	1:I:217:ILE:HD12	1.78	0.66
1:E:229:VAL:HG11	1:E:249:PHE:CD1	2.30	0.66
1:B:95:TYR:OH	1:B:98:PHE:CD1	2.49	0.65
1:D:48:LEU:HD23	1:D:69:ARG:HG3	1.76	0.65
1:K:61:ARG:HG3	1:K:105:LEU:HD13	1.78	0.65
1:I:45:ARG:NH2	1:I:47:LYS:HE2	2.12	0.65
1:A:8:ARG:HA	1:A:11:ASN:HD22	1.62	0.65
1:D:152:MSE:HE2	1:E:152:MSE:SE	2.46	0.65
1:A:145:TYR:HD2	1:A:145:TYR:O	1.79	0.65
1:A:14:LEU:HD23	1:A:15:GLN:HE21	1.62	0.65
1:D:234:SER:CB	1:D:234:SER:HG	2.08	0.65
1:K:30:THR:O	1:K:34:VAL:HG23	1.97	0.65
1:K:251:ILE:O	1:K:254:GLU:HB2	1.97	0.65
1:H:95:TYR:OH	1:H:98:PHE:HB2	1.97	0.64
1:A:255:ASN:C	1:A:256:LEU:HD12	2.18	0.64
1:E:115:PRO:HB2	1:E:117:ILE:CD1	2.27	0.64
1:H:8:ARG:HA	1:H:11:ASN:HD22	1.62	0.64
1:F:40:PHE:HB2	1:F:127:ILE:HB	1.78	0.64
1:G:214:ARG:HA	1:G:217:ILE:HD12	1.79	0.64
1:D:150:VAL:HG12	1:D:154:ILE:HD11	1.78	0.64
1:D:78:ASN:HB3	1:D:98:PHE:CE2	2.32	0.64
1:G:22:VAL:HG13	1:G:27:MSE:CE	2.28	0.64
1:A:230:ILE:HG22	1:A:244:VAL:HA	1.80	0.64
1:B:206:ILE:O	1:B:210:VAL:HG23	1.98	0.64
1:I:201:LEU:HG	1:I:202:VAL:H	1.63	0.64
1:C:122:ARG:HH21	1:C:125:THR:HG23	1.63	0.63
1:I:244:VAL:HG21	1:I:250:LEU:HD22	1.80	0.63
1:I:137:ASP:HA	1:I:140:LEU:HD12	1.79	0.63
1:B:14:LEU:HD12	1:B:149:VAL:HG13	1.81	0.63
1:F:29:GLU:HG3	1:F:52:SER:OG	1.98	0.63
1:A:11:ASN:OD1	1:A:145:TYR:OH	2.12	0.63
1:H:213:THR:CG2	1:H:214:ARG:HH21	2.11	0.63
1:I:45:ARG:HH21	1:I:47:LYS:HE2	1.63	0.63
1:K:153:GLU:OE2	1:K:153:GLU:HA	1.97	0.63
1:G:11:ASN:O	1:G:15:GLN:CG	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASN:ND2	1:A:247:ASN:H	1.96	0.63
1:B:95:TYR:OH	1:B:98:PHE:HB2	1.99	0.63
1:C:251:ILE:O	1:C:254:GLU:HB2	1.98	0.63
1:A:63:LYS:O	1:A:67:GLU:HG3	1.99	0.62
1:A:3:LEU:HD13	1:A:138:ASP:HB3	1.80	0.62
1:H:180:SER:N	1:H:183:GLU:OE1	2.22	0.62
1:E:238:LYS:HG3	1:E:238:LYS:O	1.99	0.62
1:E:247:ASN:ND2	1:E:247:ASN:N	2.43	0.62
1:G:231:GLU:HB2	1:G:245:LEU:HD21	1.80	0.62
1:I:121:GLU:OE1	1:K:182:SER:HA	1.99	0.62
1:E:214:ARG:N	1:E:214:ARG:HD3	2.10	0.62
1:E:6:LYS:HB3	1:E:34:VAL:CG1	2.28	0.62
1:G:205:LYS:HD3	1:G:209:ARG:HH22	1.63	0.62
1:B:205:LYS:HD3	1:B:209:ARG:NH2	2.15	0.62
1:H:247:ASN:H	1:H:247:ASN:ND2	1.95	0.62
1:I:95:TYR:OH	1:I:98:PHE:HB2	1.99	0.62
1:D:194:LEU:HD11	1:D:199:GLY:HA3	1.82	0.62
1:G:168:SER:O	1:G:172:VAL:HG23	2.00	0.62
1:F:35:ILE:HG22	1:F:37:SER:HB3	1.81	0.62
1:H:210:VAL:CG1	1:H:212:ILE:HG13	2.30	0.61
1:A:39:ILE:HD13	1:A:128:LEU:HG	1.82	0.61
1:A:167:ARG:HG3	1:B:174:MSE:CG	2.29	0.61
1:B:218:VAL:CG1	1:B:222:ARG:HH12	2.13	0.61
1:I:176:ILE:HA	1:I:179:LEU:HD12	1.83	0.61
1:C:8:ARG:HA	1:C:11:ASN:ND2	2.16	0.61
1:D:77:LYS:HE2	1:D:81:ASN:HD21	1.66	0.61
1:C:213:THR:HG23	1:C:214:ARG:HH22	1.66	0.61
1:F:248:LYS:N	1:F:248:LYS:HD2	2.16	0.61
1:E:233:ARG:CZ	1:H:233:ARG:HH11	2.13	0.61
1:F:167:ARG:O	1:F:171:VAL:HG13	2.01	0.61
1:H:30:THR:O	1:H:34:VAL:HG23	2.01	0.61
1:D:205:LYS:HG2	1:D:209:ARG:HH12	1.65	0.61
1:G:174:MSE:CE	1:H:170:ALA:CB	2.79	0.61
1:B:88:ASN:ND2	1:B:135:PHE:H	1.93	0.60
1:D:29:GLU:HG2	1:D:52:SER:HG	1.66	0.60
1:K:201:LEU:CD1	1:K:202:VAL:H	2.13	0.60
1:K:231:GLU:HB2	1:K:245:LEU:HD11	1.81	0.60
1:E:153:GLU:HA	1:E:153:GLU:OE2	2.01	0.60
1:G:14:LEU:CD1	1:G:149:VAL:HG13	2.31	0.60
1:H:179:LEU:HD13	1:H:183:GLU:HB3	1.83	0.60
1:A:85:THR:HG23	1:A:114:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:OG	1:B:89:LEU:HD11	2.00	0.60
1:B:213:THR:HG22	1:B:215:SER:H	1.66	0.60
1:C:30:THR:O	1:C:34:VAL:HG23	2.02	0.60
1:D:194:LEU:HD22	1:D:242:ILE:CD1	2.31	0.60
1:H:169:LYS:HG3	1:H:248:LYS:HG2	1.82	0.60
1:I:45:ARG:NH2	1:I:47:LYS:CE	2.65	0.60
1:H:24:PHE:HA	1:H:27:MSE:CE	2.31	0.60
1:A:248:LYS:N	1:A:248:LYS:HD2	2.16	0.59
1:C:169:LYS:HD2	1:E:173:GLN:NE2	2.17	0.59
1:D:32:ARG:HD2	1:D:54:ASN:HB3	1.84	0.59
1:E:130:ARG:HD2	1:E:135:PHE:CZ	2.37	0.59
1:A:234:SER:O	1:A:235:LEU:HD13	2.03	0.59
1:F:115:PRO:HB2	1:F:117:ILE:HD11	1.83	0.59
1:F:40:PHE:O	1:F:126:LEU:HD12	2.01	0.59
1:B:203:ALA:HB3	1:B:237:MSE:HE1	1.83	0.59
1:B:247:ASN:ND2	1:B:247:ASN:N	2.24	0.59
1:F:23:ASN:CB	1:F:26:GLU:HG3	2.33	0.59
1:I:88:ASN:HD21	1:I:135:PHE:H	1.51	0.59
1:G:2:ALA:HA	1:G:5:GLN:OE1	2.03	0.59
1:A:167:ARG:HG3	1:B:174:MSE:HG3	1.85	0.59
1:G:174:MSE:C	1:G:174:MSE:SE	2.91	0.59
1:K:247:ASN:ND2	1:K:247:ASN:N	2.51	0.59
1:A:170:ALA:HB3	1:B:174:MSE:CE	2.33	0.58
1:A:219:ASN:HB2	1:B:19:GLY:O	2.02	0.58
1:C:167:ARG:O	1:C:171:VAL:HG13	2.03	0.58
1:E:115:PRO:HB2	1:E:117:ILE:HD12	1.84	0.58
1:I:51:TYR:CE1	1:I:53:ILE:HD11	2.36	0.58
1:D:174:MSE:HG3	1:E:174:MSE:CE	2.31	0.58
1:K:213:THR:HG22	1:K:215:SER:H	1.68	0.58
1:B:159:ALA:O	1:B:163:GLU:HG2	2.04	0.58
1:K:171:VAL:O	1:K:174:MSE:HB3	2.03	0.58
1:K:247:ASN:H	1:K:247:ASN:ND2	2.02	0.58
1:G:199:GLY:O	1:G:241:TYR:CD1	2.57	0.58
1:G:247:ASN:H	1:G:247:ASN:HD22	1.51	0.58
1:I:127:ILE:C	1:I:128:LEU:HD12	2.24	0.58
1:K:206:ILE:HG22	1:K:210:VAL:HG21	1.86	0.58
1:A:170:ALA:HB3	1:B:174:MSE:HE1	1.86	0.58
1:A:214:ARG:NH1	1:A:214:ARG:H	2.01	0.58
1:B:88:ASN:HD21	1:B:135:PHE:N	1.96	0.58
1:B:167:ARG:O	1:B:171:VAL:HG13	2.04	0.57
1:B:205:LYS:HD3	1:B:209:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:SER:HB3	1:K:242:ILE:HG22	1.86	0.57
1:H:39:ILE:HD13	1:H:128:LEU:HD12	1.86	0.57
1:K:213:THR:HG22	1:K:215:SER:N	2.19	0.57
1:F:201:LEU:O	1:F:240:THR:HG23	2.04	0.57
1:F:12:SER:HA	1:F:15:GLN:HG2	1.85	0.57
1:H:13:MSE:HE2	1:H:30:THR:HB	1.85	0.57
1:K:230:ILE:HG22	1:K:244:VAL:HA	1.86	0.57
1:D:88:ASN:OD1	1:D:135:PHE:HB2	2.04	0.57
