



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 03:45 PM EST

PDB ID : 5C31  
Title : Constitutively active Sin recombinase catalytic domain reveals two rotational intermediates  
Authors : Trejo, C.S.; Rice, P.A.  
Deposited on : 2015-06-16  
Resolution : 3.10 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:

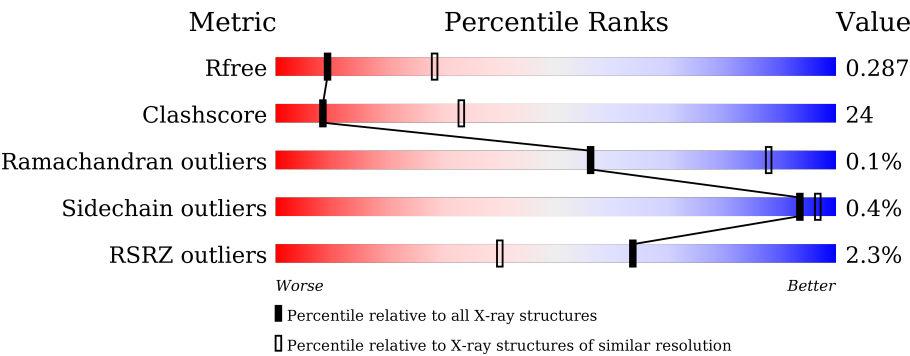
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal 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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	128	<div><div>2%</div><div>57%</div><div>41%</div><div>..</div></div>
1	B	128	<div><div>52%</div><div>47%</div><div>.</div></div>
1	C	128	<div><div>57%</div><div>41%</div><div>.</div></div>
1	D	128	<div><div>2%</div><div>55%</div><div>42%</div><div>.</div></div>
1	E	128	<div><div>9%</div><div>45%</div><div>52%</div><div>.</div></div>
1	F	128	<div><div>8%</div><div>48%</div><div>50%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	G	128	
1	H	128	
1	I	128	
1	J	128	
1	K	128	
1	L	128	

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	C	201	-	-	X	-
2	SO4	D	201	-	-	X	-
2	SO4	E	201	-	-	X	-
2	SO4	H	201	-	-	X	-
2	SO4	H	203	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13750 atoms, of which 1445 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 Sin, putative plasmid resolvase dimer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	126	Total	C	H	N	O	Se	0	0	0
			1135	645	115	175	193	7			
1	B	126	Total	C	H	N	O	Se	0	1	0
			1150	650	122	176	194	8			
1	C	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	D	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	E	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	F	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	G	122	Total	C	H	N	O	Se	0	0	0
			1105	625	117	170	186	7			
1	H	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	I	126	Total	C	H	N	O	Se	0	0	0
			1142	645	122	175	193	7			
1	J	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			
1	K	126	Total	C	H	N	O	Se	0	0	0
			1142	645	122	175	193	7			
1	L	125	Total	C	H	N	O	Se	0	0	0
			1133	641	121	173	191	7			

There are 24 discrepancies between the modelled and reference sequences:

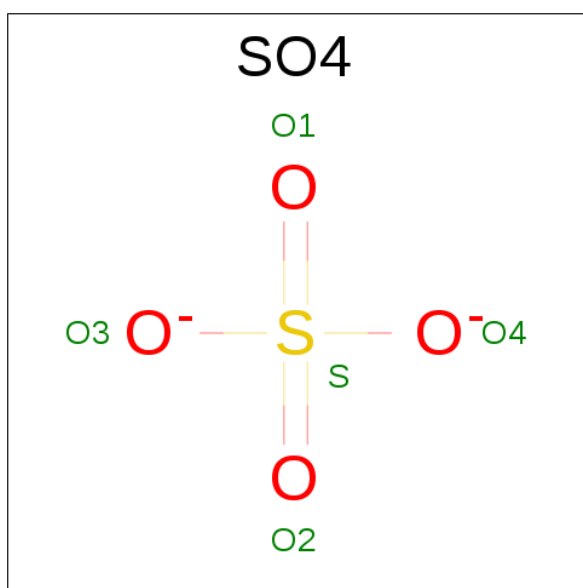
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLU	ARG	engineered mutation	UNP P20384
A	113	VAL	ILE	engineered mutation	UNP P20384
B	54	GLU	ARG	engineered mutation	UNP P20384
B	113	VAL	ILE	engineered mutation	UNP P20384
C	54	GLU	ARG	engineered mutation	UNP P20384

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Chain	Residue	Modelled	Actual	Comment	Reference
C	113	VAL	ILE	engineered mutation	UNP P20384
D	54	GLU	ARG	engineered mutation	UNP P20384
D	113	VAL	ILE	engineered mutation	UNP P20384
E	54	GLU	ARG	engineered mutation	UNP P20384
E	113	VAL	ILE	engineered mutation	UNP P20384
F	54	GLU	ARG	engineered mutation	UNP P20384
F	113	VAL	ILE	engineered mutation	UNP P20384
G	54	GLU	ARG	engineered mutation	UNP P20384
G	113	VAL	ILE	engineered mutation	UNP P20384
H	54	GLU	ARG	engineered mutation	UNP P20384
H	113	VAL	ILE	engineered mutation	UNP P20384
I	54	GLU	ARG	engineered mutation	UNP P20384
I	113	VAL	ILE	engineered mutation	UNP P20384
J	54	GLU	ARG	engineered mutation	UNP P20384
J	113	VAL	ILE	engineered mutation	UNP P20384
K	54	GLU	ARG	engineered mutation	UNP P20384
K	113	VAL	ILE	engineered mutation	UNP P20384
L	54	GLU	ARG	engineered mutation	UNP P20384
L	113	VAL	ILE	engineered mutation	UNP P20384

- 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 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	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	H	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	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

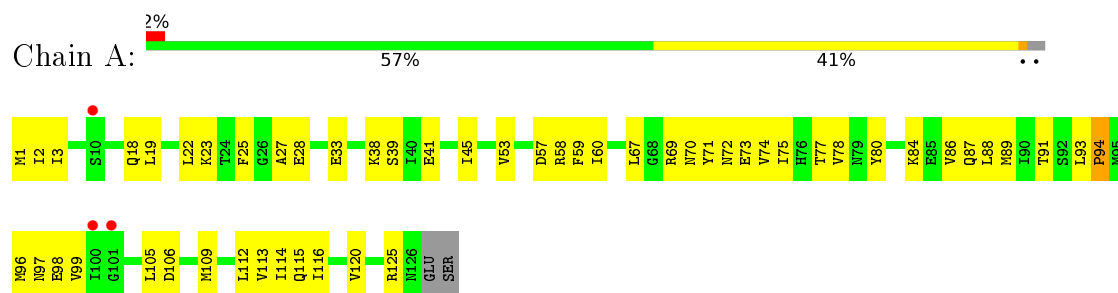
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	8	Total O 8 8	0	0
3	C	2	Total O 2 2	0	0
3	E	1	Total O 1 1	0	0
3	F	2	Total O 2 2	0	0
3	G	3	Total O 3 3	0	0
3	H	8	Total O 8 8	0	0
3	I	3	Total O 3 3	0	0
3	J	4	Total O 4 4	0	0
3	K	2	Total O 2 2	0	0
3	L	3	Total O 3 3	0	0

