Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:41 pm BST

PDB ID	:	3TTH
Title	:	Structure of the spermidine N1-acetyltransferase (speG) from Coxiella burnetii
Authors	:	Rudolph, M.; Cheung, J.; Franklin, M.C.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on	:	2011-09-14
Resolution	:	3.30 Å(reported)

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

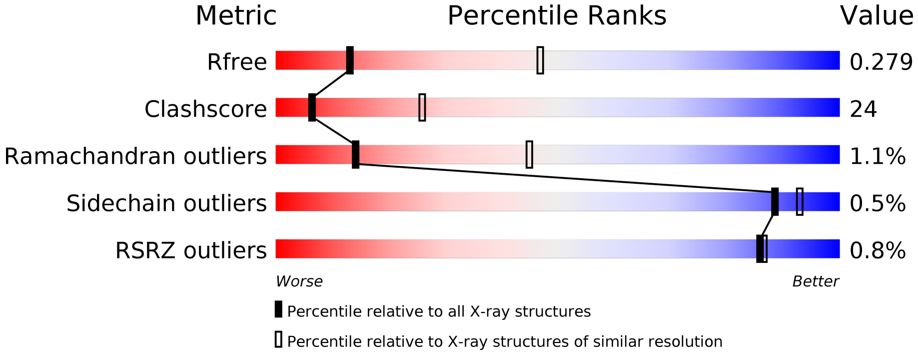
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

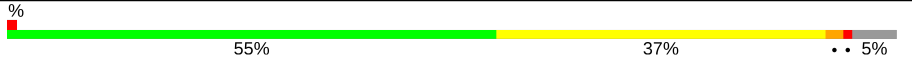
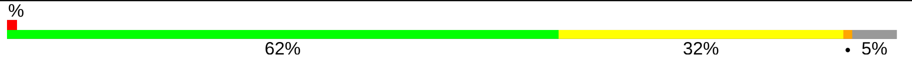
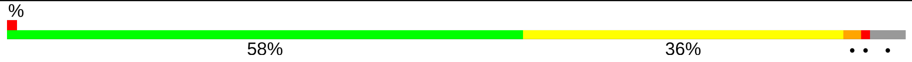
The reported resolution of this entry is 3.30 Å.

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	C	170	
1	D	170	
1	E	170	
1	F	170	

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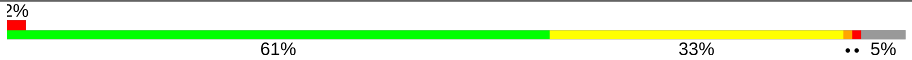
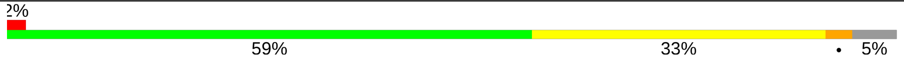
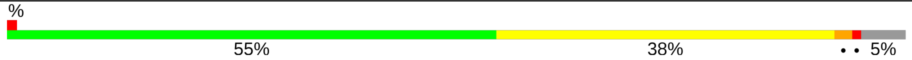
Mol	Chain	Length	Quality of chain
1	G	170	
1	H	170	
1	I	170	
1	J	170	
1	K	170	
1	L	170	

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	D	171	-	-	X	-

2 Entry composition

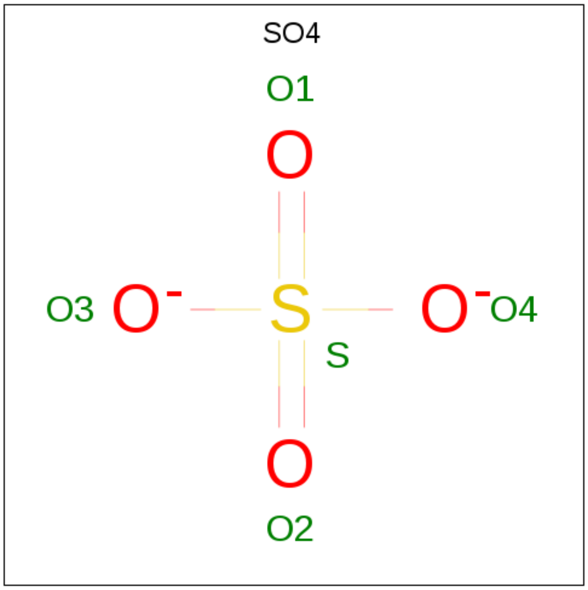
There are 3 unique types of molecules in this entry. The entry contains 16408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spermidine N1-acetyltransferase.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	162	Total C N O S Se 1361 874 231 253 1 2	0	0	0
1	B	164	Total C N O S Se 1375 883 233 256 1 2	0	0	0
1	C	162	Total C N O S Se 1358 871 230 254 1 2	0	0	0
1	D	161	Total C N O S Se 1353 868 230 252 1 2	0	0	0
1	E	163	Total C N O S Se 1366 877 231 255 1 2	0	0	0
1	F	162	Total C N O S Se 1361 874 231 253 1 2	0	0	0
1	G	164	Total C N O S Se 1375 883 233 256 1 2	0	0	0
1	H	163	Total C N O S Se 1367 877 232 255 1 2	0	0	0
1	I	162	Total C N O S Se 1362 875 230 254 1 2	0	0	0
1	J	164	Total C N O S Se 1375 883 233 256 1 2	0	0	0
1	K	162	Total C N O S Se 1358 871 230 254 1 2	0	0	0
1	L	162	Total C N O S Se 1361 874 231 253 1 2	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

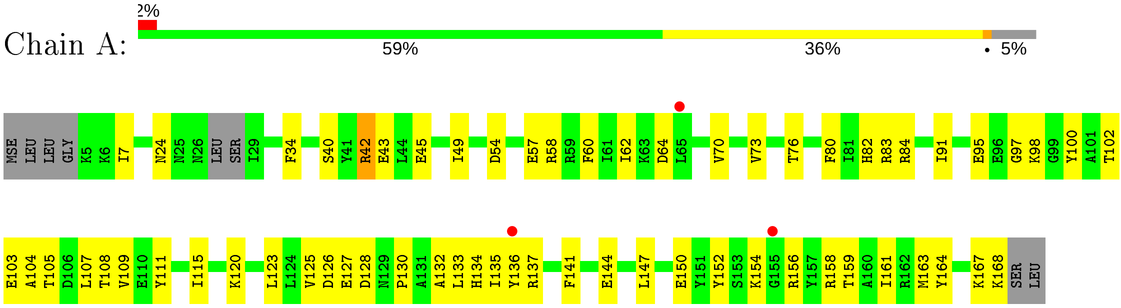
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	G	1	Total O 1 1	0	0
3	K	2	Total O 2 2	0	0

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.

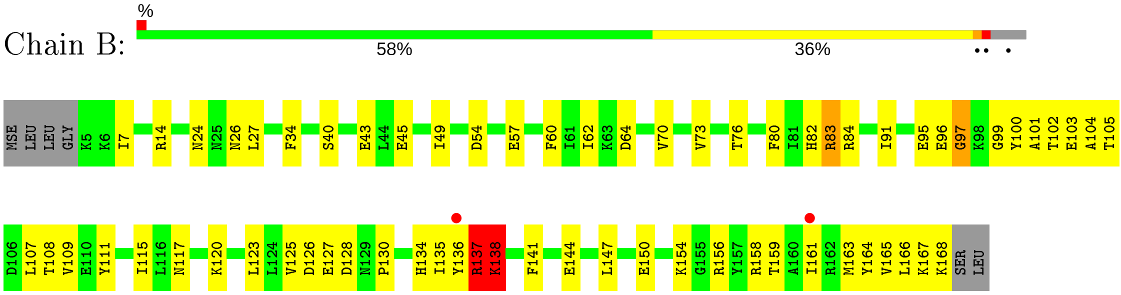
- Molecule 1: Spermidine N1-acetyltransferase

Chain A:



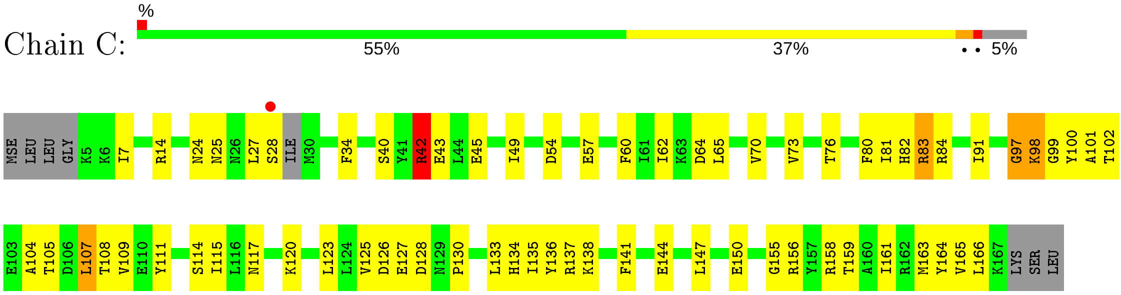
- Molecule 1: Spermidine N1-acetyltransferase

Chain B:



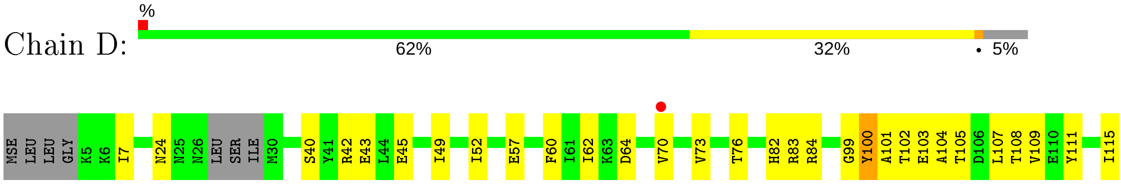
- Molecule 1: Spermidine N1-acetyltransferase

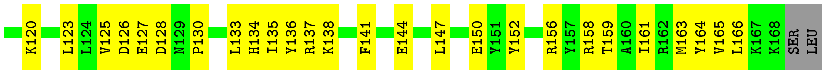
Chain C:



- Molecule 1: Spermidine N1-acetyltransferase

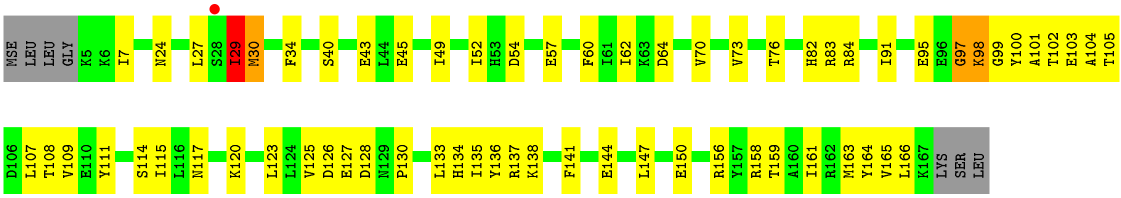
Chain D:





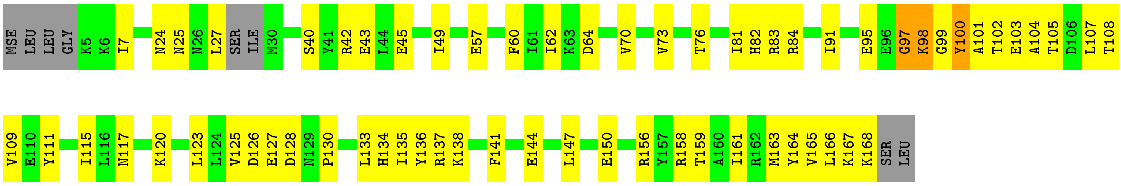
- Molecule 1: Spermidine N1-acetyltransferase