1:F:11:ASN:O	1:F:15:GLN:HG2	2.05	0.57
1:H:43:SER:HB2	1:H:45:ARG:NH1	2.20	0.57
1:A:3:LEU:CD1	1:A:138:ASP:HB3	2.35	0.57
1:I:169:LYS:NZ	1:K:173:GLN:NE2	2.52	0.57
1:K:32:ARG:HD2	1:K:54:ASN:HB3	1.87	0.57
1:C:183:GLU:HG2	1:C:220:ALA:HB2	1.85	0.57
1:G:168:SER:O	1:G:171:VAL:HG22	2.05	0.57
1:H:203:ALA:HB3	1:H:237:MSE:HE1	1.86	0.57
1:H:40:PHE:HB2	1:H:127:ILE:HB	1.86	0.56
1:B:99:PRO:HB2	1:B:101:GLU:OE1	2.04	0.56
1:D:201:LEU:HD12	1:D:202:VAL:H	1.70	0.56
1:A:234:SER:C	1:A:235:LEU:HD13	2.25	0.56
1:H:205:LYS:HE2	1:H:209:ARG:NH2	2.20	0.56
1:C:23:ASN:ND2	1:C:26:GLU:CG	2.66	0.56
1:E:213:THR:HG23	1:E:214:ARG:CZ	2.35	0.56
1:F:237:MSE:O	1:F:238:LYS:HB2	2.05	0.56
1:B:206:ILE:HG22	1:B:210:VAL:CG2	2.36	0.56
1:B:218:VAL:HG12	1:B:222:ARG:HH12	1.71	0.56
1:C:153:GLU:HA	1:C:153:GLU:OE1	2.06	0.56
1:D:165:GLU:HG3	1:D:248:LYS:NZ	2.21	0.56
1:A:229:VAL:HG12	1:A:230:ILE:HG23	1.88	0.56
1:B:46:GLY:HA3	1:B:76:THR:HG22	1.85	0.56
1:B:214:ARG:N	1:B:214:ARG:CD	2.61	0.56
1:A:45:ARG:NH2	1:A:47:LYS:HD2	2.21	0.56
1:E:173:GLN:CG	1:E:173:GLN:NE2	2.66	0.56
1:H:172:VAL:O	1:H:176:ILE:HG13	2.06	0.56
1:A:251:ILE:O	1:A:254:GLU:HB2	2.06	0.56
1:F:79:LEU:HD12	1:F:98:PHE:HZ	1.71	0.56
1:I:51:TYR:HE1	1:I:53:ILE:CD1	2.16	0.56
1:K:138:ASP:OD1	1:K:138:ASP:N	2.38	0.56
1:I:13:MSE:CE	1:I:27:MSE:HG2	2.36	0.55
1:C:89:LEU:CD1	1:C:113:ILE:HD11	2.36	0.55
1:I:137:ASP:O	1:I:141:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:ARG:O	1:I:171:VAL:HG13	2.05	0.55
1:K:14:LEU:HD13	1:K:149:VAL:HG22	1.88	0.55
1:A:2:ALA:HA	1:A:5:GLN:HE22	1.71	0.55
1:C:148:THR:O	1:C:152:MSE:HE3	2.06	0.55
1:D:16:ALA:O	1:D:20:LYS:NZ	2.39	0.55
1:I:24:PHE:HA	1:I:27:MSE:HE3	1.87	0.55
1:K:8:ARG:HA	1:K:11:ASN:HD22	1.72	0.55
1:I:212:ILE:HG22	1:I:216:VAL:HG23	1.89	0.55
1:C:179:LEU:O	1:E:162:ILE:HD11	2.07	0.55
1:I:25:LYS:O	1:I:28:ALA:HB3	2.07	0.55
1:K:38:ASN:HD22	1:K:53:ILE:CG1	2.19	0.55
1:D:4:LEU:HD11	1:D:8:ARG:NH1	2.20	0.55
1:K:85:THR:HG23	1:K:114:VAL:HG22	1.89	0.55
1:H:173:GLN:HA	1:H:176:ILE:HD12	1.89	0.55
1:A:156:ARG:HD3	1:A:160:GLU:OE2	2.06	0.55
1:D:71:PHE:HD1	1:D:72:PRO:HD2	1.71	0.55
1:H:213:THR:HB	1:H:216:VAL:HG12	1.88	0.55
1:I:169:LYS:HZ3	1:K:173:GLN:NE2	2.05	0.55
1:D:172:VAL:HG21	1:D:249:PHE:HA	1.88	0.54
1:G:218:VAL:HG12	1:G:219:ASN:N	2.22	0.54
1:K:205:LYS:HE2	1:K:209:ARG:HH22	1.71	0.54
1:D:99:PRO:HB2	1:D:101:GLU:OE2	2.08	0.54
1:G:167:ARG:O	1:G:171:VAL:HG13	2.08	0.54
1:C:113:ILE:HG23	1:C:127:ILE:HG13	1.88	0.54
1:H:99:PRO:HG2	1:H:102:ASN:ND2	2.22	0.54
1:I:121:GLU:HG2	1:I:123:LEU:HD23	1.89	0.54
1:K:200:LEU:HD23	1:K:200:LEU:C	2.27	0.54
1:B:206:ILE:HG22	1:B:210:VAL:HG21	1.90	0.54
1:A:160:GLU:O	1:A:164:GLU:HG2	2.08	0.54
1:B:172:VAL:O	1:B:176:ILE:HG13	2.08	0.54
1:D:158:LYS:CD	1:D:158:LYS:NZ	2.67	0.54
1:H:88:ASN:ND2	1:H:110:LEU:HD13	2.19	0.54
1:A:247:ASN:HD22	1:A:247:ASN:N	1.98	0.54
1:D:88:ASN:ND2	1:D:135:PHE:H	2.03	0.54
1:I:30:THR:O	1:I:34:VAL:HG23	2.08	0.54
1:I:78:ASN:OD1	1:I:102:ASN:ND2	2.41	0.54
1:D:11:ASN:O	1:D:15:GLN:HG2	2.07	0.54
1:G:201:LEU:HG	1:G:202:VAL:N	2.17	0.54
1:G:48:LEU:HD13	1:G:65:MSE:SE	2.58	0.54
1:H:24:PHE:CD1	1:H:27:MSE:HE1	2.43	0.54
1:A:171:VAL:HA	1:A:174:MSE:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MSE:HG3	1:A:238:LYS:H	1.71	0.54
1:F:6:LYS:HD2	1:F:34:VAL:HG13	1.88	0.54
1:H:218:VAL:O	1:H:222:ARG:HG3	2.07	0.54
1:I:201:LEU:HD23	1:I:206:ILE:HD11	1.89	0.54
1:H:130:ARG:HG3	1:H:135:PHE:CE1	2.43	0.53
1:H:87:SER:HA	1:H:112:THR:OG1	2.08	0.53
1:I:247:ASN:N	1:I:247:ASN:HD22	2.04	0.53
1:F:160:GLU:O	1:F:164:GLU:HG2	2.08	0.53
1:H:167:ARG:O	1:H:171:VAL:HG23	2.08	0.53
1:B:6:LYS:O	1:B:10:ILE:HD12	2.08	0.53
1:H:63:LYS:O	1:H:67:GLU:HG3	2.07	0.53
1:K:172:VAL:HG12	1:K:176:ILE:HD12	1.89	0.53
1:B:237:MSE:SE	1:B:240:THR:HG22	2.58	0.53
1:H:150:VAL:O	1:H:154:ILE:HD12	2.08	0.53
1:C:197:ASN:ND2	1:C:244:VAL:HG22	2.24	0.53
1:D:205:LYS:HG2	1:D:209:ARG:NH1	2.23	0.53
1:G:48:LEU:HD23	1:G:69:ARG:HE	1.74	0.53
1:H:116:ILE:HG22	1:H:123:LEU:HB2	1.90	0.53
1:I:190:ILE:HD11	1:I:217:ILE:HG23	1.91	0.53
1:B:34:VAL:HG12	1:B:35:ILE:HG13	1.89	0.53
1:H:16:ALA:O	1:H:20:LYS:NZ	2.41	0.53
1:H:203:ALA:HB3	1:H:237:MSE:CE	2.39	0.53
1:F:201:LEU:HG	1:F:202:VAL:H	1.74	0.53
1:C:169:LYS:HE2	1:C:248:LYS:HE2	1.90	0.53
1:C:218:VAL:HG12	1:C:219:ASN:N	2.23	0.53
1:A:40:PHE:CE2	1:A:62:MSE:HE1	2.44	0.52
1:G:206:ILE:HD13	1:G:206:ILE:N	2.24	0.52
1:H:201:LEU:HG	1:H:206:ILE:HD11	1.90	0.52
1:C:4:LEU:O	1:C:8:ARG:HG3	2.08	0.52
1:F:88:ASN:HD21	1:F:135:PHE:N	2.00	0.52
1:I:230:ILE:HG22	1:I:244:VAL:HA	1.91	0.52
1:D:6:LYS:HA	1:D:9:ILE:HD12	1.92	0.52
1:F:200:LEU:O	1:F:200:LEU:HD23	2.10	0.52
1:G:190:ILE:O	1:G:193:GLU:HB3	2.10	0.52
1:I:251:ILE:O	1:I:254:GLU:HB2	2.09	0.52
1:B:4:LEU:O	1:B:7:THR:OG1	2.23	0.52
1:D:234:SER:O	1:D:235:LEU:HD13	2.09	0.52
1:D:88:ASN:HD21	1:D:135:PHE:N	2.02	0.52
1:E:24:PHE:CD1	1:E:27:MSE:CE	2.93	0.52
1:A:174:MSE:O	1:A:177:SER:HB3	2.10	0.52
1:C:95:TYR:CE2	1:C:97:ALA:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ARG:N	1:E:214:ARG:CD	2.71	0.52
1:G:231:GLU:CB	1:G:245:LEU:HD21	2.39	0.52
1:G:32:ARG:HD3	1:G:52:SER:OG	2.09	0.52
1:C:212:ILE:HG12	1:E:121:GLU:HG3	1.92	0.52
1:H:214:ARG:HA	1:H:217:ILE:HD12	1.92	0.52
1:I:128:LEU:N	1:I:128:LEU:HD12	2.25	0.52
1:I:130:ARG:HH22	1:I:139:ASP:CG	2.14	0.52
1:B:116:ILE:HD12	1:B:125:THR:N	2.24	0.52
1:H:132:GLN:HE21	1:H:132:GLN:N	2.08	0.52
1:B:136:ASN:O	1:B:139:ASP:HB2	2.10	0.51