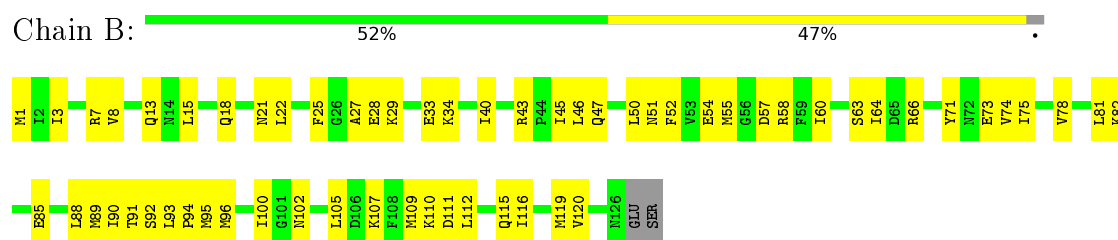
### 3 Residue-property plots

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

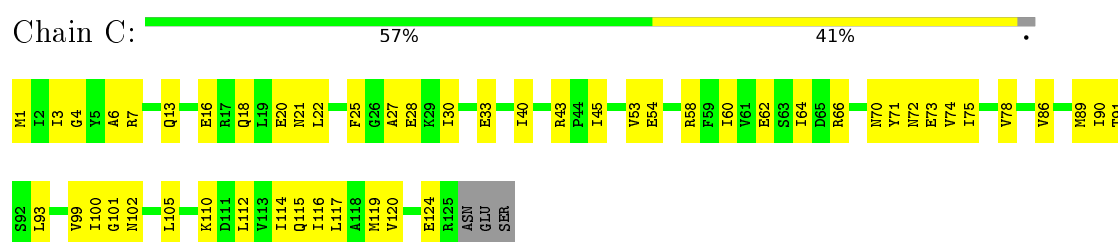
- Molecule 1: Sin, putative plasmid resolvase dimer



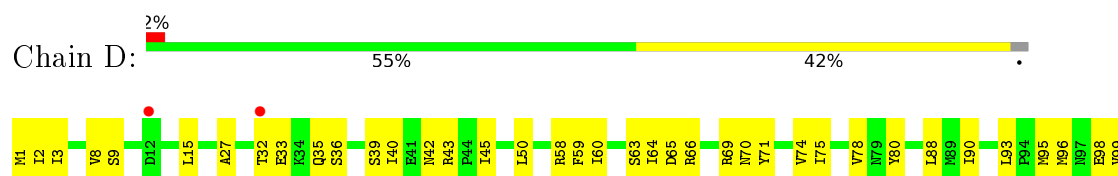
- Molecule 1: Sin, putative plasmid resolvase dimer



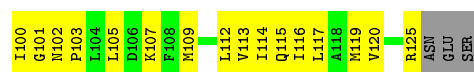
- Molecule 1: Sin, putative plasmid resolvase dimer



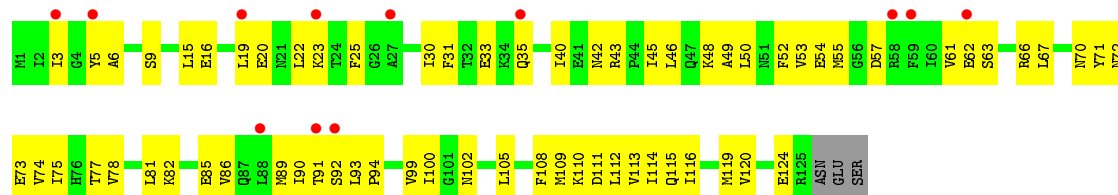
- Molecule 1: Sin, putative plasmid resolvase dimer



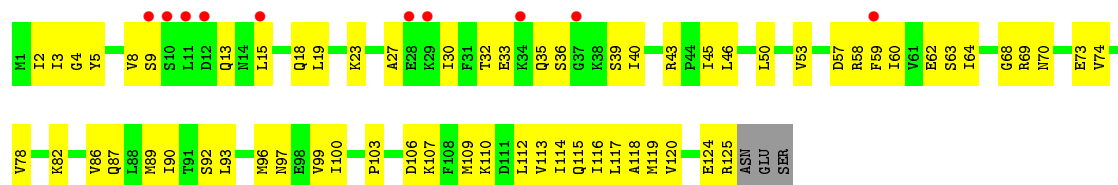




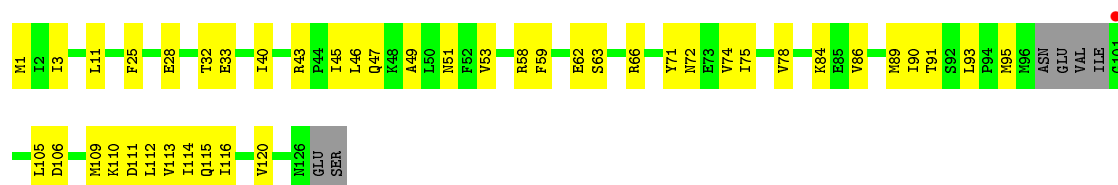
- Molecule 1: Sin, putative plasmid resolvase dimer



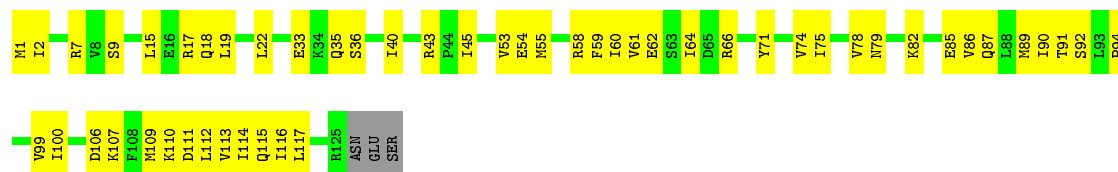
- Molecule 1: Sin, putative plasmid resolvase dimer



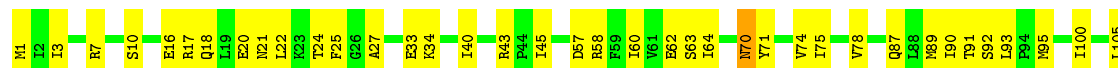
- Molecule 1: Sin, putative plasmid resolvase dimer



- Molecule 1: Sin, putative plasmid resolvase dimer

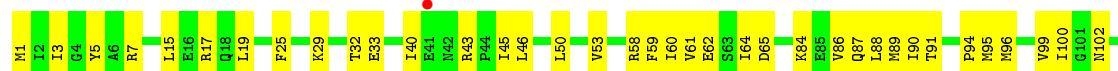


- Molecule 1: Sin, putative plasmid resolvase dimer

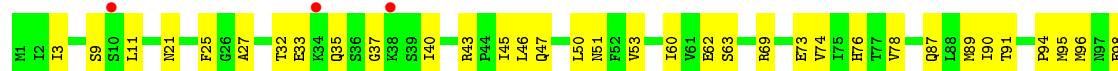




- Molecule 1: Sin, putative plasmid resolvase dimer



- Molecule 1: Sin, putative plasmid resolvase dimer



- Molecule 1: Sin, putative plasmid resolvase dimer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.59Å 152.72Å 193.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.10 49.75 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-3.10) 88.0 (49.75-3.04)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.227 , 0.286 0.226 , 0.287	Depositor DCC
$R_{free}$ test set	1753 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.20	0/1025	0.33	0/1365
1	B	0.21	0/1033	0.33	0/1375
1	C	0.20	0/1017	0.33	0/1354
1	D	0.20	0/1017	0.33	0/1354
1	E	0.20	0/1017	0.34	0/1354
1	F	0.20	0/1017	0.33	0/1354
1	G	0.20	0/992	0.33	0/1318
1	H	0.20	0/1017	0.34	0/1354
1	I	0.20	0/1025	0.34	0/1365
1	J	0.20	0/1017	0.34	0/1354
1	K	0.21	0/1025	0.34	0/1365
1	L	0.21	0/1017	0.34	0/1354
All	All	0.20	0/12219	0.34	0/16266

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1020	115	1053	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1028	122	1061	68	0
1	C	1012	121	1047	59	0
1	D	1012	121	1047	63	0
1	E	1012	121	1047	75	0
1	F	1012	121	1047	83	0
1	G	988	117	1020	44	0
1	H	1012	121	1047	52	0
1	I	1020	122	1053	39	0
1	J	1012	121	1047	48	0
1	K	1020	122	1053	48	0
1	L	1012	121	1047	39	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	2	0
2	D	5	0	0	4	0
2	E	5	0	0	2	0
2	F	5	0	0	1	0
2	G	5	0	0	0	0
2	H	15	0	0	4	0
2	I	20	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	1	0
2	L	10	0	0	1	0
3	A	4	0	0	0	0
3	B	8	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	1	0
3	G	3	0	0	0	0
3	H	8	0	0	0	0
3	I	3	0	0	0	0
3	J	4	0	0	0	0
3	K	2	0	0	0	0
3	L	3	0	0	0	0
All	All	12305	1445	12569	599	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 24.