Chain E:



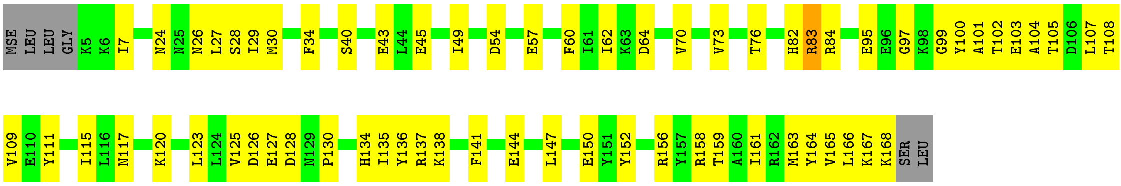
- Molecule 1: Spermidine N1-acetyltransferase

Chain F:



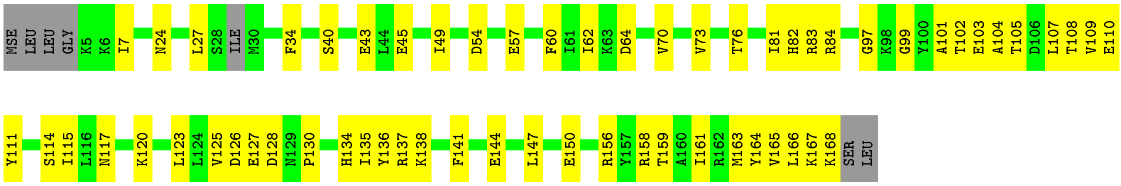
- Molecule 1: Spermidine N1-acetyltransferase

Chain G:



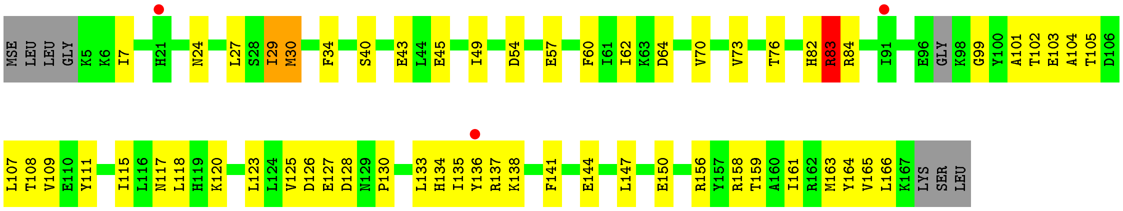
- Molecule 1: Spermidine N1-acetyltransferase

Chain H:



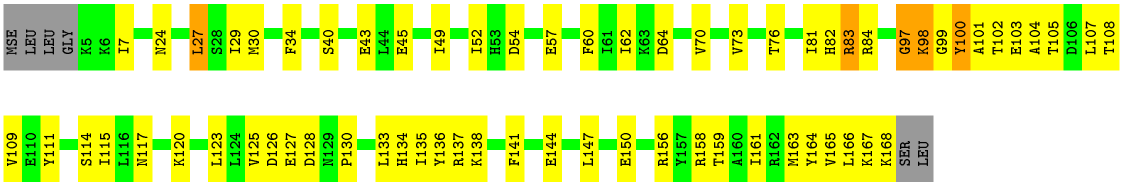
- Molecule 1: Spermidine N1-acetyltransferase

Chain I:



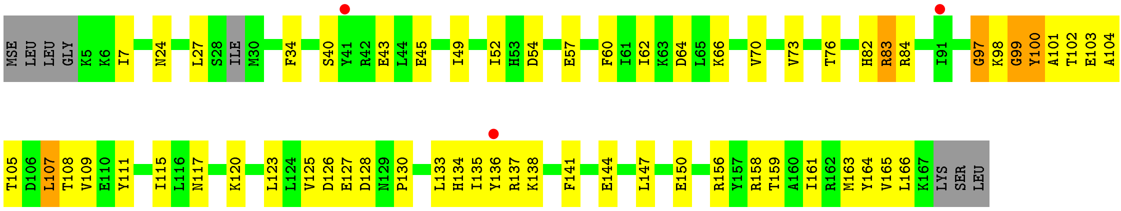
- Molecule 1: Spermidine N1-acetyltransferase

Chain J:



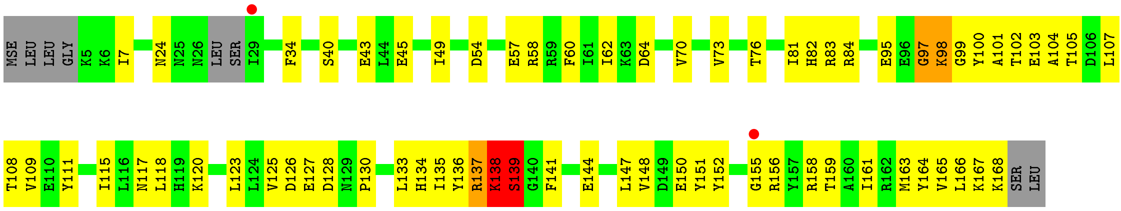
- Molecule 1: Spermidine N1-acetyltransferase

Chain K:



- Molecule 1: Spermidine N1-acetyltransferase

Chain L:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	177.89Å 106.84Å 143.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.75 – 3.30 43.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.75-3.30) 99.4 (43.75-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.238 , 0.289 0.231 , 0.279	Depositor DCC
R_{free} test set	2113 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	100.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 77.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16408	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/1387	0.40	0/1860
1	B	0.50	2/1402 (0.1%)	0.61	4/1882 (0.2%)
1	C	0.36	0/1385	0.86	5/1860 (0.3%)
1	D	0.23	0/1380	0.40	0/1852
1	E	0.38	0/1393	0.50	0/1871
1	F	0.49	2/1388 (0.1%)	0.46	0/1863
1	G	0.32	0/1402	0.49	1/1882 (0.1%)
1	H	0.30	0/1394	0.45	0/1871
1	I	0.46	1/1388 (0.1%)	0.93	3/1863 (0.2%)
1	J	0.34	0/1402	0.52	2/1882 (0.1%)
1	K	0.36	0/1385	0.53	2/1860 (0.1%)
1	L	0.39	0/1387	0.55	2/1860 (0.1%)
All	All	0.37	5/16693 (0.0%)	0.58	19/22406 (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	3
1	E	0	1
1	I	0	1
1	K	0	1
1	L	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	83	ARG	CZ-NH1	-12.99	1.16	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	24	ASN	CG-ND2	-10.55	1.06	1.32
1	B	24	ASN	CG-ND2	-10.54	1.06	1.32
1	F	24	ASN	CG-OD1	-9.71	1.02	1.24
1	B	24	ASN	CG-OD1	-9.70	1.02	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	83	ARG	NE-CZ-NH2	31.87	136.24	120.30
1	C	42	ARG	NE-CZ-NH1	-19.79	110.41	120.30
1	C	42	ARG	NE-CZ-NH2	19.59	130.09	120.30
1	I	83	ARG	NE-CZ-NH1	-10.73	114.94	120.30
1	I	83	ARG	NH1-CZ-NH2	-9.90	108.51	119.40
1	K	107	LEU	CB-CG-CD1	8.61	125.63	111.00
1	C	107	LEU	CB-CG-CD1	8.60	125.63	111.00
1	C	42	ARG	CD-NE-CZ	7.62	134.27	123.60
1	B	137	ARG	O-C-N	-7.22	111.16	122.70
1	L	138	LYS	O-C-N	-6.95	111.58	122.70
1	K	83	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	L	137	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	J	83	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	C	83	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	B	138	LYS	N-CA-C	-5.73	95.52	111.00
1	B	83	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	J	27	LEU	N-CA-C	-5.44	96.31	111.00
1	B	138	LYS	N-CA-CB	5.18	119.92	110.60
1	G	83	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	ARG	Mainchain,Peptide
1	B	96	GLU	Peptide
1	E	29	ILE	Peptide
1	I	29	ILE	Peptide
1	K	99	GLY	Peptide
1	L	138	LYS	Mainchain

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	1361	0	1348	59	3
1	B	1375	0	1365	85	1
1	C	1358	0	1340	85	5
1	D	1353	0	1337	78	0
1	E	1366	0	1352	91	1
1	F	1361	0	1348	66	3
1	G	1375	0	1365	61	1
1	H	1367	0	1353	65	1
1	I	1362	0	1348	64	0
1	J	1375	0	1365	81	0
1	K	1358	0	1340	81	0
1	L	1361	0	1348	66	2
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	3	0
2	I	10	0	0	0	0
2	K	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	K	2	0	0	0	0
All	All	16408	0	16209	782	11

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 24.