1:D:225:GLU:OE2	1:D:232:SER:HB3	2.09	0.51
1:D:194:LEU:HD22	1:D:242:ILE:HD11	1.91	0.51
1:I:165:GLU:HG3	1:I:248:LYS:NZ	2.25	0.51
1:A:145:TYR:O	1:A:145:TYR:CD2	2.61	0.51
1:B:11:ASN:O	1:B:15:GLN:HG2	2.10	0.51
1:B:95:TYR:HH	1:B:98:PHE:HD1	1.56	0.51
1:E:3:LEU:HD12	1:E:3:LEU:O	2.09	0.51
1:E:40:PHE:HB2	1:E:127:ILE:HB	1.92	0.51
1:E:168:SER:O	1:E:171:VAL:HG12	2.10	0.51
1:F:45:ARG:HD3	1:F:45:ARG:H	1.76	0.51
1:I:176:ILE:HA	1:I:179:LEU:CD1	2.40	0.51
1:G:13:MSE:HE2	1:G:13:MSE:O	2.10	0.51
1:D:44:ARG:HG3	1:D:80:PHE:HE2	1.75	0.51
1:E:237:MSE:HE2	1:E:240:THR:HB	1.93	0.51
1:I:237:MSE:HE3	1:I:239:GLY:C	2.30	0.51
1:B:99:PRO:HB2	1:B:101:GLU:CD	2.31	0.51
1:B:230:ILE:HG22	1:B:244:VAL:HA	1.92	0.51
1:B:87:SER:HB3	1:B:140:LEU:HD21	1.92	0.51
1:E:247:ASN:H	1:E:247:ASN:HD22	1.53	0.51
1:H:61:ARG:NH1	1:H:72:PRO:HG2	2.25	0.51
1:C:11:ASN:O	1:C:14:LEU:HB3	2.10	0.51
1:C:174:MSE:CG	1:D:167:ARG:HG3	2.40	0.51
1:B:167:ARG:O	1:B:170:ALA:HB3	2.11	0.51
1:G:247:ASN:H	1:G:247:ASN:ND2	2.08	0.51
1:F:247:ASN:HD22	1:F:247:ASN:N	2.04	0.51
1:A:231:GLU:HG3	1:A:245:LEU:HD11	1.92	0.51
1:F:23:ASN:CG	1:F:26:GLU:HG3	2.32	0.51
1:H:12:SER:HA	1:H:15:GLN:HG3	1.93	0.51
1:A:203:ALA:HB3	1:A:237:MSE:HE1	1.92	0.50
1:B:3:LEU:HD13	1:B:138:ASP:HB3	1.93	0.50
1:G:24:PHE:CD1	1:G:27:MSE:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:ILE:HD11	1:I:220:ALA:HB1	1.93	0.50
1:I:29:GLU:O	1:I:32:ARG:HB3	2.11	0.50
1:I:57:ILE:HG12	1:I:131:LEU:HD13	1.93	0.50
1:A:14:LEU:HD23	1:A:15:GLN:NE2	2.24	0.50
1:C:188:GLU:O	1:C:192:GLU:CG	2.57	0.50
1:E:170:ALA:HB1	1:F:174:MSE:HE3	1.92	0.50
1:K:229:VAL:HG12	1:K:230:ILE:HG23	1.93	0.50
1:A:137:ASP:O	1:A:141:ILE:HG13	2.11	0.50
1:D:165:GLU:CG	1:D:248:LYS:HZ1	2.25	0.50
1:H:130:ARG:HD2	1:H:133:ASP:HB2	1.94	0.50
1:I:45:ARG:HH21	1:I:47:LYS:CE	2.21	0.50
1:K:206:ILE:O	1:K:210:VAL:HG23	2.12	0.50
1:B:164:GLU:O	1:B:168:SER:OG	2.29	0.50
1:H:203:ALA:HB3	1:H:237:MSE:SE	2.62	0.50
1:I:244:VAL:HG21	1:I:250:LEU:CD2	2.41	0.50
1:B:205:LYS:CG	1:B:205:LYS:CE	2.88	0.50
1:C:95:TYR:HE2	1:C:97:ALA:HB3	1.76	0.50
1:E:218:VAL:HG12	1:E:219:ASN:N	2.27	0.50
1:F:156:ARG:CD	1:F:160:GLU:OE2	2.60	0.50
1:H:45:ARG:HD3	1:H:45:ARG:H	1.76	0.50
1:I:8:ARG:O	1:I:11:ASN:HB2	2.12	0.50
1:A:217:ILE:O	1:A:221:LEU:HD22	2.12	0.50
1:A:79:LEU:HD11	1:A:125:THR:HG21	1.94	0.50
1:E:201:LEU:O	1:E:240:THR:HG23	2.12	0.50
1:H:149:VAL:HA	1:H:152:MSE:CE	2.42	0.50
1:F:251:ILE:O	1:F:254:GLU:HB2	2.11	0.50
1:A:204:SER:HA	1:A:214:ARG:HG3	1.93	0.50
1:C:168:SER:O	1:C:171:VAL:HG22	2.12	0.50
1:G:88:ASN:OD1	1:G:135:PHE:HB2	2.12	0.50
1:K:179:LEU:HD23	1:K:183:GLU:HB3	1.94	0.50
1:G:163:GLU:O	1:G:167:ARG:HB2	2.12	0.49
1:B:204:SER:O	1:B:207:ALA:HB3	2.12	0.49
1:C:65:MSE:HG3	1:C:71:PHE:CE1	2.47	0.49
1:D:173:GLN:NE2	1:D:176:ILE:HD12	2.28	0.49
1:E:217:ILE:O	1:E:221:LEU:HD22	2.12	0.49
1:C:213:THR:HA	1:C:214:ARG:HH12	1.77	0.49
1:C:59:ASN:ND2	1:C:62:MSE:HG2	2.27	0.49
1:D:168:SER:O	1:D:171:VAL:HG22	2.12	0.49
1:E:11:ASN:O	1:E:15:GLN:HG2	2.11	0.49
1:E:171:VAL:O	1:E:174:MSE:HB3	2.13	0.49
1:F:214:ARG:CD	1:F:214:ARG:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:HG2	1:A:102:ASN:OD1	2.11	0.49
1:B:145:TYR:O	1:B:149:VAL:HG23	2.12	0.49
1:I:83:PRO:HG2	1:I:84:GLU:HG2	1.94	0.49
1:C:89:LEU:HD12	1:C:113:ILE:HD11	1.94	0.49
1:C:203:ALA:HB3	1:C:237:MSE:CE	2.43	0.49
1:C:88:ASN:HD21	1:C:135:PHE:N	1.99	0.49
1:D:165:GLU:HG3	1:D:248:LYS:HZ1	1.77	0.49
1:G:145:TYR:O	1:G:148:THR:HB	2.12	0.49
1:A:95:TYR:HD2	1:A:97:ALA:H	1.60	0.49
1:B:38:ASN:HB2	1:B:129:SER:OG	2.12	0.49
1:C:115:PRO:HB3	1:C:122:ARG:CZ	2.42	0.49
1:G:172:VAL:O	1:G:176:ILE:HG13	2.11	0.49
1:I:6:LYS:HA	1:I:9:ILE:HD12	1.94	0.49
1:K:213:THR:O	1:K:216:VAL:CG1	2.60	0.49
1:K:252:GLU:HA	1:K:255:ASN:ND2	2.25	0.49
1:D:156:ARG:O	1:D:160:GLU:HG3	2.12	0.49
1:G:130:ARG:NH1	1:G:134:GLN:O	2.45	0.49
1:G:171:VAL:O	1:G:174:MSE:HG3	2.12	0.49
1:H:205:LYS:HE2	1:H:209:ARG:HH21	1.76	0.49
1:D:165:GLU:CG	1:D:248:LYS:NZ	2.76	0.49
1:H:95:TYR:HE1	1:H:103:ARG:NH1	2.11	0.49
1:E:115:PRO:HB3	1:E:122:ARG:CZ	2.43	0.49
1:F:88:ASN:ND2	1:F:135:PHE:H	2.02	0.49
1:I:229:VAL:HG12	1:I:230:ILE:HG23	1.95	0.49
1:K:213:THR:O	1:K:216:VAL:HG13	2.13	0.49
1:C:62:MSE:SE	1:C:65:MSE:HE2	2.63	0.48
1:C:78:ASN:HD21	1:C:99:PRO:HD3	1.78	0.48
1:D:237:MSE:HG3	1:D:238:LYS:N	2.28	0.48
1:I:4:LEU:HB3	1:I:5:GLN:OE1	2.13	0.48
1:C:214:ARG:NH1	1:C:214:ARG:H	2.12	0.48
1:E:216:VAL:O	1:E:217:ILE:C	2.52	0.48
1:I:231:GLU:HB2	1:I:245:LEU:CD1	2.43	0.48
1:C:231:GLU:HB2	1:C:245:LEU:HD21	1.94	0.48
1:E:88:ASN:HD21	1:E:135:PHE:H	1.60	0.48
1:F:169:LYS:HG3	1:F:248:LYS:HG2	1.93	0.48
1:F:255:ASN:N	1:F:255:ASN:HD22	2.12	0.48
1:A:214:ARG:HA	1:A:217:ILE:HD12	1.95	0.48
1:A:170:ALA:HB1	1:B:174:MSE:HE1	1.95	0.48
1:I:45:ARG:H	1:I:45:ARG:HD3	1.78	0.48
1:A:162:ILE:HD12	1:G:184:LEU:HD12	1.95	0.48
1:H:252:GLU:HA	1:H:252:GLU:OE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:MSE:SE	1:H:27:MSE:HG2	2.63	0.48
1:I:37:SER:HA	1:I:55:GLN:NE2	2.28	0.48
1:A:201:LEU:HD23	1:A:206:ILE:CD1	2.44	0.48
1:B:85:THR:HB	1:G:8:ARG:NH2	2.28	0.48
1:C:15:GLN:OE1	1:C:15:GLN:HA	2.14	0.48
1:D:252:GLU:O	1:D:255:ASN:HB2	2.13	0.48
1:E:238:LYS:CG	1:E:238:LYS:O	2.61	0.48
1:E:57:ILE:HG12	1:E:131:LEU:HD12	1.95	0.48
1:E:82:VAL:HG22	1:E:97:ALA:HB1	1.96	0.48
1:A:40:PHE:CZ	1:A:62:MSE:HE1	2.48	0.48
1:D:173:GLN:HG2	1:F:169:LYS:HB2	1.96	0.48
1:H:112:THR:HG1	1:H:135:PHE:HD2	1.60	0.48
1:A:194:LEU:HD22	1:A:242:ILE:CD1	2.43	0.48