All (599) 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:E:89:MSE:HE3	1:E:94:PRO:HB3	1.40	1.02
1:B:60:ILE:HG22	1:B:89:MSE:HB3	1.45	0.97
1:B:40:ILE:HG22	1:B:43:ARG:HH21	1.32	0.95
1:F:27:ALA:HB2	1:F:60:ILE:HD11	1.49	0.94
1:H:58:ARG:HH11	1:H:89:MSE:HE1	1.34	0.91
1:J:95:MSE:HE2	1:J:110:LYS:HG2	1.51	0.91
1:J:105:LEU:HD23	1:K:120:VAL:HG13	1.55	0.89
1:C:21:ASN:HB3	1:C:91:THR:HG21	1.53	0.86
1:L:100:ILE:HD12	1:L:105:LEU:HB3	1.56	0.85
1:D:33:GLU:HG3	1:D:45:ILE:HD12	1.59	0.85
1:F:78:VAL:HG11	1:F:114:ILE:HG21	1.56	0.85
1:C:60:ILE:HG22	1:C:89:MSE:HB3	1.59	0.84
1:E:78:VAL:HG12	1:E:82:LYS:HE3	1.58	0.84
1:E:3:ILE:HD11	1:E:31:PHE:HE2	1.42	0.84
1:C:33:GLU:HG3	1:C:45:ILE:HD12	1.60	0.83
1:K:33:GLU:HG3	1:K:45:ILE:HD12	1.57	0.82
1:G:33:GLU:HG3	1:G:45:ILE:HD12	1.61	0.81
1:G:53:VAL:HG11	1:G:86:VAL:HG11	1.61	0.81
1:F:33:GLU:HG3	1:F:45:ILE:HD12	1.63	0.80
1:F:99:VAL:HG13	1:H:100:ILE:HG12	1.62	0.80
1:F:69:ARG:HH12	1:F:124:GLU:HB2	1.46	0.80
1:J:89:MSE:HE3	1:J:94:PRO:HB3	1.63	0.79
1:C:40:ILE:HG22	1:C:43:ARG:HH21	1.48	0.78
1:B:93:LEU:HD22	1:D:105:LEU:HD22	1.65	0.78
1:A:105:LEU:HD21	1:C:93:LEU:HD11	1.65	0.78
1:A:105:LEU:HD13	1:B:119:MSE:HE1	1.66	0.78
1:A:96:MSE:HG2	1:A:97:ASN:H	1.50	0.77
1:B:116:ILE:HG21	1:C:119:MSE:HE1	1.66	0.77
1:B:7:ARG:HD3	1:B:43:ARG:HH11	1.50	0.76
1:G:62:GLU:HA	1:G:91:THR:HB	1.67	0.76
1:J:33:GLU:HG3	1:J:45:ILE:HD12	1.69	0.75
1:G:93:LEU:HD13	1:G:95:MSE:HG3	1.67	0.75
1:E:3:ILE:HD11	1:E:31:PHE:CE2	2.23	0.74
1:J:3:ILE:HD13	1:J:53:VAL:HG12	1.70	0.74
1:K:95:MSE:HE2	1:K:110:LYS:HG2	1.71	0.73
1:F:53:VAL:HG11	1:F:86:VAL:HG11	1.71	0.73
1:B:109:MSE:HE3	1:D:112:LEU:HD23	1.69	0.73
1:B:27:ALA:HB2	1:B:60:ILE:HD11	1.70	0.72
1:H:22:LEU:HD22	1:H:60:ILE:HG22	1.71	0.72
1:L:102:ASN:HD22	1:L:105:LEU:HD13	1.55	0.71
1:H:9:SER:OG	2:H:201:SO4:O3	2.07	0.71
1:B:47:GLN:O	1:B:51:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:ARG:HD3	1:F:89:MSE:HE1	1.74	0.70
1:C:7:ARG:HD3	1:C:43:ARG:HH11	1.56	0.69
1:C:25:PHE:CE1	1:C:91:THR:HG23	2.27	0.69
1:L:60:ILE:HG21	1:L:89:MSE:HE2	1.75	0.69
1:L:60:ILE:CG2	1:L:89:MSE:HE2	2.23	0.68
1:B:109:MSE:HE3	1:D:112:LEU:HB3	1.75	0.68
1:F:40:ILE:HG22	1:F:43:ARG:HH21	1.58	0.68
1:E:25:PHE:CE1	1:E:91:THR:HG23	2.29	0.68
1:I:33:GLU:HG3	1:I:45:ILE:HD12	1.75	0.68
1:K:27:ALA:HB2	1:K:60:ILE:HD11	1.75	0.67
1:K:95:MSE:CE	1:K:110:LYS:HG2	2.24	0.67
1:E:89:MSE:HE3	1:E:94:PRO:CB	2.21	0.67
1:L:58:ARG:HG2	1:L:60:ILE:HG23	1.76	0.67
1:J:112:LEU:HD22	1:K:116:ILE:HD13	1.77	0.67
1:F:109:MSE:HE3	1:H:109:MSE:HE2	1.77	0.66
1:A:72:ASN:HD21	1:B:107:LYS:HD3	1.60	0.66
1:E:31:PHE:HB3	1:E:45:ILE:HG22	1.77	0.66
1:K:60:ILE:CG2	1:K:89:MSE:HE2	2.25	0.66
1:F:69:ARG:NH1	1:F:124:GLU:HB2	2.10	0.66
1:K:60:ILE:HG21	1:K:89:MSE:HE2	1.78	0.66
1:C:40:ILE:HG22	1:C:43:ARG:NH2	2.10	0.66
1:E:78:VAL:CG1	1:E:82:LYS:HE3	2.26	0.66
1:I:95:MSE:HE3	1:I:110:LYS:HG3	1.77	0.66
1:L:102:ASN:ND2	1:L:105:LEU:HD13	2.11	0.66
1:A:105:LEU:HD11	1:A:109:MSE:HE2	1.78	0.65
1:F:96:MSE:HE2	1:F:96:MSE:HA	1.78	0.65
1:A:115:GLN:OE1	1:B:115:GLN:NE2	2.30	0.65
1:H:9:SER:OG	2:H:201:SO4:S	2.54	0.65
1:A:25:PHE:CE1	1:A:91:THR:HG23	2.32	0.64
1:L:17:ARG:NH1	1:L:62:GLU:OE1	2.30	0.64
1:D:64:ILE:HD11	1:D:90:ILE:HD11	1.78	0.64
1:A:27:ALA:HB2	1:A:60:ILE:HD11	1.79	0.64
1:L:60:ILE:HG22	1:L:89:MSE:HB3	1.79	0.64
1:C:62:GLU:HA	1:C:91:THR:HB	1.80	0.64
1:E:63:SER:HA	1:E:90:ILE:CG2	2.28	0.64
1:G:25:PHE:CE1	1:G:91:THR:HG23	2.33	0.64
1:J:95:MSE:CE	1:J:110:LYS:HG2	2.27	0.64
1:K:95:MSE:HE1	1:K:110:LYS:HA	1.80	0.64
1:L:40:ILE:HG22	1:L:43:ARG:HH21	1.62	0.64
1:F:78:VAL:HG11	1:F:114:ILE:HD13	1.79	0.64
1:D:9:SER:HB3	2:D:201:SO4:O3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLN:HB3	1:D:43:ARG:HD3	1.79	0.63
1:E:43:ARG:NH1	1:E:46:LEU:HD22	2.14	0.63
1:E:109:MSE:HE2	1:G:109:MSE:HE3	1.80	0.63