All (782) 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:D:83:ARG:HE	1:E:83:ARG:NH2	1.27	1.32
1:E:91:ILE:HD11	1:E:100:TYR:O	1.44	1.15
1:H:115:ILE:HD12	1:J:29:ILE:HG12	1.31	1.13
1:J:29:ILE:HG22	1:J:30:MSE:H	1.14	1.09
1:J:83:ARG:NH2	1:K:83:ARG:NE	2.02	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:O	1:A:100:TYR:CD2	2.07	1.07
1:G:83:ARG:NH1	1:G:117:ASN:O	1.88	1.06
1:J:83:ARG:NE	1:K:83:ARG:NH2	2.02	1.05
1:B:83:ARG:NE	1:C:83:ARG:NH2	2.05	1.05
1:B:49:ILE:HD12	1:D:42:ARG:CZ	1.88	1.02
1:D:83:ARG:HE	1:E:83:ARG:CZ	1.71	1.02
1:D:83:ARG:NE	1:E:83:ARG:NH2	2.09	1.00
1:K:100:TYR:CD1	1:K:103:GLU:OE1	2.14	1.00
1:K:100:TYR:HD1	1:K:103:GLU:OE1	1.44	0.99
1:J:83:ARG:NE	1:K:83:ARG:HH21	1.61	0.98
1:J:83:ARG:HH21	1:K:83:ARG:NE	1.59	0.98
1:B:49:ILE:HD12	1:D:42:ARG:NH2	1.82	0.95
1:C:42:ARG:HG2	1:E:52:ILE:CD1	1.96	0.95
1:J:83:ARG:NH2	1:K:83:ARG:CZ	2.30	0.95
1:J:29:ILE:CG2	1:J:30:MSE:H	1.79	0.94
1:B:83:ARG:NH2	1:C:83:ARG:NE	2.16	0.93
1:A:95:GLU:O	1:A:100:TYR:HD2	1.46	0.93
1:F:83:ARG:NH1	1:F:117:ASN:O	2.01	0.93
1:E:27:LEU:C	1:E:29:ILE:H	1.72	0.93
1:J:83:ARG:CZ	1:K:83:ARG:NH2	2.31	0.93
1:B:83:ARG:HH21	1:C:83:ARG:NE	1.67	0.93
1:B:91:ILE:HD11	1:B:100:TYR:O	1.71	0.91
1:J:29:ILE:HG22	1:J:30:MSE:N	1.85	0.90
1:I:29:ILE:HB	1:I:30:MSE:O	1.72	0.90
1:C:28:SER:HB2	1:E:111:TYR:HE1	1.32	0.90
1:E:83:ARG:NH1	1:E:117:ASN:O	2.05	0.90
1:B:49:ILE:HD12	1:D:42:ARG:NH1	1.87	0.89
1:E:29:ILE:HG22	1:E:30:MSE:N	1.89	0.88
1:F:167:LYS:HG2	1:F:168:LYS:H	1.40	0.87
1:H:83:ARG:NH1	1:H:117:ASN:O	2.07	0.87
1:L:83:ARG:NH1	1:L:117:ASN:O	2.07	0.86
1:J:83:ARG:CZ	1:K:83:ARG:CZ	2.53	0.86
1:B:14:ARG:HD2	1:D:42:ARG:NH1	1.90	0.86
1:K:100:TYR:HB3	1:K:103:GLU:CG	2.05	0.85
1:B:83:ARG:NE	1:C:83:ARG:HH21	1.74	0.85
1:C:43:GLU:HG2	1:E:52:ILE:HG12	1.59	0.85
1:A:103:GLU:O	1:A:107:LEU:HG	1.78	0.84
1:D:103:GLU:O	1:D:107:LEU:HG	1.77	0.83
1:A:80:PHE:O	1:A:83:ARG:NE	2.13	0.82
1:G:27:LEU:C	1:G:29:ILE:H	1.78	0.82
1:J:83:ARG:HH21	1:K:83:ARG:HE	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:TYR:HB3	1:K:103:GLU:CD	2.00	0.81
1:J:83:ARG:NH1	1:J:117:ASN:O	2.14	0.81
1:B:83:ARG:NH1	1:B:117:ASN:O	2.14	0.80
1:C:28:SER:HB2	1:E:111:TYR:CE1	2.18	0.79
1:J:83:ARG:HE	1:K:83:ARG:HH21	1.28	0.79
1:B:83:ARG:CZ	1:C:83:ARG:CZ	2.60	0.79
1:K:100:TYR:HB3	1:K:103:GLU:HG2	1.65	0.78
1:K:83:ARG:NH1	1:K:117:ASN:O	2.15	0.78
1:C:83:ARG:NH1	1:C:117:ASN:O	2.17	0.78
1:J:167:LYS:HG2	1:J:168:LYS:H	1.48	0.78
1:C:42:ARG:HG2	1:E:52:ILE:HD12	1.66	0.77
1:E:95:GLU:O	1:E:100:TYR:CD2	2.38	0.76
1:D:83:ARG:NH1	2:D:171:SO4:S	2.59	0.76
1:F:91:ILE:HD11	1:F:100:TYR:O	1.86	0.76
1:B:83:ARG:HG3	1:C:83:ARG:HH22	1.50	0.76
1:H:137:ARG:HG3	1:H:163:MSE:HE3	1.66	0.76
1:H:115:ILE:CD1	1:J:29:ILE:HG12	2.13	0.75
1:G:103:GLU:O	1:G:107:LEU:HG	1.86	0.75
1:F:103:GLU:O	1:F:107:LEU:HG	1.86	0.75
1:K:100:TYR:O	1:K:102:THR:N	2.17	0.74
1:B:49:ILE:CD1	1:D:42:ARG:NH1	2.50	0.74
1:E:103:GLU:O	1:E:107:LEU:HG	1.86	0.74
1:I:103:GLU:O	1:I:107:LEU:HG	1.87	0.74
1:D:7:ILE:HD13	1:D:100:TYR:CE1	2.20	0.74
1:K:100:TYR:HD1	1:K:103:GLU:CD	1.90	0.74
1:L:103:GLU:O	1:L:107:LEU:HG	1.87	0.74
1:B:83:ARG:CG	1:C:83:ARG:NH2	2.50	0.74
1:A:102:THR:HG23	1:A:135:ILE:HG23	1.70	0.74
1:A:95:GLU:O	1:A:100:TYR:CE2	2.41	0.73
1:H:103:GLU:O	1:H:107:LEU:HG	1.86	0.73
1:J:103:GLU:O	1:J:107:LEU:HG	1.86	0.73
1:B:103:GLU:O	1:B:107:LEU:HG	1.86	0.73
1:D:83:ARG:NE	1:E:83:ARG:CZ	2.48	0.73
1:D:83:ARG:HE	1:E:83:ARG:HH22	1.35	0.73
1:L:137:ARG:HG3	1:L:163:MSE:HE3	1.69	0.73
1:B:83:ARG:HE	1:C:83:ARG:HH21	1.34	0.72
1:J:52:ILE:HG12	1:L:43:GLU:HG2	1.71	0.72
1:B:83:ARG:NH2	1:C:83:ARG:HG3	2.04	0.72
1:B:83:ARG:HH22	1:C:83:ARG:HG3	1.55	0.71
1:H:83:ARG:NH2	1:I:83:ARG:CZ	2.53	0.71
1:H:83:ARG:CZ	1:I:83:ARG:CZ	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:NH2	1:C:83:ARG:CZ	2.54	0.71
1:E:91:ILE:CD1	1:E:100:TYR:O	2.33	0.71
1:D:83:ARG:NH1	2:D:171:SO4:O2	2.24	0.71
1:L:141:PHE:HB3	1:L:163:MSE:HE2	1.73	0.71
1:D:83:ARG:HH21	1:E:83:ARG:CZ	2.03	0.70
1:F:97:GLY:O	1:F:99:GLY:N	2.24	0.70
1:C:137:ARG:HG3	1:C:163:MSE:HE3	1.71	0.70
1:I:137:ARG:HG3	1:I:163:MSE:HE3	1.72	0.70
1:G:27:LEU:C	1:G:29:ILE:N	2.45	0.70
1:K:137:ARG:HG3	1:K:163:MSE:HE3	1.72	0.70
1:E:141:PHE:HB3	1:E:163:MSE:HE2	1.73	0.70
1:J:137:ARG:HG3	1:J:163:MSE:HE3	1.72	0.70
1:H:141:PHE:HB3	1:H:163:MSE:HE2	1.73	0.70
1:B:141:PHE:HB3	1:B:163:MSE:HE2	1.73	0.70
1:I:141:PHE:HB3	1:I:163:MSE:HE2	1.74	0.70
1:C:137:ARG:HG3	1:C:163:MSE:CE	2.22	0.69
1:J:137:ARG:HG3	1:J:163:MSE:CE	2.22	0.69
1:G:137:ARG:HG3	1:G:163:MSE:HE3	1.72	0.69
1:B:83:ARG:NH2	1:C:83:ARG:CG	2.55	0.69
1:F:137:ARG:HG3	1:F:163:MSE:HE3	1.72	0.69
1:B:14:ARG:HD2	1:D:42:ARG:HH11	1.56	0.69
1:G:141:PHE:HB3	1:G:163:MSE:HE2	1.74	0.69
1:K:141:PHE:HB3	1:K:163:MSE:HE2	1.74	0.69
1:G:137:ARG:HG3	1:G:163:MSE:CE	2.22	0.69
1:F:141:PHE:HB3	1:F:163:MSE:HE2	1.74	0.69
1:H:137:ARG:HG3	1:H:163:MSE:CE	2.22	0.69
1:A:137:ARG:HG2	1:A:163:MSE:CE	2.23	0.69
1:C:97:GLY:O	1:C:99:GLY:N	2.25	0.69
1:D:83:ARG:NH2	1:E:83:ARG:NH1	2.40	0.69
1:I:137:ARG:HG3	1:I:163:MSE:CE	2.22	0.69
1:I:83:ARG:HD2	1:I:118:LEU:HA	1.75	0.69
1:C:141:PHE:HB3	1:C:163:MSE:HE2	1.74	0.68
1:J:141:PHE:HB3	1:J:163:MSE:HE2	1.74	0.68
1:F:137:ARG:HG3	1:F:163:MSE:CE	2.22	0.68
1:E:97:GLY:O	1:E:99:GLY:N	2.27	0.68
1:K:137:ARG:HG3	1:K:163:MSE:CE	2.22	0.68
1:A:141:PHE:HB3	1:A:163:MSE:HE2	1.75	0.68
1:D:83:ARG:HG3	1:E:83:ARG:HH22	1.59	0.68
1:J:97:GLY:O	1:J:99:GLY:N	2.27	0.68
1:E:29:ILE:HG22	1:E:30:MSE:H	1.59	0.67
1:L:137:ARG:HG3	1:L:163:MSE:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG21	1:A:108:THR:HG21	1.77	0.67
1:L:97:GLY:O	1:L:99:GLY:N	2.26	0.67
1:K:100:TYR:CD1	1:K:103:GLU:CD	2.66	0.67
1:B:7:ILE:HG12	1:B:62:ILE:HG23	1.78	0.66
1:K:100:TYR:CB	1:K:103:GLU:CD	2.64	0.66
1:D:7:ILE:HG12	1:D:62:ILE:HG23	1.77	0.66
1:B:95:GLU:O	1:B:100:TYR:CD2	2.49	0.66
1:D:83:ARG:HH21	1:E:83:ARG:NH1	1.92	0.66
1:K:7:ILE:HG12	1:K:62:ILE:HG23	1.78	0.66
1:D:73:VAL:HG21	1:D:108:THR:HG21	1.78	0.66
1:L:73:VAL:HG21	1:L:108:THR:HG21	1.78	0.65
1:L:7:ILE:HG12	1:L:62:ILE:HG23	1.78	0.65
1:H:115:ILE:HD12	1:J:29:ILE:CG1	2.17	0.65
1:I:73:VAL:HG21	1:I:108:THR:HG21	1.78	0.65
1:D:83:ARG:NE	1:E:83:ARG:HH22	1.93	0.65
1:B:83:ARG:CZ	1:C:83:ARG:NH2	2.59	0.65
1:H:7:ILE:HG12	1:H:62:ILE:HG23	1.78	0.65
1:H:137:ARG:HG2	1:H:141:PHE:O	1.97	0.65
1:I:7:ILE:HG12	1:I:62:ILE:HG23	1.78	0.65
1:D:141:PHE:HB3	1:D:163:MSE:HE2	1.78	0.64
1:G:7:ILE:HG12	1:G:62:ILE:HG23	1.78	0.64
1:K:73:VAL:HG21	1:K:108:THR:HG21	1.78	0.64
1:C:7:ILE:HG12	1:C:62:ILE:HG23	1.78	0.64
1:A:7:ILE:HG12	1:A:62:ILE:HG23	1.79	0.64
1:F:73:VAL:HG21	1:F:108:THR:HG21	1.78	0.64
1:B:73:VAL:HG21	1:B:108:THR:HG21	1.78	0.64
1:E:73:VAL:HG21	1:E:108:THR:HG21	1.79	0.64
1:J:7:ILE:HG12	1:J:62:ILE:HG23	1.78	0.64
1:H:73:VAL:HG21	1:H:108:THR:HG21	1.78	0.63
1:E:7:ILE:HG12	1:E:62:ILE:HG23	1.78	0.63
1:F:7:ILE:HG12	1:F:62:ILE:HG23	1.78	0.63
1:G:73:VAL:HG21	1:G:108:THR:HG21	1.79	0.63
1:E:82:HIS:HD2	1:E:84:ARG:HH21	1.47	0.63
1:J:73:VAL:HG21	1:J:108:THR:HG21	1.78	0.63
1:C:73:VAL:HG21	1:C:108:THR:HG21	1.78	0.63
1:H:83:ARG:NH2	1:I:83:ARG:NE	2.47	0.63
1:J:29:ILE:CG2	1:J:30:MSE:N	2.51	0.63
1:K:82:HIS:HD2	1:K:84:ARG:HH21	1.47	0.63
1:D:52:ILE:HG12	1:F:43:GLU:HG2	1.81	0.63
1:B:26:ASN:O	1:B:27:LEU:HB2	1.99	0.62
1:G:82:HIS:HD2	1:G:84:ARG:HH21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ILE:HD12	1:D:64:ASP:HA	1.81	0.62
1:I:27:LEU:HB2	1:I:29:ILE:HG12	1.82	0.62
1:A:91:ILE:HD13	1:A:100:TYR:HB2	1.82	0.61
1:B:49:ILE:CD1	1:D:42:ARG:HH12	2.11	0.61
1:D:83:ARG:CG	1:E:83:ARG:NH2	2.63	0.61
1:K:137:ARG:HG2	1:K:141:PHE:O	2.00	0.61
1:I:137:ARG:HG2	1:I:141:PHE:O	2.00	0.61
1:I:82:HIS:HD2	1:I:84:ARG:HH21	1.48	0.61
1:B:82:HIS:HD2	1:B:84:ARG:HH21	1.47	0.61
1:E:137:ARG:HG3	1:E:163:MSE:CE	2.31	0.61
1:J:137:ARG:HG2	1:J:141:PHE:O	2.00	0.61
1:E:137:ARG:HG3	1:E:163:MSE:HE3	1.82	0.61
1:D:83:ARG:CG	1:E:83:ARG:HH22	2.12	0.61
1:L:134:HIS:O	1:L:138:LYS:HG3	2.01	0.61
1:E:27:LEU:C	1:E:29:ILE:N	2.43	0.60
1:A:154:LYS:HA	1:C:114:SER:HB3	1.83	0.60
1:F:167:LYS:HG2	1:F:168:LYS:N	2.15	0.60
1:F:137:ARG:HG2	1:F:141:PHE:O	2.00	0.60
1:J:7:ILE:HD12	1:J:64:ASP:HA	1.84	0.60
1:L:137:ARG:HG2	1:L:141:PHE:O	2.02	0.60
1:L:7:ILE:HD12	1:L:64:ASP:HA	1.83	0.60
1:G:137:ARG:HG2	1:G:141:PHE:O	2.00	0.60
1:J:117:ASN:ND2	1:L:152:TYR:CD1	2.70	0.60
1:C:137:ARG:HG2	1:C:141:PHE:O	2.01	0.60
1:C:7:ILE:HD12	1:C:64:ASP:HA	1.83	0.60
1:A:128:ASP:O	1:A:130:PRO:HD3	2.02	0.60
1:B:49:ILE:HG23	1:D:42:ARG:NH2	2.16	0.60
1:A:7:ILE:HD12	1:A:64:ASP:HA	1.83	0.59
1:E:7:ILE:HD12	1:E:64:ASP:HA	1.84	0.59