1:D:164:GLU:HG2	1:D:167:ARG:HH22	1.79	0.48
1:B:31:LEU:HB3	1:B:35:ILE:HD12	1.95	0.48
1:F:145:TYR:O	1:F:149:VAL:HG23	2.14	0.48
1:I:2:ALA:HA	1:I:5:GLN:NE2	2.29	0.47
1:F:243:LYS:NZ	1:F:243:LYS:CD	2.73	0.47
1:B:153:GLU:OE2	1:B:153:GLU:HA	2.13	0.47
1:F:115:PRO:HB3	1:F:122:ARG:CZ	2.44	0.47
1:G:115:PRO:HB3	1:G:122:ARG:CZ	2.44	0.47
1:I:58:GLU:OE2	1:I:58:GLU:CA	2.50	0.47
1:B:40:PHE:HB2	1:B:127:ILE:HB	1.95	0.47
1:A:187:ILE:O	1:A:191:PHE:HD1	1.98	0.47
1:E:213:THR:CG2	1:E:214:ARG:CZ	2.92	0.47
1:E:190:ILE:CD1	1:E:221:LEU:HD11	2.44	0.47
1:E:20:LYS:N	1:E:20:LYS:CG	2.78	0.47
1:E:167:ARG:HD3	1:F:178:SER:OG	2.14	0.47
1:F:6:LYS:HB3	1:F:34:VAL:CG1	2.44	0.47
1:G:95:TYR:CE2	1:G:97:ALA:HB3	2.50	0.47
1:I:213:THR:HB	1:I:216:VAL:HG22	1.96	0.47
1:A:88:ASN:ND2	1:A:134:GLN:OE1	2.48	0.47
1:G:95:TYR:CD1	1:G:95:TYR:C	2.87	0.47
1:H:99:PRO:HG2	1:H:102:ASN:HD22	1.79	0.47
1:C:213:THR:HA	1:C:214:ARG:NH1	2.30	0.47
1:I:216:VAL:O	1:I:217:ILE:C	2.53	0.47
1:B:203:ALA:HB3	1:B:237:MSE:CE	2.44	0.47
1:B:28:ALA:HB1	1:B:52:SER:HB2	1.97	0.47
1:D:201:LEU:HD12	1:D:202:VAL:HG23	1.97	0.47
1:E:35:ILE:O	1:E:36:ASP:HB3	2.15	0.47
1:F:6:LYS:HB3	1:F:34:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:MSE:CE	1:H:170:ALA:HB1	2.45	0.47
1:H:122:ARG:NH2	1:H:125:THR:HG23	2.30	0.47
1:A:214:ARG:N	1:A:214:ARG:NH1	2.63	0.47
1:A:58:GLU:OE2	1:A:58:GLU:HA	2.15	0.47
1:C:174:MSE:HG2	1:D:167:ARG:HG3	1.97	0.47
1:F:243:LYS:HD3	1:F:245:LEU:CD2	2.45	0.47
1:K:255:ASN:C	1:K:256:LEU:HD12	2.36	0.47
1:K:56:GLN:NE2	1:K:56:GLN:HA	2.30	0.47
1:C:91:ILE:HD12	1:C:107:GLN:HA	1.97	0.46
1:D:158:LYS:O	1:D:161:GLU:HB3	2.15	0.46
1:I:183:GLU:O	1:I:186:ALA:HB3	2.15	0.46
1:K:176:ILE:O	1:K:179:LEU:HD12	2.15	0.46
1:B:229:VAL:HG11	1:B:249:PHE:CD1	2.50	0.46
1:C:204:SER:HA	1:C:214:ARG:HG3	1.97	0.46
1:E:230:ILE:HG22	1:E:244:VAL:HA	1.97	0.46
1:E:251:ILE:O	1:E:254:GLU:HB2	2.15	0.46
1:G:174:MSE:HG2	1:H:174:MSE:SE	2.65	0.46
1:I:79:LEU:HA	1:I:79:LEU:HD23	1.74	0.46
1:B:179:LEU:CD2	1:B:183:GLU:HB3	2.44	0.46
1:E:11:ASN:ND2	2:E:301:SO4:O4	2.48	0.46
1:G:32:ARG:HD2	1:G:53:ILE:C	2.36	0.46
1:H:230:ILE:HG22	1:H:244:VAL:HA	1.97	0.46
1:I:75:TYR:O	1:I:78:ASN:HB2	2.15	0.46
1:A:121:GLU:HG2	1:A:122:ARG:N	2.30	0.46
1:B:27:MSE:HE1	1:B:150:VAL:HA	1.97	0.46
1:B:27:MSE:HE3	1:B:150:VAL:HG22	1.97	0.46
1:E:4:LEU:O	1:E:7:THR:OG1	2.26	0.46
1:H:249:PHE:CD2	1:H:249:PHE:C	2.88	0.46
1:I:87:SER:HA	1:I:112:THR:HG23	1.97	0.46
1:D:202:VAL:O	1:D:206:ILE:HG12	2.15	0.46
1:C:101:GLU:CD	1:C:101:GLU:H	2.18	0.46
1:C:85:THR:HG23	1:C:114:VAL:HG22	1.98	0.46
1:G:251:ILE:HD13	1:G:251:ILE:HA	1.78	0.46
1:H:172:VAL:HG12	1:H:176:ILE:CD1	2.43	0.46
1:A:200:LEU:HD23	1:A:200:LEU:O	2.16	0.46
1:A:169:LYS:HG3	1:A:248:LYS:HG2	1.96	0.46
1:A:29:GLU:O	1:A:32:ARG:HB3	2.16	0.46
1:C:165:GLU:O	1:C:169:LYS:HG3	2.16	0.46
1:D:205:LYS:HD3	1:D:209:ARG:HH22	1.81	0.46
1:D:237:MSE:HG3	1:D:238:LYS:H	1.80	0.46
1:G:6:LYS:HA	1:G:9:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:MSE:O	1:H:31:LEU:HD23	2.16	0.46
1:G:4:LEU:CD1	1:G:8:ARG:HD2	2.46	0.46
1:H:218:VAL:HG13	1:H:219:ASN:N	2.31	0.46
1:I:148:THR:HG22	1:I:152:MSE:HE2	1.97	0.46
1:A:6:LYS:HD2	1:A:34:VAL:HG13	1.97	0.45
1:E:190:ILE:O	1:E:193:GLU:HB3	2.16	0.45
1:A:2:ALA:O	1:A:6:LYS:HG2	2.16	0.45
1:B:198:GLU:CG	1:B:243:LYS:HG3	2.41	0.45
1:G:213:THR:O	1:G:216:VAL:HG13	2.16	0.45
1:H:187:ILE:HD12	1:H:224:LEU:HD12	1.98	0.45
1:A:114:VAL:HA	1:A:115:PRO:HD2	1.83	0.45
1:B:90:ASP:HB3	1:B:110:LEU:HD23	1.98	0.45
1:C:149:VAL:HA	1:C:152:MSE:HE3	1.97	0.45
1:D:38:ASN:ND2	1:D:55:GLN:O	2.47	0.45
1:E:6:LYS:HB3	1:E:34:VAL:HG13	1.97	0.45
1:H:216:VAL:O	1:H:217:ILE:C	2.54	0.45
1:B:37:SER:HB2	1:B:130:ARG:HD2	1.99	0.45
1:B:145:TYR:O	1:B:145:TYR:HD2	1.99	0.45
1:B:34:VAL:HG12	1:B:35:ILE:N	2.31	0.45
1:E:233:ARG:NE	1:H:233:ARG:HH11	2.15	0.45
1:E:4:LEU:HG	1:E:8:ARG:HD2	1.98	0.45
1:E:95:TYR:OH	1:E:98:PHE:HB2	2.15	0.45
1:A:40:PHE:N	1:A:40:PHE:CD2	2.85	0.45
1:B:137:ASP:HA	1:B:140:LEU:HD12	1.99	0.45
1:F:115:PRO:HB2	1:F:117:ILE:CD1	2.46	0.45
1:F:172:VAL:HG12	1:F:176:ILE:HD12	1.98	0.45
1:F:183:GLU:O	1:F:186:ALA:HB3	2.17	0.45
1:F:48:LEU:HD23	1:F:69:ARG:HG3	1.99	0.45
1:G:250:LEU:CD2	1:G:250:LEU:H	2.27	0.45
1:G:62:MSE:O	1:G:65:MSE:HB3	2.16	0.45
1:G:6:LYS:HB3	1:G:34:VAL:CG1	2.46	0.45
1:H:177:SER:OG	1:H:178:SER:N	2.49	0.45
1:H:31:LEU:HD12	1:H:35:ILE:HD11	1.97	0.45
1:K:232:SER:CB	1:K:242:ILE:HG22	2.45	0.45
1:A:38:ASN:O	1:A:128:LEU:HA	2.17	0.45
1:I:249:PHE:CE1	1:I:253:LEU:HD13	2.52	0.45
1:A:150:VAL:HG12	1:A:154:ILE:CD1	2.44	0.45
1:B:24:PHE:HD1	1:B:27:MSE:CE	2.16	0.45
1:E:23:ASN:OD1	1:E:23:ASN:C	2.55	0.45
1:H:202:VAL:O	1:H:206:ILE:HG12	2.17	0.45
1:A:186:ALA:O	1:A:187:ILE:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLU:O	1:B:256:LEU:HD13	2.17	0.45
1:C:213:THR:HG23	1:C:214:ARG:NH2	2.31	0.45
1:D:203:ALA:HB3	1:D:237:MSE:CE	2.43	0.45
1:D:25:LYS:O	1:D:29:GLU:HG3	2.17	0.45
1:E:206:ILE:HD13	1:E:209:ARG:HH11	1.82	0.45
1:I:203:ALA:HB3	1:I:237:MSE:SE	2.67	0.45
1:I:5:GLN:N	1:I:5:GLN:OE1	2.49	0.45
1:A:167:ARG:HG3	1:B:174:MSE:HG2	1.97	0.45
1:B:225:GLU:HG3	1:B:230:ILE:O	2.17	0.45
1:B:95:TYR:C	1:B:95:TYR:CD1	2.90	0.45
1:D:206:ILE:HD13	1:D:206:ILE:N	2.32	0.45
1:D:218:VAL:CG1	1:D:219:ASN:N	2.69	0.45
1:G:88:ASN:HD21	1:G:134:GLN:HA	1.82	0.45
1:B:95:TYR:CG	1:B:96:THR:N	2.85	0.44
1:H:88:ASN:ND2	1:H:135:PHE:H	2.04	0.44
1:I:183:GLU:O	1:I:187:ILE:HG12	2.17	0.44