1:E:43:ARG:HH12	1:E:46:LEU:HD22	1.62	0.63
1:E:90:ILE:HG22	1:E:92:SER:H	1.64	0.63
1:D:8:VAL:CG2	1:D:15:LEU:HD13	2.28	0.63
1:J:33:GLU:CG	1:J:45:ILE:HD12	2.28	0.63
1:A:60:ILE:HG22	1:A:89:MSE:HB3	1.79	0.63
1:E:62:GLU:HA	1:E:91:THR:HB	1.81	0.63
1:B:54:GLU:HB3	1:F:58:ARG:HH22	1.64	0.63
1:J:60:ILE:HG22	1:J:89:MSE:HB3	1.81	0.63
1:G:40:ILE:HG22	1:G:43:ARG:NH2	2.14	0.62
1:G:43:ARG:HH12	1:G:46:LEU:HD22	1.64	0.62
1:D:27:ALA:HB2	1:D:60:ILE:HD11	1.80	0.62
1:F:93:LEU:CD2	1:F:117:LEU:HD21	2.30	0.62
1:B:116:ILE:HG21	1:C:119:MSE:CE	2.29	0.62
1:C:27:ALA:HB3	1:C:30:ILE:HD11	1.82	0.61
1:E:6:ALA:HB2	1:E:22:LEU:CD1	2.30	0.61
1:F:53:VAL:HG12	1:F:86:VAL:HG21	1.83	0.61
1:F:8:VAL:HG13	1:F:15:LEU:HD13	1.83	0.61
1:B:7:ARG:HD3	1:B:43:ARG:NH1	2.15	0.61
1:L:64:ILE:HG12	1:L:90:ILE:HD13	1.82	0.60
1:L:93:LEU:HD12	1:L:117:LEU:HD11	1.81	0.60
1:A:69:ARG:HG2	1:A:125:ARG:HD2	1.82	0.60
1:I:95:MSE:CE	1:I:110:LYS:HG3	2.31	0.60
1:H:75:ILE:O	1:H:79:ASN:ND2	2.33	0.60
1:C:115:GLN:NE2	1:D:115:GLN:OE1	2.35	0.60
1:H:58:ARG:HD3	1:H:89:MSE:HE3	1.84	0.60
1:H:82:LYS:NZ	1:H:111:ASP:OD1	2.33	0.59
1:F:78:VAL:CG1	1:F:114:ILE:HD13	2.33	0.59
1:B:60:ILE:HG22	1:B:89:MSE:CB	2.27	0.59
1:B:116:ILE:HD13	1:C:116:ILE:HG23	1.85	0.59
1:F:93:LEU:HD22	1:F:117:LEU:HD21	1.85	0.59
1:D:78:VAL:HG21	1:D:114:ILE:HG21	1.85	0.59
1:E:5:TYR:HB3	1:E:61:VAL:HG22	1.85	0.58
1:F:120:VAL:O	1:F:124:GLU:HG2	2.03	0.58
1:E:93:LEU:HD21	1:G:105:LEU:HD23	1.85	0.58
1:A:33:GLU:HA	1:A:45:ILE:HD12	1.85	0.58
1:A:33:GLU:HG3	1:A:45:ILE:HD12	1.86	0.58
1:B:21:ASN:HB3	1:B:91:THR:HG21	1.86	0.58
1:C:66:ARG:NH2	2:C:201:SO4:S	2.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ILE:HG22	1:F:92:SER:H	1.69	0.58
1:E:115:GLN:NE2	1:F:115:GLN:OE1	2.38	0.57
1:K:33:GLU:CG	1:K:45:ILE:HD12	2.31	0.57
1:B:25:PHE:CE2	1:B:91:THR:HG23	2.40	0.57
1:I:40:ILE:HG22	1:I:43:ARG:HH21	1.70	0.57
1:A:58:ARG:HG3	1:A:87:GLN:HG3	1.86	0.57
1:C:64:ILE:HD11	1:C:90:ILE:HD11	1.87	0.57
1:I:109:MSE:HE1	1:L:109:MSE:HE3	1.87	0.57
1:H:58:ARG:NH1	1:H:89:MSE:HE1	2.13	0.57
1:E:50:LEU:O	1:E:53:VAL:HG22	2.05	0.57
1:H:55:MSE:HE3	1:H:85:GLU:OE1	2.04	0.57
1:L:64:ILE:HD11	1:L:90:ILE:HD11	1.87	0.57
1:F:78:VAL:HG21	1:F:114:ILE:CG2	2.34	0.57
1:E:119:MSE:HE1	1:H:116:ILE:HG21	1.86	0.57
1:E:54:GLU:O	1:E:86:VAL:HG22	2.05	0.57
1:G:33:GLU:HA	1:G:45:ILE:HD12	1.86	0.57
1:J:7:ARG:NH2	1:J:65:ASP:O	2.36	0.57
1:F:112:LEU:HD23	1:H:109:MSE:HE3	1.86	0.56
1:E:108:PHE:HZ	1:F:116:ILE:HG12	1.68	0.56
1:J:112:LEU:HD22	1:K:116:ILE:CD1	2.35	0.56
1:J:15:LEU:HG	1:J:19:LEU:HD13	1.87	0.56
1:E:31:PHE:HB3	1:E:45:ILE:CG2	2.36	0.56
1:F:100:ILE:HG13	1:F:109:MSE:SE	2.56	0.56
1:F:64:ILE:CD1	1:F:90:ILE:HD11	2.36	0.56
1:L:17:ARG:O	1:L:21:ASN:ND2	2.34	0.55
1:B:109:MSE:HB3	1:D:109:MSE:HE3	1.88	0.55
1:B:40:ILE:HG22	1:B:43:ARG:NH2	2.12	0.55
1:E:102:ASN:HB3	1:E:105:LEU:HD13	1.87	0.55
1:I:60:ILE:CG2	1:I:89:MSE:HE2	2.37	0.55
1:C:1:MSE:HG3	1:C:28:GLU:OE2	2.06	0.55
1:B:55:MSE:HG3	1:B:85:GLU:CB	2.36	0.55
1:E:112:LEU:O	1:E:116:ILE:HG13	2.07	0.55
1:F:69:ARG:HG3	1:F:125:ARG:NH2	2.21	0.55
1:H:99:VAL:HA	1:H:106:ASP:OD2	2.07	0.55
1:K:87:GLN:HG2	1:K:96:MSE:HE3	1.87	0.55
1:K:87:GLN:HG2	1:K:96:MSE:CE	2.37	0.55
1:C:6:ALA:HB2	1:C:22:LEU:CD1	2.37	0.55
1:C:33:GLU:CG	1:C:45:ILE:HD12	2.33	0.55
1:E:109:MSE:HE2	1:G:109:MSE:CE	2.36	0.55
1:I:18:GLN:O	1:I:22:LEU:HG	2.07	0.55
1:B:82:LYS:NZ	1:B:111:ASP:OD2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:GLU:CG	1:G:45:ILE:HD12	2.35	0.54
1:I:25:PHE:CE1	1:I:91:THR:HG23	2.42	0.54
1:E:108:PHE:CZ	1:F:116:ILE:HG12	2.42	0.54
1:I:64:ILE:HG12	1:I:90:ILE:HD13	1.89	0.54
1:C:93:LEU:HD12	1:C:117:LEU:HD11	1.90	0.54
1:H:106:ASP:OD2	1:H:110:LYS:HE2	2.08	0.54
1:G:93:LEU:O	1:G:93:LEU:HD12	2.07	0.54
1:G:106:ASP:OD2	1:G:110:LYS:HE3	2.07	0.54