1:A:128:ASP:C	1:A:130:PRO:HD3	2.22	0.59
1:B:137:ARG:HG3	1:B:163:MSE:CE	2.32	0.59
1:K:97:GLY:O	1:K:99:GLY:N	2.36	0.59
1:I:7:ILE:HD12	1:I:64:ASP:HA	1.84	0.59
1:B:137:ARG:HG3	1:B:163:MSE:HE3	1.84	0.59
1:G:7:ILE:HD12	1:G:64:ASP:HA	1.84	0.59
1:D:83:ARG:NH1	2:D:171:SO4:O1	2.36	0.59
1:A:137:ARG:HG2	1:A:163:MSE:HE1	1.85	0.59
1:A:82:HIS:HD2	1:A:84:ARG:HH21	1.51	0.59
1:F:7:ILE:HD12	1:F:64:ASP:HA	1.83	0.59
1:B:137:ARG:HG2	1:B:141:PHE:O	2.02	0.59
1:B:7:ILE:HD12	1:B:64:ASP:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ILE:HD12	1:H:64:ASP:HA	1.84	0.58
1:A:80:PHE:O	1:A:83:ARG:CZ	2.51	0.58
1:G:27:LEU:O	1:G:29:ILE:HG13	2.02	0.58
1:A:102:THR:CG2	1:A:135:ILE:HG23	2.33	0.58
1:J:27:LEU:C	1:J:29:ILE:H	2.02	0.58
1:K:7:ILE:HD12	1:K:64:ASP:HA	1.84	0.58
1:D:133:LEU:O	1:D:137:ARG:HG3	2.03	0.58
1:D:82:HIS:HD2	1:D:84:ARG:HH21	1.51	0.58
1:F:167:LYS:O	1:F:168:LYS:C	2.41	0.58
1:A:97:GLY:O	1:A:98:LYS:C	2.41	0.57
1:A:111:TYR:O	1:A:115:ILE:HB	2.05	0.57
1:I:27:LEU:CB	1:I:29:ILE:HG12	2.34	0.57
1:J:99:GLY:O	1:J:101:ALA:N	2.37	0.57
1:E:99:GLY:O	1:E:100:TYR:C	2.40	0.57
1:D:99:GLY:O	1:D:101:ALA:N	2.38	0.57
1:G:97:GLY:O	1:G:99:GLY:N	2.38	0.57
1:A:137:ARG:HG2	1:A:163:MSE:HE3	1.86	0.56
1:B:49:ILE:HD12	1:D:42:ARG:HH22	1.65	0.56
1:H:83:ARG:NH2	1:I:83:ARG:CG	2.68	0.56
1:L:111:TYR:O	1:L:115:ILE:HB	2.06	0.56
1:C:111:TYR:O	1:C:115:ILE:HB	2.06	0.56
1:H:111:TYR:O	1:H:115:ILE:HB	2.05	0.56
1:K:111:TYR:O	1:K:115:ILE:HB	2.06	0.56
1:H:97:GLY:O	1:H:99:GLY:N	2.39	0.56
1:J:111:TYR:O	1:J:115:ILE:HB	2.06	0.56
1:D:111:TYR:O	1:D:115:ILE:HB	2.06	0.56
1:B:111:TYR:O	1:B:115:ILE:HB	2.06	0.56
1:E:137:ARG:HG2	1:E:141:PHE:O	2.06	0.56
1:E:91:ILE:HD13	1:E:100:TYR:HB2	1.87	0.56
1:L:7:ILE:HG12	1:L:62:ILE:CG2	2.36	0.56
1:D:7:ILE:HG12	1:D:62:ILE:CG2	2.36	0.55
1:G:111:TYR:O	1:G:115:ILE:HB	2.06	0.55
1:I:7:ILE:HG12	1:I:62:ILE:CG2	2.36	0.55
1:J:167:LYS:O	1:J:168:LYS:C	2.44	0.55
1:A:125:VAL:HG21	1:A:136:TYR:CE2	2.41	0.55
1:B:7:ILE:HG12	1:B:62:ILE:CG2	2.36	0.55
1:E:7:ILE:HG12	1:E:62:ILE:CG2	2.36	0.55
1:G:7:ILE:HG12	1:G:62:ILE:CG2	2.36	0.55
1:H:134:HIS:O	1:H:138:LYS:HG3	2.06	0.55
1:C:97:GLY:C	1:C:99:GLY:N	2.60	0.55
1:D:83:ARG:NH2	1:E:83:ARG:CZ	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:TYR:O	1:E:115:ILE:HB	2.06	0.55
1:F:7:ILE:HG12	1:F:62:ILE:CG2	2.36	0.55
1:H:7:ILE:HG12	1:H:62:ILE:CG2	2.36	0.55
1:I:111:TYR:O	1:I:115:ILE:HB	2.06	0.55
1:J:7:ILE:HG12	1:J:62:ILE:CG2	2.36	0.55
1:K:7:ILE:HG12	1:K:62:ILE:CG2	2.36	0.55
1:J:114:SER:HA	1:L:155:GLY:HA2	1.89	0.55
1:E:27:LEU:HB2	1:E:29:ILE:H	1.71	0.55
1:B:83:ARG:HH21	1:C:83:ARG:HE	1.49	0.55
1:B:83:ARG:NE	1:C:83:ARG:CZ	2.67	0.55
1:D:126:ASP:OD1	1:D:127:GLU:N	2.39	0.55
1:E:7:ILE:HD11	1:E:70:VAL:HG21	1.89	0.55
1:G:7:ILE:HD11	1:G:70:VAL:HG21	1.89	0.55
1:H:7:ILE:HD11	1:H:70:VAL:HG21	1.89	0.55
1:C:7:ILE:HG12	1:C:62:ILE:CG2	2.36	0.55
1:C:126:ASP:OD1	1:C:127:GLU:N	2.41	0.54
1:E:126:ASP:OD1	1:E:127:GLU:N	2.41	0.54
1:F:7:ILE:HD11	1:F:70:VAL:HG21	1.89	0.54
1:H:126:ASP:OD1	1:H:127:GLU:N	2.41	0.54
1:B:7:ILE:HD11	1:B:70:VAL:HG21	1.89	0.54
1:F:111:TYR:O	1:F:115:ILE:HB	2.06	0.54
1:J:97:GLY:C	1:J:99:GLY:N	2.59	0.54
1:K:134:HIS:O	1:K:138:LYS:HG3	2.07	0.54
1:F:126:ASP:OD1	1:F:127:GLU:N	2.41	0.54
1:J:7:ILE:HD11	1:J:70:VAL:HG21	1.89	0.54
1:L:97:GLY:C	1:L:99:GLY:N	2.60	0.54
1:B:49:ILE:HD12	1:D:42:ARG:HH12	1.70	0.54
1:B:83:ARG:HH21	1:C:83:ARG:CG	2.20	0.54
1:G:126:ASP:OD1	1:G:127:GLU:N	2.41	0.54
1:J:134:HIS:O	1:J:138:LYS:HG3	2.07	0.54
1:L:126:ASP:OD1	1:L:127:GLU:N	2.40	0.54
1:B:83:ARG:CD	1:C:83:ARG:NH2	2.71	0.54
1:E:134:HIS:O	1:E:138:LYS:HG3	2.07	0.54
1:G:134:HIS:O	1:G:138:LYS:HG3	2.07	0.54
1:A:125:VAL:HG21	1:A:136:TYR:HE2	1.73	0.54
1:C:134:HIS:O	1:C:138:LYS:HG3	2.08	0.54
1:C:7:ILE:HD11	1:C:70:VAL:HG21	1.89	0.54
1:G:104:ALA:O	1:G:108:THR:HG23	2.08	0.54
1:K:100:TYR:HD1	1:K:103:GLU:CG	2.21	0.54
1:J:126:ASP:OD1	1:J:127:GLU:N	2.41	0.54
1:K:7:ILE:HD11	1:K:70:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:ALA:O	1:I:108:THR:HG23	2.08	0.54
1:I:126:ASP:OD1	1:I:127:GLU:N	2.41	0.54
1:D:144:GLU:HB3	1:D:164:TYR:CD2	2.43	0.54
1:F:134:HIS:O	1:F:138:LYS:HG3	2.08	0.54
1:H:104:ALA:O	1:H:108:THR:HG23	2.08	0.54
1:J:104:ALA:O	1:J:108:THR:HG23	2.08	0.54
1:C:104:ALA:O	1:C:108:THR:HG23	2.08	0.53
1:B:80:PHE:HB3	1:C:80:PHE:HB3	1.90	0.53
1:F:104:ALA:O	1:F:108:THR:HG23	2.08	0.53
1:L:104:ALA:O	1:L:108:THR:HG23	2.08	0.53
1:F:97:GLY:C	1:F:99:GLY:N	2.58	0.53
1:I:134:HIS:O	1:I:138:LYS:HG3	2.07	0.53
1:K:104:ALA:O	1:K:108:THR:HG23	2.08	0.53
1:H:83:ARG:HG3	1:I:83:ARG:HH22	1.73	0.53
1:I:7:ILE:HD11	1:I:70:VAL:HG21	1.89	0.53
1:K:126:ASP:OD1	1:K:127:GLU:N	2.40	0.53
1:A:126:ASP:OD1	1:A:127:GLU:N	2.42	0.53
1:B:104:ALA:O	1:B:108:THR:HG23	2.08	0.53
1:B:126:ASP:OD1	1:B:127:GLU:N	2.41	0.53
1:I:147:LEU:O	1:I:159:THR:HG23	2.09	0.53
1:A:147:LEU:O	1:A:159:THR:HG23	2.09	0.53
1:B:147:LEU:O	1:B:159:THR:HG23	2.09	0.53
1:E:128:ASP:C	1:E:130:PRO:HD3	2.29	0.53
1:K:147:LEU:O	1:K:159:THR:HG23	2.09	0.53
1:A:7:ILE:HG12	1:A:62:ILE:CG2	2.39	0.53
1:E:104:ALA:O	1:E:108:THR:HG23	2.08	0.53
1:E:147:LEU:O	1:E:159:THR:HG23	2.09	0.53
1:K:147:LEU:HD12	1:L:144:GLU:CD	2.29	0.53
1:C:147:LEU:O	1:C:159:THR:HG23	2.09	0.53
1:G:27:LEU:O	1:G:28:SER:OG	2.21	0.53
1:H:147:LEU:O	1:H:159:THR:HG23	2.09	0.53
1:F:147:LEU:O	1:F:159:THR:HG23	2.09	0.53
1:L:7:ILE:HD11	1:L:70:VAL:HG21	1.89	0.53
1:A:24:ASN:HD22	1:A:24:ASN:N	2.07	0.52
1:L:147:LEU:O	1:L:159:THR:HG23	2.09	0.52
1:A:104:ALA:O	1:A:108:THR:HG23	2.09	0.52
1:H:83:ARG:HH22	1:I:83:ARG:HG3	1.73	0.52
1:D:147:LEU:O	1:D:159:THR:HG23	2.10	0.52
1:G:27:LEU:O	1:G:29:ILE:N	2.43	0.52
1:G:147:LEU:O	1:G:159:THR:HG23	2.09	0.52
1:J:147:LEU:O	1:J:159:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HB3	1:A:164:TYR:CD2	2.45	0.52
1:C:155:GLY:HA2	1:E:114:SER:HA	1.92	0.52
1:D:104:ALA:O	1:D:108:THR:HG23	2.09	0.52
1:D:24:ASN:N	1:D:24:ASN:HD22	2.06	0.52
1:C:91:ILE:HD11	1:C:100:TYR:O	2.09	0.52
1:B:144:GLU:HB3	1:B:164:TYR:CD2	2.45	0.52
1:K:144:GLU:HB3	1:K:164:TYR:CD2	2.45	0.52
1:A:102:THR:HG23	1:A:135:ILE:CG2	2.38	0.52
1:B:134:HIS:O	1:B:138:LYS:HG3	2.09	0.52
1:E:144:GLU:HB3	1:E:164:TYR:CD2	2.45	0.52
1:F:144:GLU:HB3	1:F:164:TYR:CD2	2.45	0.52
1:I:102:THR:HG23	1:I:135:ILE:HG23	1.92	0.52
1:I:144:GLU:HB3	1:I:164:TYR:CD2	2.45	0.52
1:K:120:LYS:HD2	1:L:148:VAL:O	2.10	0.51
1:B:117:ASN:ND2	1:D:152:TYR:CG	2.78	0.51
1:B:97:GLY:O	1:B:99:GLY:N	2.43	0.51
1:J:144:GLU:HB3	1:J:164:TYR:CD2	2.45	0.51
1:I:43:GLU:HG2	1:K:52:ILE:HG12	1.92	0.51
1:G:144:GLU:HB3	1:G:164:TYR:CD2	2.45	0.51
1:K:100:TYR:C	1:K:102:THR:H	2.10	0.51
1:A:156:ARG:HG3	1:A:158:ARG:HE	1.75	0.51
1:B:83:ARG:HG3	1:C:83:ARG:NH2	2.16	0.51
1:E:29:ILE:CG2	1:E:30:MSE:N	2.60	0.51
1:J:156:ARG:HG3	1:J:158:ARG:HE	1.75	0.51
1:L:102:THR:HG23	1:L:135:ILE:HG23	1.92	0.51
1:A:7:ILE:HD11	1:A:70:VAL:HG21	1.90	0.51
1:B:156:ARG:HG3	1:B:158:ARG:HE	1.76	0.51
1:K:102:THR:HG23	1:K:135:ILE:HG23	1.92	0.51
1:L:144:GLU:HB3	1:L:164:TYR:CD2	2.46	0.51
1:B:102:THR:HG23	1:B:135:ILE:HG23	1.92	0.51
1:C:144:GLU:HB3	1:C:164:TYR:CD2	2.45	0.51
1:B:117:ASN:ND2	1:D:152:TYR:CD1	2.79	0.51
1:D:7:ILE:HD11	1:D:70:VAL:HG21	1.91	0.51
1:H:144:GLU:HB3	1:H:164:TYR:CD2	2.46	0.51
1:J:117:ASN:HB2	1:L:152:TYR:CD2	2.46	0.51
1:K:156:ARG:HG3	1:K:158:ARG:HE	1.76	0.51
1:L:156:ARG:HG3	1:L:158:ARG:HE	1.76	0.51
1:C:128:ASP:C	1:C:130:PRO:HD3	2.32	0.51
1:H:128:ASP:C	1:H:130:PRO:HD3	2.32	0.51
1:C:156:ARG:HG3	1:C:158:ARG:HE	1.76	0.51
1:H:102:THR:HG23	1:H:135:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:SER:OG	1:H:43:GLU:HG3	2.11	0.51
1:L:128:ASP:C	1:L:130:PRO:HD3	2.32	0.51
1:B:83:ARG:NH2	1:C:83:ARG:CD	2.74	0.51
1:E:147:LEU:HB3	1:E:150:GLU:HB2	1.93	0.51
1:F:128:ASP:C	1:F:130:PRO:HD3	2.32	0.51
1:D:147:LEU:HB3	1:D:150:GLU:HB2	1.92	0.50
1:F:102:THR:HG23	1:F:135:ILE:HG23	1.92	0.50
1:G:128:ASP:C	1:G:130:PRO:HD3	2.32	0.50
1:H:147:LEU:HB3	1:H:150:GLU:HB2	1.93	0.50
1:E:102:THR:HG23	1:E:135:ILE:HG23	1.92	0.50
1:I:128:ASP:C	1:I:130:PRO:HD3	2.32	0.50
1:J:102:THR:HG23	1:J:135:ILE:HG23	1.92	0.50
1:K:97:GLY:C	1:K:99:GLY:N	2.64	0.50
1:G:147:LEU:HB3	1:G:150:GLU:HB2	1.93	0.50
1:J:147:LEU:HB3	1:J:150:GLU:HB2	1.93	0.50
1:B:99:GLY:O	1:B:100:TYR:C	2.49	0.50
1:G:40:SER:OG	1:G:43:GLU:HG3	2.11	0.50
1:E:156:ARG:HG3	1:E:158:ARG:HE	1.76	0.50
1:G:102:THR:HG23	1:G:135:ILE:HG23	1.92	0.50
1:C:102:THR:HG23	1:C:135:ILE:HG23	1.92	0.50
1:F:40:SER:OG	1:F:43:GLU:HG3	2.11	0.50
1:H:156:ARG:HG3	1:H:158:ARG:HE	1.76	0.50
1:H:83:ARG:HH22	1:I:83:ARG:CG	2.25	0.50