1:D:204:SER:HA	1:D:214:ARG:HG3	2.00	0.44
1:G:91:ILE:HD13	1:G:107:GLN:HA	1.99	0.44
1:H:182:SER:HA	1:H:185:GLU:HB2	2.00	0.44
1:K:137:ASP:HA	1:K:140:LEU:HD12	2.00	0.44
1:D:179:LEU:HD13	1:D:184:LEU:HA	2.00	0.44
1:D:241:TYR:CG	1:D:242:ILE:N	2.85	0.44
1:A:121:GLU:HG3	1:G:212:ILE:HG12	1.98	0.44
1:H:39:ILE:CD1	1:H:128:LEU:HD12	2.46	0.44
1:K:214:ARG:HD3	1:K:214:ARG:H	1.82	0.44
1:E:162:ILE:HG13	1:E:163:GLU:N	2.31	0.44
1:F:251:ILE:O	1:F:255:ASN:ND2	2.51	0.44
1:H:86:SER:HB3	1:H:89:LEU:HD11	1.99	0.44
1:A:241:TYR:CD2	1:A:241:TYR:C	2.91	0.44
1:B:95:TYR:OH	1:B:98:PHE:CB	2.66	0.44
1:D:214:ARG:H	1:D:214:ARG:CD	2.30	0.44
1:D:8:ARG:NH1	1:E:144:GLU:OE2	2.50	0.44
1:H:23:ASN:C	1:H:23:ASN:OD1	2.55	0.44
1:I:70:GLN:HG3	1:I:71:PHE:N	2.32	0.44
1:K:121:GLU:HG2	1:K:122:ARG:N	2.32	0.44
1:K:8:ARG:O	1:K:11:ASN:HB2	2.18	0.44
1:E:250:LEU:HG	1:E:251:ILE:H	1.83	0.44
1:F:237:MSE:HG3	1:F:238:LYS:H	1.83	0.44
1:G:174:MSE:HE2	1:H:170:ALA:HB1	1.99	0.44
1:K:216:VAL:O	1:K:217:ILE:C	2.56	0.44
1:H:51:TYR:HE2	1:H:69:ARG:HH21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HA	1:B:19:GLY:HA3	1.99	0.44
1:C:78:ASN:HD21	1:C:99:PRO:CD	2.31	0.44
1:D:217:ILE:O	1:D:220:ALA:HB3	2.18	0.44
1:B:99:PRO:HB2	1:B:101:GLU:OE2	2.17	0.43
1:D:169:LYS:HD2	1:F:173:GLN:NE2	2.33	0.43
1:D:213:THR:HG22	1:D:215:SER:H	1.83	0.43
1:D:214:ARG:HA	1:D:217:ILE:HD12	1.99	0.43
1:E:148:THR:O	1:E:152:MSE:HE3	2.18	0.43
1:A:114:VAL:HG23	1:A:126:LEU:HB3	2.00	0.43
1:A:179:LEU:HD22	1:A:183:GLU:HB3	1.99	0.43
1:A:6:LYS:HA	1:A:9:ILE:HD12	2.00	0.43
1:D:23:ASN:OD1	1:D:23:ASN:C	2.56	0.43
1:E:11:ASN:OD1	1:E:145:TYR:OH	2.31	0.43
1:F:17:ALA:O	1:F:18:ALA:C	2.57	0.43
1:K:250:LEU:H	1:K:250:LEU:CD2	2.13	0.43
1:C:38:ASN:OD1	1:C:55:GLN:HG2	2.19	0.43
1:E:95:TYR:CG	1:E:96:THR:N	2.84	0.43
1:H:12:SER:HA	1:H:15:GLN:CG	2.47	0.43
1:H:218:VAL:CG1	1:H:219:ASN:N	2.81	0.43
1:I:17:ALA:O	1:I:18:ALA:C	2.56	0.43
1:I:234:SER:O	1:I:235:LEU:HD13	2.19	0.43
1:K:14:LEU:HD23	1:K:15:GLN:NE2	2.34	0.43
1:F:216:VAL:O	1:F:217:ILE:C	2.56	0.43
1:H:61:ARG:HH12	1:H:72:PRO:HG2	1.83	0.43
1:K:61:ARG:O	1:K:61:ARG:HD3	2.18	0.43
1:C:187:ILE:HD11	1:C:220:ALA:HB1	2.00	0.43
1:K:65:MSE:HG3	1:K:71:PHE:CZ	2.53	0.43
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.68	0.43
1:C:255:ASN:C	1:C:256:LEU:HD12	2.38	0.43
1:D:65:MSE:C	1:D:65:MSE:SE	3.07	0.43
1:H:210:VAL:HG13	1:H:212:ILE:HG13	2.00	0.43
1:C:216:VAL:O	1:C:217:ILE:C	2.57	0.43
1:C:87:SER:O	1:C:89:LEU:HD23	2.19	0.43
1:D:130:ARG:HD2	1:D:133:ASP:O	2.19	0.43
1:D:47:LYS:HG2	1:D:48:LEU:N	2.33	0.43
1:F:213:THR:HG22	1:F:215:SER:N	2.34	0.43
1:G:100:VAL:HA	1:G:103:ARG:HE	1.84	0.43
1:G:252:GLU:OE1	1:G:252:GLU:HA	2.19	0.43
1:K:78:ASN:CB	1:K:98:PHE:CE2	2.97	0.43
1:A:136:ASN:OD1	1:A:139:ASP:OD1	2.36	0.43
1:B:150:VAL:O	1:B:154:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:HE2	2:B:302:SO4:O2	2.19	0.43
1:C:238:LYS:HD3	1:C:238:LYS:HA	1.87	0.43
1:E:237:MSE:HA	1:E:239:GLY:O	2.17	0.43
1:H:187:ILE:HD12	1:H:224:LEU:CD1	2.49	0.43
1:H:247:ASN:N	1:H:247:ASN:ND2	2.63	0.43
1:I:37:SER:HA	1:I:55:GLN:HE21	1.83	0.43
1:A:252:GLU:O	1:A:256:LEU:HD13	2.19	0.43
1:B:82:VAL:HA	1:B:83:PRO:HD3	1.84	0.43
1:F:153:GLU:OE2	1:F:153:GLU:HA	2.18	0.43
1:G:230:ILE:HG22	1:G:244:VAL:HA	2.01	0.43
1:D:35:ILE:HD13	1:D:128:LEU:HD21	2.00	0.43
1:D:234:SER:C	1:D:235:LEU:HD13	2.39	0.43
1:F:232:SER:HB2	1:F:242:ILE:CG2	2.49	0.43
1:G:255:ASN:HD22	1:G:255:ASN:N	2.17	0.43
1:H:201:LEU:HG	1:H:206:ILE:CD1	2.49	0.43
1:A:256:LEU:HD12	1:A:256:LEU:N	2.34	0.42
1:K:123:LEU:HA	1:K:123:LEU:HD23	1.81	0.42
1:I:203:ALA:H	1:I:237:MSE:CE	2.28	0.42
1:A:15:GLN:OE1	1:H:117:ILE:HG22	2.19	0.42
1:A:156:ARG:O	1:A:160:GLU:HG3	2.19	0.42
1:A:17:ALA:O	1:A:18:ALA:C	2.57	0.42
1:E:212:ILE:CG2	1:E:216:VAL:HG22	2.49	0.42
1:F:4:LEU:O	1:F:8:ARG:HG3	2.19	0.42
1:H:11:ASN:OD1	1:H:145:TYR:OH	2.09	0.42
1:H:150:VAL:HG12	1:H:154:ILE:HD11	2.02	0.42
1:I:148:THR:O	1:I:152:MSE:HE3	2.19	0.42
1:A:19:GLY:O	1:B:219:ASN:HB2	2.20	0.42
1:A:94:GLU:HG3	1:A:94:GLU:O	2.19	0.42
1:B:78:ASN:HA	1:B:78:ASN:HD22	1.63	0.42
1:D:101:GLU:CD	1:D:101:GLU:H	2.23	0.42
1:D:229:VAL:HG11	1:D:249:PHE:CD1	2.54	0.42
1:E:206:ILE:HD13	1:E:209:ARG:HD3	2.01	0.42
1:G:156:ARG:HD2	1:G:160:GLU:OE1	2.18	0.42
1:G:58:GLU:OE2	1:G:58:GLU:HA	2.19	0.42
1:K:38:ASN:O	1:K:128:LEU:HA	2.19	0.42
1:A:11:ASN:O	1:A:15:GLN:HG2	2.19	0.42
1:B:27:MSE:CE	1:B:150:VAL:HG22	2.50	0.42
1:C:22:VAL:HG13	1:C:27:MSE:CE	2.49	0.42
1:C:27:MSE:HE1	1:C:153:GLU:OE2	2.20	0.42
1:D:148:THR:HG22	1:D:152:MSE:HE3	2.01	0.42
1:D:42:VAL:HG21	1:D:127:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.72	0.42
1:K:115:PRO:HB3	1:K:122:ARG:CZ	2.49	0.42
1:K:95:TYR:OH	1:K:98:PHE:HB2	2.19	0.42
1:B:145:TYR:CD2	1:B:145:TYR:O	2.73	0.42
1:D:87:SER:HA	1:D:112:THR:OG1	2.18	0.42
1:F:230:ILE:HG22	1:F:244:VAL:HA	2.00	0.42
1:F:32:ARG:HD2	1:F:54:ASN:HB3	2.01	0.42
1:G:197:ASN:HD22	1:G:197:ASN:H	1.67	0.42
1:K:95:TYR:CD1	1:K:95:TYR:N	2.87	0.42
1:B:171:VAL:O	1:B:174:MSE:HB3	2.20	0.42
1:C:19:GLY:N	1:D:216:VAL:HG12	2.35	0.42
1:E:229:VAL:CG1	1:E:249:PHE:CD1	2.99	0.42
1:I:31:LEU:HB3	1:I:35:ILE:HD12	2.01	0.42
1:A:217:ILE:O	1:A:221:LEU:CD2	2.68	0.42
1:B:237:MSE:HG3	1:B:238:LYS:H	1.85	0.42
1:B:95:TYR:OH	1:B:98:PHE:N	2.52	0.42
1:C:85:THR:OG1	1:C:114:VAL:HG13	2.20	0.42
1:C:84:GLU:HA	1:C:115:PRO:HG2	2.01	0.42
1:F:59:ASN:HB3	1:F:62:MSE:HB2	2.01	0.42
1:I:4:LEU:HD21	1:I:8:ARG:NH1	2.34	0.42