1:F:99:VAL:CG1	1:H:100:ILE:HG12	2.35	0.54
1:D:66:ARG:NH2	2:D:201:SO4:O1	2.30	0.54
1:H:61:VAL:O	1:H:90:ILE:HA	2.08	0.54
1:H:66:ARG:NH2	2:H:201:SO4:O2	2.40	0.54
1:D:35:GLN:HG3	1:D:36:SER:H	1.73	0.54
1:H:7:ARG:HD3	1:H:43:ARG:HH11	1.73	0.54
1:F:39:SER:O	1:F:43:ARG:NE	2.42	0.53
1:F:78:VAL:O	1:F:82:LYS:HG2	2.08	0.53
1:F:35:GLN:HG3	1:F:36:SER:H	1.72	0.53
1:B:55:MSE:HE3	1:F:89:MSE:HE1	1.90	0.53
1:H:112:LEU:O	1:H:116:ILE:HG13	2.09	0.53
1:K:47:GLN:O	1:K:51:ASN:ND2	2.33	0.53
1:L:55:MSE:HG3	1:L:85:GLU:HB2	1.90	0.53
1:C:66:ARG:NH2	2:C:201:SO4:O1	2.41	0.53
1:A:25:PHE:CZ	1:A:91:THR:HG23	2.44	0.53
1:A:113:VAL:HG13	1:C:100:ILE:CD1	2.39	0.53
1:I:1:MSE:N	1:I:57:ASP:OD1	2.42	0.53
1:B:18:GLN:O	1:B:22:LEU:HG	2.08	0.53
1:I:64:ILE:HG12	1:I:90:ILE:CD1	2.39	0.53
1:J:108:PHE:CZ	1:J:112:LEU:HD12	2.44	0.53
1:C:112:LEU:HD13	1:D:112:LEU:HD13	1.90	0.53
1:D:69:ARG:HD3	1:D:125:ARG:HB2	1.91	0.53
1:K:35:GLN:HB3	1:K:43:ARG:HG2	1.91	0.53
1:I:105:LEU:HD13	1:L:116:ILE:CG2	2.39	0.52
1:D:64:ILE:HG12	1:D:90:ILE:HD13	1.92	0.52
1:F:58:ARG:NH1	3:F:301:HOH:O	2.43	0.52
1:E:6:ALA:HB2	1:E:22:LEU:HD11	1.92	0.52
1:H:18:GLN:O	1:H:22:LEU:HG	2.09	0.52
1:G:53:VAL:HG12	1:G:86:VAL:HG21	1.91	0.52
1:E:67:LEU:O	1:E:67:LEU:HD23	2.09	0.52
1:F:32:THR:O	1:F:45:ILE:HG21	2.09	0.52
1:G:74:VAL:O	1:G:78:VAL:HG23	2.09	0.52
1:A:39:SER:HA	1:A:73:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HD11	1:B:52:PHE:CE2	2.44	0.52
1:E:48:LYS:O	1:E:52:PHE:HB2	2.10	0.52
1:F:87:GLN:NE2	1:F:97:ASN:OD1	2.39	0.52
1:K:98:GLU:O	1:K:98:GLU:HG3	2.09	0.52
1:H:40:ILE:HG22	1:H:43:ARG:HH21	1.75	0.52
1:L:66:ARG:NH1	2:L:201:SO4:O1	2.42	0.52
1:H:64:ILE:HD11	1:H:90:ILE:HD11	1.91	0.52
1:K:63:SER:HA	1:K:90:ILE:HG23	1.91	0.52
1:C:74:VAL:O	1:C:78:VAL:HG23	2.10	0.51
1:E:55:MSE:HE3	1:E:85:GLU:OE1	2.10	0.51
1:J:100:ILE:HG22	1:J:102:ASN:H	1.75	0.51
1:C:33:GLU:CD	1:C:45:ILE:HB	2.30	0.51
1:F:62:GLU:O	1:F:92:SER:OG	2.25	0.51
1:B:74:VAL:O	1:B:78:VAL:HG23	2.11	0.51
1:D:116:ILE:O	1:D:120:VAL:HG23	2.11	0.51
1:D:33:GLU:CD	1:D:45:ILE:HB	2.31	0.51
1:E:63:SER:HA	1:E:90:ILE:HG23	1.91	0.51
1:F:93:LEU:HD22	1:F:117:LEU:HD11	1.92	0.51
1:K:3:ILE:HD13	1:K:53:VAL:HG12	1.91	0.51
1:A:70:ASN:ND2	1:A:73:GLU:HG3	2.26	0.51
1:I:92:SER:C	1:I:93:LEU:HD12	2.31	0.51
1:A:99:VAL:HB	1:A:106:ASP:OD2	2.11	0.51
1:E:74:VAL:O	1:E:78:VAL:HG23	2.11	0.51
1:A:94:PRO:HD2	1:C:99:VAL:O	2.10	0.51
1:C:18:GLN:O	1:C:22:LEU:HG	2.11	0.51
1:I:33:GLU:CD	1:I:45:ILE:HB	2.32	0.51
1:A:59:PHE:O	1:A:88:LEU:HD12	2.11	0.51
1:F:63:SER:HA	1:F:90:ILE:CG2	2.41	0.51
1:A:78:VAL:HG21	1:A:114:ILE:HG21	1.92	0.51
1:A:96:MSE:HG2	1:A:97:ASN:N	2.24	0.51
1:B:89:MSE:HA	1:B:96[A]:MSE:HE1	1.93	0.51
1:C:116:ILE:O	1:C:120:VAL:HG23	2.11	0.51
1:E:19:LEU:HD22	1:E:30:ILE:HG21	1.92	0.51
1:F:109:MSE:CE	1:H:109:MSE:HE2	2.40	0.51
1:J:3:ILE:CD1	1:J:53:VAL:HG12	2.39	0.51
1:K:25:PHE:CE1	1:K:91:THR:HG23	2.46	0.51
1:B:89:MSE:HA	1:B:96[A]:MSE:CE	2.42	0.50
1:D:66:ARG:NH2	2:D:201:SO4:O4	2.44	0.50
1:L:105:LEU:O	1:L:109:MSE:HG2	2.12	0.50
1:A:2:ILE:N	1:A:2:ILE:HD12	2.26	0.50
1:A:70:ASN:HD22	1:A:73:GLU:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:O	1:B:109:MSE:HG3	2.12	0.50
1:B:71:TYR:O	1:B:75:ILE:HG12	2.12	0.50
1:F:33:GLU:CG	1:F:45:ILE:HD12	2.36	0.50
1:G:33:GLU:CD	1:G:45:ILE:HB	2.32	0.50
1:J:33:GLU:CB	1:J:45:ILE:HD12	2.41	0.50
1:B:8:VAL:HG13	1:B:15:LEU:HD13	1.93	0.50
1:D:109:MSE:O	1:D:113:VAL:HG23	2.12	0.50
1:G:112:LEU:O	1:G:116:ILE:HG13	2.10	0.50
1:G:1:MSE:HG3	1:G:28:GLU:CD	2.32	0.50
1:E:16:GLU:O	1:E:20:GLU:HB2	2.12	0.50
1:G:78:VAL:HG21	1:G:114:ILE:HG21	1.93	0.50
1:G:90:ILE:HD12	1:G:90:ILE:N	2.27	0.50
1:J:17:ARG:NH1	1:J:62:GLU:OE1	2.45	0.50
1:A:74:VAL:O	1:A:78:VAL:HG23	2.12	0.50
1:C:102:ASN:CG	1:C:105:LEU:HD13	2.33	0.50
1:B:100:ILE:HD13	1:D:99:VAL:HG11	1.94	0.49