1:I:156:ARG:HG3	1:I:158:ARG:HE	1.76	0.50
1:B:147:LEU:HB3	1:B:150:GLU:HB2	1.93	0.50
1:C:147:LEU:HB3	1:C:150:GLU:HB2	1.93	0.50
1:E:97:GLY:C	1:E:99:GLY:N	2.62	0.50
1:J:27:LEU:C	1:J:29:ILE:N	2.63	0.50
1:K:40:SER:OG	1:K:43:GLU:HG3	2.11	0.50
1:C:40:SER:OG	1:C:43:GLU:HG3	2.11	0.49
1:E:40:SER:OG	1:E:43:GLU:HG3	2.11	0.49
1:F:156:ARG:HG3	1:F:158:ARG:HE	1.76	0.49
1:J:167:LYS:HG2	1:J:168:LYS:N	2.23	0.49
1:J:40:SER:OG	1:J:43:GLU:HG3	2.11	0.49
1:K:128:ASP:C	1:K:130:PRO:HD3	2.32	0.49
1:C:99:GLY:O	1:C:101:ALA:N	2.46	0.49
1:D:165:VAL:HG22	1:D:166:LEU:O	2.12	0.49
1:F:147:LEU:HB3	1:F:150:GLU:HB2	1.93	0.49
1:G:156:ARG:HG3	1:G:158:ARG:HE	1.75	0.49
1:L:40:SER:OG	1:L:43:GLU:HG3	2.11	0.49
1:I:40:SER:OG	1:I:43:GLU:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:LEU:HB3	1:L:150:GLU:HB2	1.93	0.49
1:A:147:LEU:HB3	1:A:150:GLU:HB2	1.93	0.49
1:D:156:ARG:HG3	1:D:158:ARG:HE	1.75	0.49
1:J:99:GLY:C	1:J:101:ALA:H	2.15	0.49
1:J:128:ASP:C	1:J:130:PRO:HD3	2.32	0.49
1:K:147:LEU:HB3	1:K:150:GLU:HB2	1.93	0.49
1:L:82:HIS:O	1:L:83:ARG:HB2	2.11	0.49
1:B:40:SER:OG	1:B:43:GLU:HG3	2.11	0.49
1:C:42:ARG:HG2	1:E:52:ILE:HD11	1.90	0.49
1:I:147:LEU:HB3	1:I:150:GLU:HB2	1.93	0.49
1:F:99:GLY:O	1:F:101:ALA:N	2.46	0.49
1:G:26:ASN:C	1:G:28:SER:N	2.66	0.49
1:B:128:ASP:C	1:B:130:PRO:HD3	2.32	0.49
1:B:137:ARG:CG	1:B:163:MSE:HE3	2.42	0.49
1:B:97:GLY:C	1:B:99:GLY:N	2.65	0.49
1:I:99:GLY:O	1:I:101:ALA:N	2.46	0.49
1:D:102:THR:HG23	1:D:135:ILE:HG23	1.95	0.49
1:J:100:TYR:O	1:J:103:GLU:HG2	2.12	0.49
1:H:99:GLY:O	1:H:101:ALA:N	2.46	0.48
1:H:82:HIS:O	1:H:83:ARG:HB2	2.12	0.48
1:J:100:TYR:HA	1:J:103:GLU:CD	2.34	0.48
1:J:82:HIS:O	1:J:83:ARG:HB2	2.13	0.48
1:F:84:ARG:HA	1:F:120:LYS:O	2.13	0.48
1:A:40:SER:OG	1:A:43:GLU:HG3	2.12	0.48
1:G:82:HIS:O	1:G:83:ARG:HB2	2.12	0.48
1:G:99:GLY:O	1:G:101:ALA:N	2.47	0.48
1:F:104:ALA:O	1:F:107:LEU:HB2	2.14	0.48
1:F:105:THR:O	1:F:109:VAL:HG23	2.14	0.48
1:G:104:ALA:O	1:G:107:LEU:HB2	2.14	0.48
1:H:83:ARG:CZ	1:I:83:ARG:NH2	2.77	0.48
1:D:40:SER:OG	1:D:43:GLU:HG3	2.12	0.48
1:E:104:ALA:O	1:E:107:LEU:HB2	2.14	0.48
1:H:104:ALA:O	1:H:107:LEU:HB2	2.14	0.48
1:L:99:GLY:O	1:L:101:ALA:N	2.46	0.48
1:C:84:ARG:HA	1:C:120:LYS:O	2.14	0.48
1:E:105:THR:O	1:E:109:VAL:HG23	2.14	0.48
1:K:100:TYR:CD1	1:K:103:GLU:CG	2.97	0.48
1:K:100:TYR:CD1	1:K:103:GLU:HG3	2.48	0.48
1:C:105:THR:O	1:C:109:VAL:HG23	2.14	0.48
1:K:84:ARG:HA	1:K:120:LYS:O	2.14	0.48
1:L:105:THR:O	1:L:109:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:ARG:HA	1:J:120:LYS:O	2.14	0.48
1:L:104:ALA:O	1:L:107:LEU:HB2	2.14	0.48
1:B:104:ALA:O	1:B:107:LEU:HB2	2.14	0.47
1:E:84:ARG:HA	1:E:120:LYS:O	2.13	0.47
1:C:82:HIS:O	1:C:83:ARG:HB2	2.15	0.47
1:J:104:ALA:O	1:J:107:LEU:HB2	2.14	0.47
1:L:84:ARG:HA	1:L:120:LYS:O	2.14	0.47
1:B:99:GLY:O	1:B:101:ALA:N	2.47	0.47
1:D:105:THR:O	1:D:109:VAL:HG23	2.14	0.47
1:D:134:HIS:HA	1:D:137:ARG:HD2	1.96	0.47
1:D:123:LEU:CD1	1:D:125:VAL:HG23	2.44	0.47
1:G:29:ILE:HG22	1:G:30:MSE:N	2.29	0.47
1:H:84:ARG:HA	1:H:120:LYS:O	2.14	0.47
1:H:97:GLY:C	1:H:99:GLY:N	2.67	0.47
1:I:24:ASN:N	1:I:24:ASN:HD22	2.13	0.47
1:B:14:ARG:CD	1:D:42:ARG:NH1	2.70	0.47
1:E:82:HIS:O	1:E:83:ARG:HB2	2.14	0.47
1:J:105:THR:O	1:J:109:VAL:HG23	2.14	0.47
1:A:105:THR:O	1:A:109:VAL:HG23	2.15	0.47
1:E:24:ASN:HD22	1:E:24:ASN:N	2.13	0.47
1:H:105:THR:O	1:H:109:VAL:HG23	2.14	0.47
1:H:24:ASN:N	1:H:24:ASN:HD22	2.13	0.47
1:J:123:LEU:CD1	1:J:125:VAL:HG23	2.45	0.47
1:K:82:HIS:O	1:K:83:ARG:HB2	2.14	0.47
1:B:105:THR:O	1:B:109:VAL:HG23	2.14	0.47
1:C:123:LEU:CD1	1:C:125:VAL:HG23	2.45	0.47
1:E:123:LEU:CD1	1:E:125:VAL:HG23	2.45	0.47
1:F:95:GLU:HB3	1:F:100:TYR:CD2	2.49	0.47
1:G:84:ARG:HA	1:G:120:LYS:O	2.14	0.47
1:G:123:LEU:CD1	1:G:125:VAL:HG23	2.45	0.47
1:G:24:ASN:N	1:G:24:ASN:HD22	2.13	0.47
1:I:84:ARG:HA	1:I:120:LYS:O	2.15	0.47
1:I:123:LEU:CD1	1:I:125:VAL:HG23	2.45	0.47
1:K:105:THR:O	1:K:109:VAL:HG23	2.14	0.47
1:E:156:ARG:HG3	1:E:158:ARG:NE	2.30	0.47
1:F:25:ASN:O	1:F:27:LEU:HG	2.15	0.47
1:H:123:LEU:CD1	1:H:125:VAL:HG23	2.45	0.47
1:C:24:ASN:N	1:C:24:ASN:HD22	2.13	0.47
1:F:156:ARG:HG3	1:F:158:ARG:NE	2.30	0.47
1:G:156:ARG:HG3	1:G:158:ARG:NE	2.30	0.47
1:H:156:ARG:HG3	1:H:158:ARG:NE	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:ALA:O	1:I:107:LEU:HB2	2.14	0.47
1:J:137:ARG:HG3	1:J:163:MSE:HE1	1.97	0.47
1:J:24:ASN:HD22	1:J:24:ASN:N	2.13	0.47
1:B:156:ARG:HG3	1:B:158:ARG:NE	2.30	0.47
1:F:123:LEU:CD1	1:F:125:VAL:HG23	2.45	0.47
1:L:156:ARG:HG3	1:L:158:ARG:NE	2.30	0.47
1:A:42:ARG:HH21	1:C:14:ARG:NH2	2.13	0.47
1:B:84:ARG:HA	1:B:120:LYS:O	2.14	0.47
1:B:123:LEU:CD1	1:B:125:VAL:HG23	2.45	0.47
1:D:156:ARG:HG3	1:D:158:ARG:NE	2.30	0.47
1:G:97:GLY:C	1:G:99:GLY:N	2.67	0.47
1:A:156:ARG:HG3	1:A:158:ARG:NE	2.30	0.46
1:G:105:THR:O	1:G:109:VAL:HG23	2.14	0.46
1:G:137:ARG:HG3	1:G:163:MSE:HE1	1.97	0.46
1:K:57:GLU:HG2	1:K:76:THR:HA	1.97	0.46
1:B:57:GLU:HG2	1:B:76:THR:HA	1.97	0.46
1:E:27:LEU:HB2	1:E:29:ILE:N	2.31	0.46
1:G:167:LYS:O	1:G:168:LYS:C	2.54	0.46
1:I:156:ARG:HG3	1:I:158:ARG:NE	2.30	0.46
1:K:24:ASN:N	1:K:24:ASN:HD22	2.13	0.46
1:L:81:ILE:HG22	1:L:82:HIS:HD2	1.80	0.46
1:A:62:ILE:HG22	1:A:70:VAL:HB	1.97	0.46
1:F:137:ARG:HG3	1:F:163:MSE:HE1	1.97	0.46
1:K:123:LEU:CD1	1:K:125:VAL:HG23	2.45	0.46
1:K:156:ARG:HG3	1:K:158:ARG:NE	2.30	0.46
1:A:123:LEU:CD1	1:A:125:VAL:HG23	2.45	0.46
1:D:57:GLU:HG2	1:D:76:THR:HA	1.96	0.46
1:D:7:ILE:HD13	1:D:100:TYR:CD1	2.51	0.46
1:D:83:ARG:CZ	1:E:83:ARG:NH1	2.79	0.46
1:H:81:ILE:HG22	1:H:82:HIS:HD2	1.80	0.46
1:I:105:THR:O	1:I:109:VAL:HG23	2.14	0.46
1:L:123:LEU:CD1	1:L:125:VAL:HG23	2.45	0.46
1:L:24:ASN:HD22	1:L:24:ASN:N	2.13	0.46
1:A:144:GLU:HB3	1:A:164:TYR:CE2	2.51	0.46
1:E:99:GLY:O	1:E:101:ALA:N	2.49	0.46
1:C:156:ARG:HG3	1:C:158:ARG:NE	2.30	0.46
1:F:165:VAL:HG22	1:F:166:LEU:O	2.15	0.46
1:J:165:VAL:HG22	1:J:166:LEU:O	2.15	0.46
1:J:81:ILE:HG22	1:J:82:HIS:HD2	1.80	0.46
1:L:141:PHE:CB	1:L:163:MSE:HE2	2.45	0.46
1:H:24:ASN:HA	1:H:27:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:ARG:CG	1:I:163:MSE:HE3	2.45	0.46
1:D:144:GLU:HB3	1:D:164:TYR:CE2	2.50	0.46
1:A:141:PHE:CB	1:A:163:MSE:HE2	2.46	0.46
1:B:91:ILE:HD13	1:B:100:TYR:HB2	1.98	0.46
1:B:82:HIS:O	1:B:83:ARG:HB2	2.16	0.46
1:I:144:GLU:HB3	1:I:164:TYR:CE2	2.51	0.46
1:I:57:GLU:HG2	1:I:76:THR:HA	1.97	0.46
1:F:81:ILE:HG22	1:F:82:HIS:HD2	1.80	0.46
1:I:27:LEU:O	1:I:29:ILE:O	2.33	0.46
1:J:156:ARG:HG3	1:J:158:ARG:NE	2.30	0.46
1:L:144:GLU:HB3	1:L:164:TYR:CE2	2.51	0.46
1:E:57:GLU:HG2	1:E:76:THR:HA	1.97	0.45
1:J:57:GLU:HG2	1:J:76:THR:HA	1.97	0.45
1:D:83:ARG:HG3	1:E:83:ARG:NH2	2.23	0.45
1:F:45:GLU:O	1:F:49:ILE:HG12	2.16	0.45
1:K:100:TYR:HD1	1:K:103:GLU:HG3	1.79	0.45
1:K:144:GLU:HB3	1:K:164:TYR:CE2	2.51	0.45
1:C:155:GLY:N	1:E:114:SER:HB3	2.30	0.45
1:F:57:GLU:HG2	1:F:76:THR:HA	1.97	0.45
1:C:81:ILE:HG22	1:C:82:HIS:HD2	1.81	0.45
1:A:136:TYR:O	1:A:141:PHE:HB2	2.15	0.45
1:B:167:LYS:O	1:B:168:LYS:C	2.54	0.45
1:C:57:GLU:HG2	1:C:76:THR:HA	1.97	0.45
1:D:62:ILE:HG22	1:D:70:VAL:HB	1.98	0.45
1:L:57:GLU:HG2	1:L:76:THR:HA	1.97	0.45
1:A:57:GLU:HG2	1:A:76:THR:HA	1.97	0.45
1:C:144:GLU:HB3	1:C:164:TYR:CE2	2.51	0.45
1:F:144:GLU:HB3	1:F:164:TYR:CE2	2.51	0.45
1:I:82:HIS:O	1:I:83:ARG:HB2	2.17	0.45
1:K:165:VAL:HG22	1:K:166:LEU:O	2.17	0.45
1:L:45:GLU:O	1:L:49:ILE:HG12	2.16	0.45
1:B:144:GLU:HB3	1:B:164:TYR:CE2	2.51	0.45
1:C:137:ARG:HG3	1:C:163:MSE:HE1	1.98	0.45
1:G:57:GLU:HG2	1:G:76:THR:HA	1.97	0.45
1:H:57:GLU:HG2	1:H:76:THR:HA	1.97	0.45
1:K:100:TYR:CA	1:K:103:GLU:OE2	2.64	0.45
1:E:62:ILE:HG22	1:E:70:VAL:HB	1.99	0.45
1:I:137:ARG:HG3	1:I:163:MSE:HE1	1.97	0.45
1:J:144:GLU:HB3	1:J:164:TYR:CE2	2.51	0.45
1:A:45:GLU:O	1:A:49:ILE:HG12	2.16	0.45
1:B:141:PHE:CB	1:B:163:MSE:HE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PHE:CB	1:C:163:MSE:HE2	2.45	0.45
1:F:62:ILE:HG22	1:F:70:VAL:HB	1.99	0.45
1:G:144:GLU:HB3	1:G:164:TYR:CE2	2.51	0.45
1:H:62:ILE:HG22	1:H:70:VAL:HB	1.99	0.45
1:E:144:GLU:CD	1:F:147:LEU:HD12	2.38	0.44
1:G:62:ILE:HG22	1:G:70:VAL:HB	1.99	0.44
1:I:62:ILE:HG22	1:I:70:VAL:HB	1.99	0.44
1:J:141:PHE:CB	1:J:163:MSE:HE2	2.46	0.44
1:J:117:ASN:HB2	1:L:152:TYR:CE2	2.52	0.44
1:D:45:GLU:O	1:D:49:ILE:HG12	2.17	0.44
1:E:144:GLU:HB3	1:E:164:TYR:CE2	2.51	0.44
1:F:161:ILE:N	1:F:161:ILE:HD12	2.32	0.44
1:G:45:GLU:O	1:G:49:ILE:HG12	2.18	0.44
1:I:161:ILE:HD12	1:I:161:ILE:N	2.32	0.44
1:I:165:VAL:HG22	1:I:166:LEU:O	2.17	0.44
1:J:62:ILE:HG22	1:J:70:VAL:HB	1.99	0.44
1:K:84:ARG:NE	1:L:150:GLU:O	2.49	0.44
1:L:136:TYR:O	1:L:139:SER:HB2	2.16	0.44