1:D:38:ASN:O	1:D:128:LEU:HA	2.19	0.42
1:F:213:THR:HB	1:F:216:VAL:HG23	2.02	0.42
1:H:132:GLN:H	1:H:132:GLN:HE21	1.67	0.42
1:H:149:VAL:HA	1:H:152:MSE:HE2	2.02	0.42
1:H:215:SER:O	1:H:218:VAL:HG12	2.20	0.42
1:I:202:VAL:HA	1:I:237:MSE:CE	2.48	0.42
1:I:38:ASN:HD21	1:I:55:GLN:HG3	1.85	0.42
1:K:185:GLU:O	1:K:189:HIS:HD2	2.03	0.42
1:A:216:VAL:O	1:A:217:ILE:C	2.57	0.42
1:A:8:ARG:O	1:A:11:ASN:HB2	2.20	0.42
1:D:248:LYS:HA	1:D:248:LYS:HD2	1.74	0.42
1:I:201:LEU:HG	1:I:202:VAL:HG23	2.02	0.42
1:I:8:ARG:HA	1:I:11:ASN:ND2	2.28	0.42
1:B:35:ILE:O	1:B:36:ASP:HB3	2.20	0.41
1:E:250:LEU:CD2	1:E:250:LEU:H	2.13	0.41
1:F:43:SER:HB2	1:F:45:ARG:NH1	2.35	0.41
1:G:169:LYS:HG3	1:G:248:LYS:HG2	2.00	0.41
1:H:155:LEU:HA	1:H:155:LEU:HD23	1.74	0.41
1:I:41:VAL:HG22	1:I:126:LEU:CD1	2.50	0.41
1:A:95:TYR:CD2	1:A:97:ALA:N	2.88	0.41
1:G:204:SER:O	1:G:208:ASP:OD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:LYS:HG2	1:I:48:LEU:N	2.34	0.41
1:B:190:ILE:O	1:B:193:GLU:HB2	2.19	0.41
1:C:144:GLU:OE2	1:F:8:ARG:NE	2.53	0.41
1:K:206:ILE:HG22	1:K:210:VAL:CG2	2.50	0.41
1:A:103:ARG:C	1:A:105:LEU:H	2.21	0.41
1:B:37:SER:OG	1:B:38:ASN:N	2.53	0.41
1:B:78:ASN:HB3	1:B:98:PHE:CE2	2.55	0.41
1:C:222:ARG:HB2	1:C:222:ARG:CZ	2.50	0.41
1:E:27:MSE:SE	1:E:153:GLU:HG3	2.70	0.41
1:F:103:ARG:C	1:F:105:LEU:H	2.23	0.41
1:G:26:GLU:O	1:G:29:GLU:HB2	2.21	0.41
1:H:24:PHE:CD1	1:H:27:MSE:CE	3.03	0.41
1:K:176:ILE:HA	1:K:179:LEU:HD13	2.00	0.41
1:K:82:VAL:HA	1:K:83:PRO:HD3	1.85	0.41
1:B:103:ARG:C	1:B:105:LEU:H	2.23	0.41
1:E:45:ARG:HD3	1:E:45:ARG:H	1.86	0.41
1:F:218:VAL:O	1:F:222:ARG:HG3	2.20	0.41
1:H:214:ARG:H	1:H:214:ARG:HG3	1.60	0.41
1:K:172:VAL:HG12	1:K:176:ILE:CD1	2.51	0.41
1:K:190:ILE:HG22	1:K:191:PHE:N	2.35	0.41
1:K:45:ARG:H	1:K:45:ARG:HD3	1.85	0.41
1:A:103:ARG:C	1:A:105:LEU:N	2.74	0.41
1:C:63:LYS:HA	1:C:66:LEU:HD12	2.02	0.41
1:E:14:LEU:HD12	1:E:149:VAL:HG13	2.02	0.41
1:G:249:PHE:CD2	1:G:249:PHE:C	2.94	0.41
1:I:205:LYS:HG2	1:I:209:ARG:NH1	2.32	0.41
1:B:200:LEU:HB2	1:B:240:THR:O	2.21	0.41
1:F:243:LYS:HD3	1:F:245:LEU:HD23	2.01	0.41
1:G:231:GLU:OE2	1:G:243:LYS:HD3	2.21	0.41
1:H:10:ILE:HA	1:H:13:MSE:HE3	2.01	0.41
1:I:250:LEU:H	1:I:250:LEU:CD2	2.18	0.41
1:C:44:ARG:HH21	1:C:45:ARG:HG3	1.86	0.41
1:D:212:ILE:CG2	1:D:216:VAL:HG22	2.51	0.41
1:F:165:GLU:HG2	1:F:248:LYS:NZ	2.36	0.41
1:G:12:SER:CA	1:G:15:GLN:HG3	2.33	0.41
1:B:153:GLU:CD	1:B:156:ARG:HH21	2.23	0.41
1:C:65:MSE:HG3	1:C:71:PHE:CZ	2.56	0.41
1:F:24:PHE:HA	1:F:27:MSE:HE2	2.02	0.41
1:I:88:ASN:HD22	1:I:110:LEU:HD22	1.86	0.41
1:K:162:ILE:HG12	1:K:162:ILE:H	1.56	0.41
1:K:174:MSE:HE2	1:K:174:MSE:HB2	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:ILE:HG22	1:K:191:PHE:CD1	2.56	0.41
1:B:101:GLU:HG2	1:B:102:ASN:OD1	2.21	0.41
1:D:251:ILE:O	1:D:254:GLU:HB2	2.21	0.41
1:F:219:ASN:HA	1:F:222:ARG:HG3	2.03	0.41
1:G:205:LYS:HG2	1:G:209:ARG:NH1	2.36	0.41
1:I:78:ASN:CB	1:I:98:PHE:CE2	3.01	0.41
1:B:206:ILE:HG22	1:B:210:VAL:HG23	2.03	0.41
1:D:200:LEU:HB2	1:D:240:THR:O	2.21	0.41
1:D:63:LYS:HE2	1:D:67:GLU:HG3	2.03	0.41
1:G:206:ILE:HG22	1:G:210:VAL:CG2	2.51	0.41
1:K:32:ARG:CD	1:K:54:ASN:HB3	2.51	0.41
1:K:95:TYR:HE2	1:K:97:ALA:HB3	1.86	0.41
1:H:153:GLU:O	1:H:157:GLU:HB2	2.21	0.40
1:H:48:LEU:HD13	1:H:65:MSE:SE	2.71	0.40
1:C:38:ASN:HB2	1:C:129:SER:OG	2.22	0.40
1:E:42:VAL:HG23	1:E:125:THR:O	2.21	0.40
1:E:170:ALA:HB1	1:F:174:MSE:CE	2.51	0.40
1:D:169:LYS:CB	1:F:173:GLN:HE21	2.27	0.40
1:F:183:GLU:HG2	1:F:220:ALA:HB2	2.04	0.40
1:G:132:GLN:NE2	1:G:133:ASP:OD1	2.47	0.40
1:H:135:PHE:HA	1:H:139:ASP:OD1	2.20	0.40
1:H:32:ARG:N	1:H:39:ILE:HG13	2.36	0.40
1:I:70:GLN:HE21	1:I:71:PHE:H	1.69	0.40
1:K:160:GLU:O	1:K:164:GLU:HG2	2.21	0.40
1:K:79:LEU:HA	1:K:79:LEU:HD23	1.79	0.40
1:C:225:GLU:HB2	1:C:230:ILE:CD1	2.50	0.40
1:E:187:ILE:HD12	1:E:224:LEU:CD1	2.52	0.40
1:F:208:ASP:OD2	1:F:208:ASP:N	2.53	0.40
1:H:250:LEU:HD22	1:H:250:LEU:HA	1.69	0.40
1:H:78:ASN:HB3	1:H:98:PHE:CZ	2.57	0.40
1:I:38:ASN:O	1:I:128:LEU:HA	2.21	0.40
1:B:110:LEU:HD13	1:B:134:GLN:OE1	2.22	0.40
1:D:234:SER:OG	1:D:234:SER:CA	2.58	0.40
1:K:203:ALA:HB3	1:K:237:MSE:SE	2.71	0.40
1:K:237:MSE:HA	1:K:239:GLY:O	2.21	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	253/263 (96%)	229 (90%)	19 (8%)	5 (2%)	9	41
1	B	253/263 (96%)	229 (90%)	22 (9%)	2 (1%)	24	66
1	C	253/263 (96%)	231 (91%)	18 (7%)	4 (2%)	12	48
1	D	253/263 (96%)	229 (90%)	20 (8%)	4 (2%)	12	48
1	E	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	16	56
1	F	253/263 (96%)	228 (90%)	22 (9%)	3 (1%)	16	56
1	G	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	16	56
1	H	253/263 (96%)	235 (93%)	16 (6%)	2 (1%)	24	66
1	I	253/263 (96%)	227 (90%)	23 (9%)	3 (1%)	16	56
1	K	253/263 (96%)	228 (90%)	23 (9%)	2 (1%)	24	66
All	All	2530/2630 (96%)	2294 (91%)	205 (8%)	31 (1%)	16	56

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	237	MSE
1	B	18	ALA
1	B	237	MSE
1	C	18	ALA
1	C	237	MSE
1	D	18	ALA
1	D	237	MSE
1	E	18	ALA
1	E	237	MSE
1	F	18	ALA
1	F	237	MSE
1	G	18	ALA
1	G	237	MSE

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Mol	Chain	Res	Type
1	H	18	ALA
1	H	237	MSE
1	I	18	ALA
1	I	237	MSE
1	K	18	ALA
1	K	237	MSE
1	A	74	GLU
1	E	74	GLU
1	A	58	GLU
1	D	74	GLU
1	G	74	GLU
1	D	218	VAL
1	C	58	GLU
1	A	218	VAL
1	C	151	GLY
1	I	151	GLY
1	F	218	VAL

### 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	221/222 (100%)	187 (85%)	34 (15%)	3	16
1	B	221/222 (100%)	184 (83%)	37 (17%)	3	13