1:B:57:ASP:OD1	1:F:97:ASN:ND2	2.44	0.49
1:D:98:GLU:OE1	1:H:1:MSE:N	2.41	0.49
1:J:58:ARG:HG2	1:J:60:ILE:HG23	1.94	0.49
1:D:8:VAL:HG21	1:D:15:LEU:HD13	1.94	0.49
1:K:3:ILE:N	1:K:3:ILE:HD12	2.27	0.49
1:C:64:ILE:HG12	1:C:90:ILE:HD13	1.93	0.49
1:D:105:LEU:O	1:D:109:MSE:HG3	2.11	0.49
1:G:93:LEU:CD1	1:G:95:MSE:HE3	2.42	0.49
1:J:25:PHE:CE1	1:J:91:THR:HB	2.47	0.49
1:E:90:ILE:N	1:E:90:ILE:HD12	2.27	0.49
1:A:105:LEU:CD2	1:C:93:LEU:HD11	2.40	0.49
1:F:64:ILE:HG12	1:F:90:ILE:CD1	2.42	0.49
1:H:33:GLU:CD	1:H:45:ILE:HB	2.32	0.49
1:I:62:GLU:HA	1:I:91:THR:HB	1.94	0.49
1:L:1:MSE:HG2	1:L:3:ILE:CD1	2.43	0.49
1:I:40:ILE:HG22	1:I:43:ARG:NH2	2.28	0.49
1:J:95:MSE:HE1	1:J:110:LYS:HA	1.94	0.49
1:G:3:ILE:N	1:G:3:ILE:HD12	2.28	0.49
1:D:78:VAL:HG21	1:D:114:ILE:CG2	2.43	0.49
1:E:120:VAL:O	1:E:124:GLU:HG3	2.12	0.49
1:F:63:SER:HA	1:F:90:ILE:HG21	1.94	0.49
1:H:15:LEU:O	1:H:19:LEU:HD13	2.12	0.49
1:D:96:MSE:HE1	1:H:87:GLN:OE1	2.12	0.49
1:B:54:GLU:HB3	1:F:58:ARG:NH2	2.27	0.49
1:E:66:ARG:HA	1:E:66:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:ILE:HG21	1:I:89:MSE:HE2	1.94	0.49
1:K:112:LEU:O	1:K:116:ILE:HG13	2.13	0.49
1:G:32:THR:O	1:G:45:ILE:HD13	2.13	0.48
1:K:32:THR:O	1:K:45:ILE:HG21	2.13	0.48
1:L:3:ILE:HG13	1:L:29:LYS:HB3	1.95	0.48
1:B:109:MSE:HE1	1:D:109:MSE:O	2.13	0.48
1:E:3:ILE:HD13	1:E:49:ALA:HB1	1.94	0.48
1:F:58:ARG:HD3	1:F:89:MSE:CE	2.40	0.48
1:F:43:ARG:HH22	1:F:68:GLY:HA2	1.78	0.48
1:G:49:ALA:O	1:G:53:VAL:HG23	2.12	0.48
1:F:64:ILE:HG13	1:F:117:LEU:HB3	1.95	0.48
1:J:3:ILE:N	1:J:3:ILE:HD12	2.29	0.48
1:K:109:MSE:HE3	1:K:110:LYS:CG	2.43	0.48
1:K:62:GLU:HA	1:K:91:THR:HB	1.95	0.48
1:B:25:PHE:HE2	1:B:91:THR:HG23	1.77	0.48
1:C:112:LEU:O	1:C:116:ILE:HG13	2.13	0.48
1:E:66:ARG:NH2	2:E:201:SO4:O1	2.31	0.48
1:J:116:ILE:HD11	1:K:116:ILE:HD11	1.95	0.48
1:J:50:LEU:O	1:J:84:LYS:NZ	2.41	0.48
1:F:18:GLN:HG3	1:F:62:GLU:OE2	2.13	0.48
1:A:1:MSE:HE3	1:A:28:GLU:CD	2.34	0.48
1:B:109:MSE:HE3	1:D:112:LEU:CD2	2.41	0.48
1:F:64:ILE:HD11	1:F:90:ILE:HD11	1.96	0.48
1:D:39:SER:HB3	1:D:42:ASN:OD1	2.14	0.48
1:I:10:SER:HA	1:I:34:LYS:HE2	1.96	0.48
1:B:1:MSE:HG3	1:B:28:GLU:OE1	2.13	0.48
1:H:54:GLU:O	1:H:86:VAL:HG22	2.14	0.48
1:D:35:GLN:HG2	1:D:43:ARG:HG2	1.96	0.48
1:H:113:VAL:O	1:H:117:LEU:HG	2.13	0.48
1:B:8:VAL:CG1	1:B:15:LEU:HD13	2.44	0.48
1:E:35:GLN:NE2	1:E:42:ASN:HB3	2.28	0.47
1:L:62:GLU:HA	1:L:91:THR:OG1	2.13	0.47
1:A:1:MSE:HG2	1:A:3:ILE:CD1	2.45	0.47
1:B:13:GLN:NE2	2:B:201:SO4:O4	2.47	0.47
1:A:99:VAL:HG13	1:C:93:LEU:CD2	2.44	0.47
1:E:54:GLU:N	1:E:57:ASP:OD2	2.44	0.47
1:L:116:ILE:O	1:L:120:VAL:HG23	2.14	0.47
1:H:58:ARG:HD3	1:H:89:MSE:CE	2.44	0.47
1:K:21:ASN:OD1	1:K:91:THR:HG21	2.14	0.47
1:B:95:MSE:HE2	1:D:101:GLY:CA	2.44	0.47
1:B:109:MSE:CE	1:D:112:LEU:HD23	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:TYR:O	1:D:75:ILE:HG12	2.14	0.47
1:H:33:GLU:HG3	1:H:45:ILE:HD12	1.97	0.47
1:J:123:GLN:NE2	1:L:123:GLN:OE1	2.47	0.47
1:C:16:GLU:O	1:C:20:GLU:HG2	2.13	0.47
1:C:3:ILE:N	1:C:3:ILE:HD12	2.29	0.47
1:I:1:MSE:HG3	1:I:3:ILE:CD1	2.45	0.47
1:F:2:ILE:HG12	1:F:58:ARG:HD2	1.97	0.47
1:A:105:LEU:O	1:A:109:MSE:HG2	2.15	0.47
1:F:99:VAL:O	1:F:100:ILE:HD13	2.14	0.47
1:J:99:VAL:HG21	1:J:109:MSE:HE1	1.97	0.47
1:L:109:MSE:O	1:L:113:VAL:HG23	2.15	0.47
1:F:100:ILE:O	1:F:100:ILE:HG22	2.15	0.47
1:G:93:LEU:HD11	1:G:95:MSE:HE3	1.96	0.47
1:J:46:LEU:O	1:J:50:LEU:HG	2.14	0.47
1:K:108:PHE:CZ	1:K:112:LEU:HD11	2.50	0.47
1:L:40:ILE:HG22	1:L:43:ARG:NH2	2.29	0.47
1:E:9:SER:HA	1:E:35:GLN:O	2.15	0.47
1:F:53:VAL:HG13	1:F:57:ASP:HB2	1.97	0.47
1:G:47:GLN:O	1:G:51:ASN:ND2	2.36	0.47
1:D:112:LEU:O	1:D:116:ILE:HG13	2.15	0.47
1:F:19:LEU:HB3	1:F:23:LYS:HE3	1.97	0.47
1:C:40:ILE:HG23	1:C:73:GLU:OE2	2.15	0.47
1:D:66:ARG:NH2	2:D:201:SO4:S	2.88	0.47
1:H:9:SER:OG	2:H:201:SO4:O4	2.33	0.47