1:C:165:VAL:HG22	1:C:166:LEU:O	2.17	0.44
1:D:161:ILE:N	1:D:161:ILE:HD12	2.32	0.44
1:D:83:ARG:CZ	1:E:83:ARG:CZ	2.95	0.44
1:G:29:ILE:CG2	1:G:30:MSE:N	2.80	0.44
1:K:137:ARG:HG3	1:K:163:MSE:HE1	1.97	0.44
1:K:161:ILE:HD12	1:K:161:ILE:N	2.33	0.44
1:H:144:GLU:HB3	1:H:164:TYR:CE2	2.51	0.44
1:G:161:ILE:HD12	1:G:161:ILE:N	2.32	0.44
1:I:45:GLU:O	1:I:49:ILE:HG12	2.18	0.44
1:C:62:ILE:HG22	1:C:70:VAL:HB	1.99	0.44
1:J:161:ILE:HD12	1:J:161:ILE:N	2.32	0.44
1:J:137:ARG:CG	1:J:163:MSE:HE3	2.45	0.44
1:L:161:ILE:HD12	1:L:161:ILE:N	2.32	0.44
1:D:134:HIS:O	1:D:138:LYS:HG3	2.18	0.44
1:F:97:GLY:C	1:F:99:GLY:H	2.21	0.44
1:H:161:ILE:HD12	1:H:161:ILE:N	2.32	0.44
1:H:83:ARG:NH2	1:I:83:ARG:CD	2.80	0.44
1:K:144:GLU:CD	1:L:147:LEU:HD12	2.37	0.44
1:B:161:ILE:N	1:B:161:ILE:HD12	2.32	0.44
1:C:161:ILE:HD12	1:C:161:ILE:N	2.32	0.44
1:D:125:VAL:HG21	1:D:136:TYR:HE2	1.83	0.44
1:D:134:HIS:HA	1:D:137:ARG:HG3	1.98	0.44
1:F:82:HIS:O	1:F:83:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:GLU:O	1:K:49:ILE:HG12	2.18	0.44
1:L:62:ILE:HG22	1:L:70:VAL:HB	1.99	0.44
1:A:60:PHE:HB2	1:A:73:VAL:CG1	2.48	0.44
1:E:161:ILE:HD12	1:E:161:ILE:N	2.32	0.44
1:E:165:VAL:HG22	1:E:166:LEU:O	2.17	0.44
1:K:141:PHE:CB	1:K:163:MSE:HE2	2.46	0.44
1:L:125:VAL:HG21	1:L:136:TYR:CE2	2.53	0.44
1:C:125:VAL:HG21	1:C:136:TYR:CE2	2.54	0.43
1:C:45:GLU:O	1:C:49:ILE:HG12	2.18	0.43
1:K:137:ARG:CG	1:K:163:MSE:HE3	2.45	0.43
1:D:52:ILE:CD1	1:F:42:ARG:HG2	2.48	0.43
1:K:62:ILE:HG22	1:K:70:VAL:HB	1.99	0.43
1:A:130:PRO:O	1:A:134:HIS:CD2	2.71	0.43
1:A:161:ILE:N	1:A:161:ILE:HD12	2.32	0.43
1:B:125:VAL:HG21	1:B:136:TYR:CE2	2.54	0.43
1:B:165:VAL:HG22	1:B:166:LEU:O	2.18	0.43
1:D:130:PRO:HA	1:D:133:LEU:HB3	2.00	0.43
1:H:45:GLU:O	1:H:49:ILE:HG12	2.18	0.43
1:J:60:PHE:HB2	1:J:73:VAL:CG1	2.49	0.43
1:K:125:VAL:HG21	1:K:136:TYR:CE2	2.53	0.43
1:L:60:PHE:HB2	1:L:73:VAL:CG1	2.49	0.43
1:B:62:ILE:HG22	1:B:70:VAL:HB	1.99	0.43
1:E:45:GLU:O	1:E:49:ILE:HG12	2.18	0.43
1:B:60:PHE:HB2	1:B:73:VAL:CG1	2.49	0.43
1:C:60:PHE:HB2	1:C:73:VAL:CG1	2.49	0.43
1:H:141:PHE:CB	1:H:163:MSE:HE2	2.45	0.43
1:J:97:GLY:O	1:J:98:LYS:C	2.56	0.43
1:K:136:TYR:O	1:K:141:PHE:HB2	2.19	0.43
1:G:141:PHE:CB	1:G:163:MSE:HE2	2.46	0.43
1:H:136:TYR:O	1:H:141:PHE:HB2	2.18	0.43
1:J:125:VAL:HG21	1:J:136:TYR:CE2	2.54	0.43
1:L:83:ARG:HD3	1:L:118:LEU:HA	2.01	0.43
1:E:141:PHE:CB	1:E:163:MSE:HE2	2.45	0.43
1:G:125:VAL:HG21	1:G:136:TYR:CE2	2.53	0.43
1:K:60:PHE:HB2	1:K:73:VAL:CG1	2.49	0.43
1:B:136:TYR:O	1:B:141:PHE:HB2	2.18	0.43
1:F:95:GLU:HB3	1:F:100:TYR:HD2	1.83	0.43
1:F:141:PHE:CB	1:F:163:MSE:HE2	2.46	0.43
1:H:60:PHE:HB2	1:H:73:VAL:CG1	2.49	0.43
1:J:81:ILE:HG22	1:J:82:HIS:CD2	2.54	0.43
1:C:65:LEU:O	1:K:66:LYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:VAL:HG21	1:D:136:TYR:CE2	2.54	0.43
1:D:164:TYR:HE1	1:D:166:LEU:HD23	1.84	0.43
1:F:125:VAL:HG21	1:F:136:TYR:CE2	2.53	0.43
1:G:60:PHE:HB2	1:G:73:VAL:CG1	2.49	0.43
1:H:167:LYS:O	1:H:168:LYS:C	2.56	0.43
1:I:136:TYR:O	1:I:141:PHE:HB2	2.19	0.43
1:I:141:PHE:CB	1:I:163:MSE:HE2	2.46	0.43
1:J:45:GLU:O	1:J:49:ILE:HG12	2.18	0.43
1:L:97:GLY:O	1:L:98:LYS:C	2.58	0.43
1:L:167:LYS:O	1:L:168:LYS:C	2.57	0.43
1:E:27:LEU:CB	1:E:29:ILE:H	2.32	0.42
1:G:95:GLU:O	1:G:100:TYR:CD2	2.73	0.42
1:G:165:VAL:HG22	1:G:166:LEU:O	2.19	0.42
1:L:136:TYR:O	1:L:141:PHE:HB2	2.19	0.42
1:F:60:PHE:HB2	1:F:73:VAL:CG1	2.49	0.42
1:K:7:ILE:CG1	1:K:62:ILE:HG23	2.49	0.42
1:E:136:TYR:O	1:E:141:PHE:HB2	2.19	0.42
1:G:137:ARG:CG	1:G:163:MSE:HE3	2.45	0.42
1:I:125:VAL:HG21	1:I:136:TYR:CE2	2.53	0.42
1:I:60:PHE:HB2	1:I:73:VAL:CG1	2.49	0.42
1:C:97:GLY:O	1:C:98:LYS:C	2.57	0.42
1:F:81:ILE:HG22	1:F:82:HIS:CD2	2.55	0.42
1:G:136:TYR:O	1:G:141:PHE:HB2	2.19	0.42
1:H:125:VAL:HG21	1:H:136:TYR:CE2	2.54	0.42
1:D:128:ASP:C	1:D:130:PRO:HD3	2.39	0.42
1:E:60:PHE:HB2	1:E:73:VAL:CG1	2.49	0.42
1:H:165:VAL:HG22	1:H:166:LEU:O	2.19	0.42
1:L:81:ILE:HG22	1:L:82:HIS:CD2	2.55	0.42
1:D:60:PHE:HB2	1:D:73:VAL:CG1	2.49	0.42
1:E:125:VAL:HG21	1:E:136:TYR:CE2	2.53	0.42
1:L:165:VAL:HG22	1:L:166:LEU:O	2.19	0.42
1:L:58:ARG:HB2	1:L:58:ARG:HE	1.76	0.42
1:B:27:LEU:HD13	1:B:154:LYS:NZ	2.35	0.42
1:E:133:LEU:CD1	1:E:163:MSE:SE	3.17	0.42
1:B:45:GLU:O	1:B:49:ILE:HG12	2.20	0.42
1:E:147:LEU:HD12	1:F:144:GLU:CD	2.40	0.42
1:F:136:TYR:O	1:F:141:PHE:HB2	2.19	0.42
1:H:81:ILE:HG22	1:H:82:HIS:CD2	2.55	0.42
1:L:141:PHE:HA	1:L:164:TYR:O	2.20	0.42
1:G:7:ILE:CG1	1:G:62:ILE:HG23	2.49	0.42
1:I:7:ILE:CG1	1:I:62:ILE:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:TYR:O	1:J:141:PHE:HB2	2.19	0.42
1:A:84:ARG:HA	1:A:120:LYS:O	2.20	0.42
1:F:99:GLY:O	1:F:100:TYR:C	2.58	0.42
1:G:164:TYR:HE1	1:G:166:LEU:HD23	1.85	0.42
1:A:125:VAL:CG2	1:A:136:TYR:HE2	2.32	0.41
1:A:58:ARG:HB2	1:A:58:ARG:HE	1.77	0.41
1:C:81:ILE:HG22	1:C:82:HIS:CD2	2.55	0.41
1:J:97:GLY:C	1:J:99:GLY:H	2.23	0.41
1:A:34:PHE:CE2	1:A:54:ASP:HB3	2.55	0.41
1:F:164:TYR:HE1	1:F:166:LEU:HD23	1.85	0.41
1:F:97:GLY:O	1:F:98:LYS:C	2.56	0.41
1:L:95:GLU:O	1:L:100:TYR:CD2	2.72	0.41
1:C:136:TYR:O	1:C:141:PHE:HB2	2.19	0.41
1:E:164:TYR:HE1	1:E:166:LEU:HD23	1.85	0.41
1:H:60:PHE:HB2	1:H:73:VAL:HG13	2.03	0.41
1:I:164:TYR:HE1	1:I:166:LEU:HD23	1.85	0.41
1:K:125:VAL:HG21	1:K:136:TYR:HE2	1.86	0.41
1:C:25:ASN:O	1:C:27:LEU:O	2.38	0.41
1:F:60:PHE:HB2	1:F:73:VAL:HG13	2.03	0.41
1:H:164:TYR:HE1	1:H:166:LEU:HD23	1.85	0.41
1:A:167:LYS:O	1:A:168:LYS:C	2.59	0.41
1:F:137:ARG:CG	1:F:163:MSE:HE3	2.45	0.41
1:K:164:TYR:HE1	1:K:166:LEU:HD23	1.85	0.41
1:A:132:ALA:HA	1:A:135:ILE:HD12	2.02	0.41
1:A:167:LYS:HG2	1:A:168:LYS:H	1.85	0.41
1:C:125:VAL:HG21	1:C:136:TYR:HE2	1.86	0.41
1:C:137:ARG:CG	1:C:163:MSE:HE3	2.47	0.41
1:E:60:PHE:HB2	1:E:73:VAL:HG13	2.03	0.41
1:G:60:PHE:HB2	1:G:73:VAL:HG13	2.03	0.41
1:H:110:GLU:O	1:H:114:SER:N	2.45	0.41
1:B:34:PHE:CE2	1:B:54:ASP:HB3	2.56	0.41
1:F:125:VAL:HG21	1:F:136:TYR:HE2	1.86	0.41
1:G:152:TYR:CD1	1:I:117:ASN:ND2	2.89	0.41
1:I:60:PHE:HB2	1:I:73:VAL:HG13	2.03	0.41
1:K:34:PHE:CE2	1:K:54:ASP:HB3	2.56	0.41
1:A:60:PHE:HB2	1:A:73:VAL:HG13	2.02	0.41
1:E:141:PHE:HA	1:E:164:TYR:O	2.21	0.41
1:E:97:GLY:O	1:E:98:LYS:C	2.59	0.41
1:A:152:TYR:CG	1:C:117:ASN:ND2	2.89	0.41
1:I:34:PHE:CE2	1:I:54:ASP:HB3	2.56	0.41
1:L:125:VAL:HG21	1:L:136:TYR:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:TYR:HE1	1:L:166:LEU:HD23	1.85	0.41
1:E:34:PHE:CE2	1:E:54:ASP:HB3	2.56	0.41
1:G:125:VAL:HG21	1:G:136:TYR:HE2	1.86	0.41
1:H:34:PHE:CE2	1:H:54:ASP:HB3	2.56	0.41
1:H:7:ILE:CG1	1:H:62:ILE:HG23	2.49	0.41
1:J:133:LEU:HD12	1:J:163:MSE:SE	2.71	0.41
1:K:82:HIS:NE2	1:L:151:TYR:CD1	2.88	0.41
1:L:34:PHE:CE2	1:L:54:ASP:HB3	2.56	0.41
1:C:164:TYR:HE1	1:C:166:LEU:HD23	1.85	0.40
1:C:34:PHE:CE2	1:C:54:ASP:HB3	2.56	0.40
1:D:60:PHE:HB2	1:D:73:VAL:HG13	2.03	0.40
1:G:34:PHE:CE2	1:G:54:ASP:HB3	2.56	0.40
1:B:164:TYR:HE1	1:B:166:LEU:HD23	1.85	0.40
1:D:84:ARG:HA	1:D:120:LYS:O	2.21	0.40
1:D:24:ASN:H	1:D:24:ASN:HD22	1.70	0.40
1:H:83:ARG:NH2	1:I:83:ARG:NH1	2.69	0.40
1:J:141:PHE:HA	1:J:164:TYR:O	2.21	0.40
1:J:34:PHE:CE2	1:J:54:ASP:HB3	2.56	0.40
1:K:133:LEU:CD1	1:K:163:MSE:SE	3.20	0.40
1:K:97:GLY:O	1:K:98:LYS:C	2.57	0.40
1:C:133:LEU:HD12	1:C:163:MSE:SE	2.71	0.40
1:E:125:VAL:HG21	1:E:136:TYR:HE2	1.86	0.40
1:F:133:LEU:HD12	1:F:163:MSE:SE	2.71	0.40
1:F:141:PHE:HA	1:F:164:TYR:O	2.21	0.40
1:F:70:VAL:HG11	1:F:100:TYR:CD2	2.56	0.40
1:I:133:LEU:HD12	1:I:163:MSE:SE	2.71	0.40
1:J:133:LEU:CD1	1:J:163:MSE:SE	3.20	0.40
1:L:133:LEU:HD12	1:L:163:MSE:SE	2.72	0.40
1:A:123:LEU:HD23	1:A:141:PHE:CE1	2.57	0.40
1:C:133:LEU:CD1	1:C:163:MSE:SE	3.20	0.40
1:C:141:PHE:HA	1:C:164:TYR:O	2.21	0.40
1:E:137:ARG:HG3	1:E:163:MSE:HE1	2.02	0.40
1:F:167:LYS:CG	1:F:168:LYS:N	2.81	0.40
1:A:130:PRO:O	1:A:133:LEU:HB3	2.20	0.40
1:D:83:ARG:CD	1:E:83:ARG:HH22	2.34	0.40
1:H:125:VAL:HG21	1:H:136:TYR:HE2	1.86	0.40
1:K:133:LEU:HD12	1:K:163:MSE:SE	2.71	0.40
1:K:141:PHE:HA	1:K:164:TYR:O	2.21	0.40
1:L:60:PHE:HB2	1:L:73:VAL:HG13	2.03	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:HIS:ND1	1:C:134:HIS:ND1[2_565]	1.14	1.06
1:C:137:ARG:NH1	1:C:137:ARG:NH1[2_565]	1.57	0.63
1:E:134:HIS:NE2	1:L:138:LYS:O[4_455]	1.64	0.56
1:C:134:HIS:ND1	1:C:134:HIS:CE1[2_565]	1.77	0.43
1:A:83:ARG:NE	1:F:83:ARG:NH2[2_555]	1.97	0.23
1:G:83:ARG:NE	1:L:83:ARG:NH2[2_555]	1.99	0.21
1:B:138:LYS:NZ	1:F:134:HIS:ND1[4_554]	2.08	0.12
1:A:134:HIS:CE1	1:H:138:LYS:O[4_555]	2.08	0.12
1:C:137:ARG:CZ	1:C:137:ARG:NH1[2_565]	2.12	0.08
1:C:137:ARG:CD	1:C:137:ARG:NH1[2_565]	2.16	0.04
1:A:83:ARG:NH2	1:F:83:ARG:NE[2_555]	2.17	0.03