1	C	221/222 (100%)	185 (84%)	36 (16%)	3	14
1	D	221/222 (100%)	192 (87%)	29 (13%)	5	22
1	E	221/222 (100%)	177 (80%)	44 (20%)	1	8
1	F	221/222 (100%)	191 (86%)	30 (14%)	5	20
1	G	221/222 (100%)	182 (82%)	39 (18%)	2	12
1	H	221/222 (100%)	179 (81%)	42 (19%)	2	10
1	I	221/222 (100%)	178 (80%)	43 (20%)	2	9
1	K	221/222 (100%)	184 (83%)	37 (17%)	3	13
All	All	2210/2220 (100%)	1839 (83%)	371 (17%)	2	13

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	40	PHE
1	A	45	ARG
1	A	52	SER
1	A	69	ARG
1	A	79	LEU
1	A	93	SER
1	A	94	GLU
1	A	100	VAL
1	A	114	VAL
1	A	122	ARG
1	A	132	GLN
1	A	136	ASN
1	A	145	TYR
1	A	152	MSE
1	A	162	ILE
1	A	163	GLU
1	A	165	GLU
1	A	171	VAL
1	A	185	GLU
1	A	193	GLU
1	A	200	LEU
1	A	205	LYS
1	A	206	ILE
1	A	208	ASP
1	A	213	THR
1	A	214	ARG
1	A	234	SER
1	A	235	LEU
1	A	238	LYS
1	A	240	THR
1	A	247	ASN
1	A	248	LYS
1	A	254	GLU
1	B	12	SER
1	B	31	LEU
1	B	45	ARG
1	B	69	ARG
1	B	76	THR
1	B	78	ASN
1	B	84	GLU
1	B	94	GLU

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Mol	Chain	Res	Type
1	B	95	TYR
1	B	96	THR
1	B	105	LEU
1	B	130	ARG
1	B	132	GLN
1	B	137	ASP
1	B	145	TYR
1	B	148	THR
1	B	152	MSE
1	B	162	ILE
1	B	165	GLU
1	B	168	SER
1	B	171	VAL
1	B	174	MSE
1	B	184	LEU
1	B	208	ASP
1	B	210	VAL
1	B	214	ARG
1	B	216	VAL
1	B	221	LEU
1	B	226	SER
1	B	235	LEU
1	B	238	LYS
1	B	240	THR
1	B	245	LEU
1	B	247	ASN
1	B	248	LYS
1	B	251	ILE
1	B	256	LEU
1	C	14	LEU
1	C	30	THR
1	C	37	SER
1	C	45	ARG
1	C	52	SER
1	C	65	MSE
1	C	69	ARG
1	C	84	GLU
1	C	86	SER
1	C	87	SER
1	C	89	LEU
1	C	93	SER
1	C	95	TYR

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Mol	Chain	Res	Type
1	C	100	VAL
1	C	101	GLU
1	C	111	THR
1	C	113	ILE
1	C	125	THR
1	C	132	GLN
1	C	162	ILE
1	C	164	GLU
1	C	188	GLU
1	C	201	LEU
1	C	204	SER
1	C	206	ILE
1	C	210	VAL
1	C	214	ARG
1	C	221	LEU
1	C	224	LEU
1	C	233	ARG
1	C	235	LEU
1	C	238	LYS
1	C	242	ILE
1	C	245	LEU
1	C	247	ASN
1	C	250	LEU
1	D	8	ARG
1	D	10	ILE
1	D	33	ASP
1	D	45	ARG
1	D	52	SER
1	D	56	GLN
1	D	69	ARG
1	D	77	LYS
1	D	78	ASN
1	D	112	THR
1	D	132	GLN
1	D	133	ASP
1	D	138	ASP
1	D	152	MSE
1	D	156	ARG
1	D	164	GLU
1	D	173	GLN
1	D	188	GLU
1	D	201	LEU

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Mol	Chain	Res	Type
1	D	208	ASP
1	D	214	ARG
1	D	216	VAL
1	D	230	ILE
1	D	231	GLU
1	D	235	LEU
1	D	238	LYS
1	D	247	ASN
1	D	248	LYS
1	D	250	LEU
1	E	3	LEU
1	E	6	LYS
1	E	10	ILE
1	E	13	MSE
1	E	14	LEU
1	E	26	GLU
1	E	42	VAL
1	E	43	SER
1	E	45	ARG
1	E	60	ASP
1	E	61	ARG
1	E	69	ARG
1	E	78	ASN
1	E	85	THR
1	E	87	SER
1	E	95	TYR
1	E	101	GLU
1	E	103	ARG
1	E	114	VAL
1	E	125	THR
1	E	133	ASP
1	E	141	ILE
1	E	148	THR
1	E	152	MSE
1	E	154	ILE
1	E	165	GLU
1	E	184	LEU
1	E	185	GLU
1	E	192	GLU
1	E	200	LEU
1	E	201	LEU
1	E	214	ARG

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Mol	Chain	Res	Type
1	E	219	ASN
1	E	221	LEU
1	E	222	ARG
1	E	225	GLU
1	E	234	SER
1	E	235	LEU
1	E	238	LYS
1	E	240	THR
1	E	242	ILE
1	E	247	ASN
1	E	248	LYS
1	E	250	LEU
1	F	20	LYS
1	F	37	SER
1	F	41	VAL
1	F	45	ARG
1	F	52	SER
1	F	56	GLN
1	F	77	LYS
1	F	96	THR
1	F	148	THR
1	F	156	ARG
1	F	164	GLU
1	F	165	GLU
1	F	171	VAL
1	F	173	GLN
1	F	174	MSE
1	F	188	GLU
1	F	200	LEU
1	F	202	VAL
1	F	206	ILE
1	F	214	ARG
1	F	221	LEU
1	F	231	GLU
1	F	232	SER
1	F	235	LEU
1	F	240	THR
1	F	242	ILE
1	F	244	VAL
1	F	247	ASN
1	F	248	LYS
1	F	256	LEU

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Mol	Chain	Res	Type
1	G	10	ILE
1	G	13	MSE
1	G	14	LEU
1	G	15	GLN
1	G	42	VAL
1	G	43	SER
1	G	45	ARG
1	G	47	LYS
1	G	69	ARG
1	G	95	TYR
1	G	100	VAL
1	G	101	GLU
1	G	103	ARG
1	G	111	THR
1	G	125	THR
1	G	132	GLN
1	G	154	ILE
1	G	155	LEU
1	G	164	GLU
1	G	165	GLU
1	G	167	ARG
1	G	174	MSE
1	G	177	SER
1	G	194	LEU
1	G	200	LEU
1	G	204	SER
1	G	206	ILE
1	G	208	ASP
1	G	214	ARG
1	G	216	VAL
1	G	221	LEU
1	G	238	LYS
1	G	240	THR
1	G	242	ILE
1	G	245	LEU
1	G	247	ASN
1	G	250	LEU
1	G	251	ILE
1	G	256	LEU
1	H	7	THR
1	H	8	ARG
1	H	13	MSE

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Mol	Chain	Res	Type
1	H	14	LEU
1	H	15	GLN
1	H	30	THR
1	H	35	ILE
1	H	41	VAL
1	H	42	VAL
1	H	45	ARG
1	H	56	GLN
1	H	66	LEU
1	H	69	ARG
1	H	78	ASN
1	H	86	SER
1	H	94	GLU
1	H	95	TYR
1	H	101	GLU
1	H	103	ARG
1	H	125	THR
1	H	128	LEU
1	H	132	GLN
1	H	145	TYR
1	H	157	GLU
1	H	163	GLU
1	H	164	GLU
1	H	165	GLU
1	H	179	LEU
1	H	192	GLU
1	H	201	LEU
1	H	204	SER
1	H	206	ILE
1	H	214	ARG
1	H	216	VAL
1	H	221	LEU
1	H	235	LEU
1	H	238	LYS
1	H	242	ILE
1	H	245	LEU
1	H	247	ASN
1	H	250	LEU
1	H	256	LEU
1	I	5	GLN
1	I	7	THR
1	I	10	ILE

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Mol	Chain	Res	Type
1	I	13	MSE
1	I	14	LEU
1	I	15	GLN
1	I	26	GLU
1	I	37	SER
1	I	45	ARG
1	I	56	GLN
1	I	58	GLU
1	I	60	ASP
1	I	69	ARG
1	I	74	GLU
1	I	93	SER
1	I	95	TYR
1	I	96	THR
1	I	100	VAL
1	I	103	ARG
1	I	136	ASN
1	I	155	LEU
1	I	162	ILE
1	I	164	GLU
1	I	173	GLN
1	I	174	MSE
1	I	177	SER
1	I	184	LEU
1	I	185	GLU
1	I	200	LEU
1	I	202	VAL
1	I	213	THR
1	I	214	ARG
1	I	216	VAL
1	I	221	LEU
1	I	225	GLU
1	I	234	SER
1	I	235	LEU
1	I	242	ILE
1	I	247	ASN
1	I	248	LYS
1	I	250	LEU
1	I	255	ASN
1	I	256	LEU
1	K	10	ILE
1	K	13	MSE

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Mol	Chain	Res	Type
1	K	14	LEU
1	K	20	LYS
1	K	25	LYS
1	K	30	THR
1	K	37	SER
1	K	43	SER
1	K	44	ARG
1	K	45	ARG
1	K	69	ARG
1	K	70	GLN
1	K	101	GLU
1	K	103	ARG
1	K	106	PHE
1	K	111	THR
1	K	132	GLN
1	K	138	ASP
1	K	148	THR
1	K	152	MSE
1	K	155	LEU
1	K	162	ILE
1	K	184	LEU