1:J:87:GLN:OE1	1:J:96:MSE:HE1	2.15	0.47
1:C:120:VAL:O	1:C:124:GLU:HG3	2.15	0.46
1:C:58:ARG:HG2	1:C:60:ILE:HG23	1.96	0.46
1:E:109:MSE:O	1:E:113:VAL:HG23	2.15	0.46
1:F:74:VAL:O	1:F:78:VAL:HG23	2.15	0.46
1:F:40:ILE:HG22	1:F:43:ARG:NH2	2.29	0.46
1:B:33:GLU:HG3	1:B:45:ILE:HD12	1.97	0.46
1:D:78:VAL:HG11	1:D:114:ILE:HD13	1.96	0.46
1:I:7:ARG:HD3	1:I:43:ARG:HH11	1.80	0.46
1:K:69:ARG:HA	1:K:121:SER:OG	2.15	0.46
1:A:38:LYS:HB2	1:A:125:ARG:NH2	2.31	0.46
1:D:32:THR:O	1:D:45:ILE:HG21	2.15	0.46
1:D:3:ILE:N	1:D:3:ILE:HD12	2.29	0.46
1:E:15:LEU:HG	1:E:19:LEU:CD1	2.45	0.46
1:I:27:ALA:HB2	1:I:60:ILE:HD11	1.96	0.46
1:B:116:ILE:O	1:B:120:VAL:HG23	2.15	0.46
1:B:46:LEU:O	1:B:50:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:O	1:E:82:LYS:HG3	2.15	0.46
1:H:74:VAL:O	1:H:78:VAL:HG23	2.15	0.46
1:J:15:LEU:O	1:J:19:LEU:HD13	2.16	0.46
1:K:9:SER:HB3	2:K:201:SO4:O4	2.16	0.46
1:E:35:GLN:HE21	1:E:42:ASN:HB3	1.81	0.46
1:J:99:VAL:HG11	1:J:109:MSE:SE	2.65	0.46
1:E:110:LYS:O	1:E:114:ILE:HG13	2.15	0.46
1:H:110:LYS:O	1:H:114:ILE:HG13	2.16	0.46
1:I:63:SER:HA	1:I:90:ILE:HG23	1.97	0.46
1:J:59:PHE:O	1:J:88:LEU:HD12	2.16	0.46
1:F:109:MSE:O	1:F:113:VAL:HG23	2.16	0.46
1:G:32:THR:O	1:G:45:ILE:HG21	2.16	0.46
1:K:109:MSE:HE3	1:K:110:LYS:HG2	1.96	0.46
1:B:3:ILE:HG13	1:B:52:PHE:HD2	1.81	0.46
1:B:63:SER:OG	1:B:66:ARG:HG2	2.16	0.46
1:D:50:LEU:HB3	1:D:80:TYR:CE2	2.51	0.46
1:F:3:ILE:HD12	1:F:3:ILE:N	2.30	0.46
1:I:16:GLU:O	1:I:20:GLU:HG3	2.16	0.46
1:J:95:MSE:CE	1:J:109:MSE:HE3	2.46	0.46
1:D:40:ILE:HG22	1:D:43:ARG:HH21	1.81	0.46
1:E:93:LEU:HD21	1:G:105:LEU:CD2	2.46	0.46
1:F:106:ASP:O	1:F:110:LYS:HG3	2.16	0.46
1:E:15:LEU:HG	1:E:19:LEU:HG	1.98	0.45
1:L:74:VAL:O	1:L:78:VAL:HG23	2.16	0.45
1:D:70:ASN:O	1:D:74:VAL:HG23	2.17	0.45
1:L:40:ILE:HG23	1:L:73:GLU:OE2	2.16	0.45
1:C:70:ASN:O	1:C:74:VAL:HG23	2.15	0.45
1:D:1:MSE:HG2	1:D:2:ILE:N	2.32	0.45
1:H:62:GLU:HA	1:H:91:THR:OG1	2.16	0.45
1:A:25:PHE:CE2	1:A:89:MSE:HE2	2.51	0.45
1:I:21:ASN:HB3	1:I:91:THR:HG21	1.99	0.45
1:E:33:GLU:OE1	1:E:43:ARG:HA	2.17	0.45
1:G:111:ASP:O	1:G:115:GLN:HG3	2.16	0.45
1:I:17:ARG:O	1:I:21:ASN:ND2	2.34	0.45
1:B:96[B]:MSE:HE3	1:B:110:LYS:HD2	1.99	0.45
1:C:64:ILE:HG12	1:C:90:ILE:CD1	2.47	0.45
1:J:109:MSE:O	1:J:113:VAL:HG23	2.16	0.45
1:J:64:ILE:HD11	1:J:90:ILE:HD11	1.99	0.45
1:B:64:ILE:HG12	1:B:90:ILE:HD13	1.99	0.45
1:A:99:VAL:HG13	1:C:93:LEU:HD21	1.98	0.45
1:D:63:SER:OG	1:D:65:ASP:OD1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASN:OD1	1:F:107:LYS:HD3	2.17	0.45
1:G:33:GLU:HA	1:G:45:ILE:CD1	2.46	0.45
1:G:93:LEU:CD1	1:G:95:MSE:HG3	2.43	0.45
1:K:106:ASP:O	1:K:110:LYS:HG3	2.17	0.45
1:A:112:LEU:HD13	1:B:112:LEU:HD13	1.99	0.45
1:A:113:VAL:HG13	1:C:100:ILE:HD11	1.99	0.45
1:D:95:MSE:SE	1:D:113:VAL:HG11	2.67	0.45
1:A:105:LEU:HD23	1:C:93:LEU:HD21	1.99	0.45
1:K:37:GLY:HA2	1:K:43:ARG:HD3	1.97	0.45
1:K:32:THR:O	1:K:45:ILE:HD13	2.17	0.45
1:D:74:VAL:O	1:D:78:VAL:HG23	2.16	0.44
1:F:109:MSE:HB3	1:H:109:MSE:HE1	1.99	0.44
1:K:25:PHE:CZ	1:K:91:THR:HG23	2.52	0.44
1:G:109:MSE:O	1:G:113:VAL:HG23	2.17	0.44
1:I:21:ASN:HA	1:I:24:THR:HG22	1.99	0.44
1:A:67:LEU:HD11	1:A:77:THR:HG21	2.00	0.44
1:C:102:ASN:CB	1:C:105:LEU:HD13	2.47	0.44
1:E:116:ILE:O	1:E:120:VAL:HG23	2.17	0.44
1:G:53:VAL:HG11	1:G:86:VAL:CG1	2.42	0.44
1:L:54:GLU:O	1:L:86:VAL:HG22	2.18	0.44
1:L:64:ILE:HG12	1:L:90:ILE:CD1	2.47	0.44
1:L:71:TYR:O	1:L:75:ILE:HG12	2.17	0.44
1:C:6:ALA:HB2	1:C:22:LEU:HD11	1.99	0.44
1:F:78:VAL:HG21	1:F:114:ILE:HG21	2.00	0.44
1:J:62:GLU:HA	1:J:91:THR:OG1	2.18	0.44
1:E:112:LEU:O	1:E:112:LEU:HD23	2.17	0.44
1:E:119:MSE:CE	1:H:116:ILE:HG21	2.48	0.44
1:E:75:ILE:HD12	1:E:115:GLN:HG2	1.99	0.44
1:H:22:LEU:CD2	1:H:60:ILE:HG22	2.45	0.44
1:K:40:ILE:HG23	1:K:73:GLU:OE2	2.17	0.44
1:B:102:ASN:HD21	1:B:105:LEU:HD13	1.83	0.44