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	158/170 (93%)	145 (92%)	13 (8%)	0	100	100
1	B	162/170 (95%)	143 (88%)	17 (10%)	2 (1%)	13	42
1	C	158/170 (93%)	142 (90%)	14 (9%)	2 (1%)	12	40
1	D	157/170 (92%)	145 (92%)	11 (7%)	1 (1%)	25	57
1	E	161/170 (95%)	142 (88%)	15 (9%)	4 (2%)	5	27
1	F	158/170 (93%)	141 (89%)	15 (10%)	2 (1%)	12	40
1	G	162/170 (95%)	145 (90%)	17 (10%)	0	100	100
1	H	159/170 (94%)	144 (91%)	15 (9%)	0	100	100
1	I	158/170 (93%)	145 (92%)	12 (8%)	1 (1%)	25	57
1	J	162/170 (95%)	145 (90%)	14 (9%)	3 (2%)	8	34
1	K	158/170 (93%)	144 (91%)	11 (7%)	3 (2%)	8	34
1	L	158/170 (93%)	140 (89%)	15 (10%)	3 (2%)	8	34
All	All	1911/2040 (94%)	1721 (90%)	169 (9%)	21 (1%)	14	45

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	LYS
1	D	100	TYR
1	E	98	LYS
1	L	139	SER
1	B	97	GLY
1	C	98	LYS
1	F	97	GLY
1	F	98	LYS
1	J	98	LYS
1	L	98	LYS
1	C	97	GLY
1	E	29	ILE
1	E	30	MSE
1	E	97	GLY
1	J	97	GLY
1	K	100	TYR
1	L	97	GLY
1	I	30	MSE
1	J	100	TYR
1	K	101	ALA
1	K	97	GLY