1	K	194	LEU
1	K	195	ASP
1	K	200	LEU
1	K	201	LEU
1	K	206	ILE
1	K	208	ASP
1	K	214	ARG
1	K	217	ILE
1	K	224	LEU
1	K	240	THR
1	K	244	VAL
1	K	247	ASN
1	K	248	LYS
1	K	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	70	GLN
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	132	GLN
1	A	173	GLN
1	A	219	ASN
1	A	247	ASN
1	B	70	GLN
1	B	88	ASN
1	B	173	GLN
1	B	189	HIS
1	B	247	ASN
1	C	23	ASN
1	C	59	ASN
1	C	78	ASN
1	C	88	ASN
1	C	173	GLN
1	C	197	ASN
1	C	247	ASN
1	D	70	GLN
1	D	78	ASN
1	D	81	ASN
1	D	88	ASN
1	D	102	ASN
1	D	173	GLN
1	D	247	ASN
1	E	173	GLN
1	E	247	ASN
1	F	70	GLN
1	F	88	ASN
1	F	173	GLN
1	F	189	HIS
1	F	247	ASN
1	F	255	ASN
1	G	88	ASN
1	G	134	GLN
1	G	189	HIS
1	G	197	ASN
1	G	247	ASN
1	G	255	ASN
1	H	55	GLN
1	H	70	GLN
1	H	78	ASN
1	H	88	ASN
1	H	102	ASN

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Mol	Chain	Res	Type
1	H	132	GLN
1	H	173	GLN
1	I	70	GLN
1	I	88	ASN
1	I	189	HIS
1	I	247	ASN
1	K	15	GLN
1	K	56	GLN
1	K	78	ASN
1	K	88	ASN
1	K	173	GLN
1	K	189	HIS
1	K	247	ASN
1	K	255	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	301	-	4,4,4	0.57	0	6,6,6	0.26	0
2	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.26	0
2	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	C	301	-	4,4,4	1.96	3 (75%)	6,6,6	0.74	0
2	SO4	E	301	-	4,4,4	0.96	0	6,6,6	0.42	0
2	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	F	301	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	H	301	-	4,4,4	0.83	0	6,6,6	0.12	0
2	SO4	I	301	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	K	301	-	4,4,4	1.21	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
2	SO4	G	301	-	-	0/0/0/0	0/0/0/0
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	I	301	-	-	0/0/0/0	0/0/0/0
2	SO4	K	301	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SO4	O4-S	2.07	1.54	1.47
2	C	301	SO4	O3-S	2.10	1.55	1.47
2	C	301	SO4	O2-S	2.43	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	SO4	1	0
2	E	301	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	248/263 (94%)	0.27	4 (1%) 74 47	69, 86, 96, 106	0
1	B	248/263 (94%)	0.23	4 (1%) 74 47	69, 86, 96, 106	0
1	C	248/263 (94%)	0.25	10 (4%) 42 17	69, 86, 96, 106	0
1	D	248/263 (94%)	0.53	31 (12%) 5 2	69, 86, 96, 106	0
1	E	248/263 (94%)	0.15	6 (2%) 62 32	69, 86, 96, 106	0
1	F	248/263 (94%)	0.28	12 (4%) 34 14	69, 86, 96, 106	0
1	G	248/263 (94%)	0.24	11 (4%) 38 16	69, 86, 96, 106	0
1	H	248/263 (94%)	0.48	24 (9%) 10 4	69, 86, 96, 106	0
1	I	248/263 (94%)	0.17	5 (2%) 68 39	69, 86, 96, 106	0
1	K	248/263 (94%)	0.08	7 (2%) 56 27	69, 86, 96, 106	0
All	All	2480/2630 (94%)	0.27	114 (4%) 36 14	69, 86, 97, 106	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	THR	6.0
1	H	108	ALA	4.9
1	D	60	ASP	4.5
1	H	105	LEU	4.5
1	D	97	ALA	4.5
1	D	108	ALA	4.3
1	E	96	THR	4.2
1	D	113	ILE	3.9
1	D	131	LEU	3.8
1	D	98	PHE	3.8
1	C	92	ASN	3.7
1	D	94	GLU	3.7
1	F	131	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	98	PHE	3.6
1	H	110	LEU	3.6
1	D	107	GLN	3.5
1	D	111	THR	3.4
1	C	200	LEU	3.4
1	H	109	GLY	3.3
1	E	100	VAL	3.3
1	D	132	GLN	3.3
1	F	132	GLN	3.3
1	D	239	GLY	3.3
1	I	97	ALA	3.2
1	I	96	THR	3.2
1	F	51	TYR	3.2
1	E	108	ALA	3.2
1	K	236	GLY	3.2
1	K	131	LEU	3.2
1	H	92	ASN	3.2
1	G	95	TYR	3.1
1	H	107	GLN	3.1
1	C	56	GLN	3.1
1	H	58	GLU	3.1
1	F	238	LYS	3.1
1	H	91	ILE	3.1
1	H	239	GLY	3.1
1	D	197	ASN	3.0
1	H	56	GLN	3.0
1	D	95	TYR	2.9
1	A	239	GLY	2.9
1	F	57	ILE	2.9
1	D	99	PRO	2.9
1	B	100	VAL	2.9
1	D	89	LEU	2.9
1	K	67	GLU	2.8
1	G	98	PHE	2.8
1	G	196	GLY	2.8
1	D	59	ASN	2.8
1	F	71	PHE	2.8
1	G	195	ASP	2.8
1	H	60	ASP	2.8
1	H	131	LEU	2.8
1	C	236	GLY	2.8
1	C	201	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	98	PHE	2.8
1	H	195	ASP	2.7
1	D	92	ASN	2.7
1	D	83	PRO	2.7
1	D	109	GLY	2.7
1	F	58	GLU	2.7
1	G	131	LEU	2.6
1	D	235	LEU	2.6
1	A	96	THR	2.6
1	G	58	GLU	2.6
1	I	95	TYR	2.6
1	H	94	GLU	2.6
1	H	57	ILE	2.6
1	E	98	PHE	2.5
1	G	100	VAL	2.5
1	I	94	GLU	2.5
1	D	200	LEU	2.5
1	G	238	LYS	2.5
1	E	73	GLU	2.5
1	E	74	GLU	2.5
1	K	40	PHE	2.4
1	D	100	VAL	2.4
1	F	55	GLN	2.4
1	H	127	ILE	2.4
1	K	238	LYS	2.4
1	C	50	GLY	2.4
1	D	40	PHE	2.4
1	F	133	ASP	2.4
1	I	200	LEU	2.4
1	H	42	VAL	2.3
1	D	129	SER	2.3
1	K	51	TYR	2.3
1	D	80	PHE	2.3
1	K	235	LEU	2.3
1	B	96	THR	2.3
1	B	195	ASP	2.3
1	D	112	THR	2.3
1	H	97	ALA	2.3
1	G	59	ASN	2.3
1	B	242	ILE	2.2
1	D	238	LYS	2.2
1	C	40	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	102	ASN	2.2
1	H	59	ASN	2.2
1	G	199	GLY	2.2
1	D	93	SER	2.1
1	C	52	SER	2.1
1	C	239	GLY	2.1
1	D	90	ASP	2.1
1	H	101	GLU	2.1
1	A	200	LEU	2.1
1	D	127	ILE	2.1
1	A	235	LEU	2.1
1	G	200	LEU	2.1
1	H	236	GLY	2.1
1	F	91	ILE	2.1
1	F	53	ILE	2.1
1	F	56	GLN	2.1
1	H	40	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	F	301	5/5	0.42	0.64	7.60	180,180,180,181	0
2	SO4	K	301	5/5	0.72	0.41	5.76	184,185,185,185	0
2	SO4	A	301	5/5	0.78	0.50	4.92	157,158,158,159	0
2	SO4	H	301	5/5	0.58	0.47	4.63	173,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	301	5/5	0.78	0.36	3.99	148,149,149,150	0
2	SO4	E	302	5/5	0.66	0.44	3.72	198,199,199,199	0
2	SO4	G	301	5/5	0.79	0.36	2.47	140,140,141,141	0
2	SO4	E	301	5/5	0.86	0.31	2.23	160,160,160,160	0
2	SO4	B	301	5/5	0.84	0.36	1.84	143,143,144,144	0
2	SO4	I	301	5/5	0.90	0.27	0.30	148,148,148,149	0
2	SO4	A	302	5/5	0.75	0.16	-	160,160,160,160	0
2	SO4	B	302	5/5	0.86	0.16	-	162,162,163,163	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.