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	146/150 (97%)	145 (99%)	1 (1%)	84	90
1	B	148/150 (99%)	148 (100%)	0	100	100
1	C	146/150 (97%)	144 (99%)	2 (1%)	67	82
1	D	145/150 (97%)	145 (100%)	0	100	100
1	E	147/150 (98%)	147 (100%)	0	100	100
1	F	146/150 (97%)	145 (99%)	1 (1%)	84	90
1	G	148/150 (99%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	147/150 (98%)	147 (100%)	0	100	100
1	I	147/150 (98%)	146 (99%)	1 (1%)	84	90
1	J	148/150 (99%)	148 (100%)	0	100	100
1	K	146/150 (97%)	144 (99%)	2 (1%)	67	82
1	L	146/150 (97%)	145 (99%)	1 (1%)	84	90
All	All	1760/1800 (98%)	1752 (100%)	8 (0%)	88	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	C	42	ARG
1	C	107	LEU
1	F	100	TYR
1	I	83	ARG
1	K	27	LEU
1	K	107	LEU
1	L	139	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	134	HIS
1	B	82	HIS
1	C	24	ASN
1	D	24	ASN
1	E	24	ASN
1	G	24	ASN
1	H	24	ASN
1	I	24	ASN
1	J	24	ASN
1	K	24	ASN
1	L	24	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	171	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	171	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	I	172	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	K	171	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	I	171	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	171	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	171	SO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	160/170 (94%)	-0.10	3 (1%)	66	65	68, 131, 188, 207	0
1	B	162/170 (95%)	0.03	2 (1%)	79	78	85, 129, 186, 247	0
1	C	160/170 (94%)	-0.11	1 (0%)	89	90	75, 123, 180, 228	0
1	D	159/170 (93%)	-0.07	1 (0%)	89	90	91, 135, 191, 222	0
1	E	161/170 (94%)	-0.10	1 (0%)	89	90	77, 122, 182, 229	0
1	F	160/170 (94%)	-0.04	0	100	100	78, 125, 180, 227	0
1	G	162/170 (95%)	0.07	0	100	100	96, 133, 187, 222	0
1	H	161/170 (94%)	-0.12	0	100	100	86, 127, 182, 218	0
1	I	160/170 (94%)	0.19	3 (1%)	66	65	94, 139, 195, 230	0
1	J	162/170 (95%)	-0.08	0	100	100	85, 130, 181, 227	0
1	K	160/170 (94%)	0.04	3 (1%)	66	65	96, 133, 182, 223	0
1	L	160/170 (94%)	-0.10	2 (1%)	77	77	77, 125, 180, 220	0
All	All	1927/2040 (94%)	-0.03	16 (0%)	86	86	68, 131, 185, 247	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	TYR	3.0
1	E	28	SER	3.0
1	L	29	ILE	2.9
1	B	136	TYR	2.9
1	C	28	SER	2.9
1	I	91	ILE	2.8
1	A	155	GLY	2.8
1	B	161	ILE	2.7
1	K	41	TYR	2.5
1	D	70	VAL	2.5
1	A	65	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	155	GLY	2.3
1	I	21	HIS	2.2
1	K	136	TYR	2.0
1	K	91	ILE	2.0
1	I	136	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled '$Q< 0.9$' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	171	5/5	0.82	0.15	181,194,216,226	0
2	SO4	I	172	5/5	0.84	0.31	158,165,197,215	0
2	SO4	C	171	5/5	0.87	0.19	125,188,212,225	0
2	SO4	I	171	5/5	0.88	0.14	161,161,180,186	0
2	SO4	K	171	5/5	0.88	0.17	151,160,194,207	0
2	SO4	A	171	5/5	0.91	0.15	97,169,181,187	0

6.5 Other polymers ⓘ

There are no such residues in this entry.