1:F:96:MSE:CA	1:F:96:MSE:HE2	2.47	0.44
1:G:84:LYS:HB3	1:G:86:VAL:HG23	2.00	0.44
1:A:1:MSE:HG2	1:A:3:ILE:HD12	1.99	0.44
1:E:112:LEU:CD2	1:E:116:ILE:HD11	2.48	0.44
1:H:75:ILE:HD12	1:H:115:GLN:HG2	2.00	0.44
1:L:35:GLN:HG3	1:L:36:SER:H	1.82	0.44
1:A:19:LEU:O	1:A:23:LYS:HG3	2.17	0.44
1:C:72:ASN:OD1	1:D:107:LYS:HD3	2.18	0.44
1:E:100:ILE:HG22	1:E:102:ASN:H	1.81	0.44
1:E:105:LEU:HG	1:F:119:MSE:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:O	1:E:91:THR:HB	2.17	0.44
1:K:74:VAL:O	1:K:78:VAL:HG23	2.18	0.44
1:L:61:VAL:O	1:L:90:ILE:HA	2.18	0.44
1:B:55:MSE:HG3	1:B:85:GLU:HB2	1.99	0.44
1:E:31:PHE:HD1	1:E:45:ILE:HG23	1.83	0.44
1:F:53:VAL:HG21	1:F:59:PHE:HD2	1.82	0.44
1:A:80:TYR:CZ	1:A:84:LYS:HD2	2.53	0.43
1:C:54:GLU:O	1:C:86:VAL:HG22	2.18	0.43
1:F:64:ILE:HG21	1:F:118:ALA:HA	2.00	0.43
1:D:100:ILE:HG22	1:D:101:GLY:N	2.33	0.43
1:D:93:LEU:HB3	1:D:95:MSE:CE	2.48	0.43
1:E:61:VAL:HG12	1:E:62:GLU:N	2.33	0.43
1:K:46:LEU:O	1:K:50:LEU:HG	2.18	0.43
1:B:102:ASN:OD1	1:B:105:LEU:HD13	2.18	0.43
1:C:13:GLN:HE22	1:C:66:ARG:HH12	1.66	0.43
1:I:1:MSE:HG3	1:I:3:ILE:HD12	1.99	0.43
1:A:112:LEU:O	1:A:116:ILE:HG13	2.18	0.43
1:E:77:THR:O	1:E:81:LEU:HG	2.18	0.43
1:F:113:VAL:HG22	1:H:109:MSE:SE	2.69	0.43
1:G:116:ILE:O	1:G:120:VAL:HG23	2.18	0.43
1:K:69:ARG:HD3	1:K:125:ARG:HB2	2.00	0.43
1:C:21:ASN:ND2	1:C:62:GLU:OE1	2.47	0.43
1:D:33:GLU:CG	1:D:45:ILE:HB	2.48	0.43
1:E:23:LYS:HG2	1:E:30:ILE:HD11	2.00	0.43
1:E:62:GLU:HA	1:E:91:THR:CB	2.48	0.43
1:E:70:ASN:O	1:E:74:VAL:HG23	2.18	0.43
1:C:71:TYR:O	1:C:75:ILE:HG12	2.19	0.43
1:G:71:TYR:O	1:G:75:ILE:HG12	2.18	0.43
1:I:100:ILE:HD12	1:I:105:LEU:HB3	2.00	0.43
1:F:112:LEU:O	1:F:116:ILE:HG13	2.18	0.43
1:K:35:GLN:CB	1:K:43:ARG:HG2	2.48	0.43
1:C:102:ASN:HB3	1:C:105:LEU:HD13	1.99	0.43
1:B:58:ARG:NH2	1:F:96:MSE:HG3	2.33	0.43
1:G:11:LEU:HD23	1:G:11:LEU:H	1.83	0.43
1:G:72:ASN:OD1	1:H:107:LYS:HE2	2.18	0.43
1:D:58:ARG:NH1	1:H:55:MSE:O	2.47	0.43
1:H:53:VAL:HG11	1:H:59:PHE:HD1	1.83	0.43
1:J:33:GLU:OE1	1:J:43:ARG:HA	2.19	0.43
1:G:58:ARG:HD3	1:G:89:MSE:HE2	2.01	0.43
1:H:35:GLN:HG3	1:H:36:SER:N	2.34	0.43
1:B:81:LEU:CD1	1:B:88:LEU:HD13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LEU:O	1:E:23:LYS:HG3	2.19	0.42
1:I:110:LYS:O	1:I:114:ILE:HG13	2.19	0.42
1:L:119:MSE:HE3	1:L:120:VAL:HG23	2.01	0.42
1:C:66:ARG:NE	1:C:66:ARG:HA	2.34	0.42
1:K:90:ILE:N	1:K:90:ILE:HD12	2.34	0.42
1:F:46:LEU:O	1:F:50:LEU:HG	2.20	0.42
1:H:58:ARG:HH11	1:H:89:MSE:CE	2.19	0.42
1:I:116:ILE:O	1:I:120:VAL:HG23	2.19	0.42
1:K:109:MSE:HB3	1:K:109:MSE:HE2	1.88	0.42
1:K:76:HIS:ND1	1:L:83:ASP:OD1	2.52	0.42
1:B:64:ILE:HD11	1:B:90:ILE:HD11	2.01	0.42
1:K:110:LYS:O	1:K:114:ILE:HG13	2.20	0.42
1:B:102:ASN:OD1	1:B:105:LEU:HB2	2.20	0.42
1:D:113:VAL:O	1:D:117:LEU:HG	2.19	0.42
1:E:71:TYR:O	1:E:75:ILE:HG12	2.20	0.42
1:F:70:ASN:OD1	1:F:73:GLU:HG3	2.19	0.42
1:K:95:MSE:SE	1:K:113:VAL:HG11	2.69	0.42
1:A:58:ARG:NE	1:A:87:GLN:OE1	2.47	0.42
1:A:99:VAL:HG11	1:A:105:LEU:HD23	2.00	0.42
1:C:13:GLN:HE22	1:C:66:ARG:NH1	2.17	0.42
1:E:99:VAL:HG13	1:E:100:ILE:HG13	2.02	0.42
1:J:100:ILE:HG13	1:K:120:VAL:HG11	2.01	0.42
1:B:92:SER:O	1:B:94:PRO:HD3	2.19	0.42
1:H:71:TYR:O	1:H:75:ILE:HG12	2.19	0.42
1:J:112:LEU:HD23	1:J:112:LEU:O	2.20	0.42
1:J:1:MSE:HE2	1:J:29:LYS:HB2	2.02	0.42
1:A:70:ASN:O	1:A:74:VAL:HG23	2.20	0.42
1:D:8:VAL:HG23	1:D:15:LEU:HD13	2.00	0.42
1:E:9:SER:HB2	2:E:201:SO4:O2	2.20	0.42
1:B:40:ILE:HG23	1:B:73:GLU:OE2	2.20	0.42
1:D:102:ASN:HA	1:D:103:PRO:HD3	1.91	0.42
1:F:109:MSE:HE3	1:H:109:MSE:HB3	2.02	0.42
1:K:11:LEU:N	1:K:11:LEU:HD22	2.35	0.42
1:B:3:ILE:CD1	1:B:29:LYS:HB3	2.50	0.41
1:D:78:VAL:HG11	1:D:114:ILE:HG21	2.01	0.41
1:A:71:TYR:O	1:A:75:ILE:HG12	2.19	0.41
1:F:35:GLN:HG3	1:F:36:SER:N	2.34	0.41
1:J:1:MSE:CE	1:J:29:LYS:HB2	2.50	0.41
1:J:33:GLU:CD	1:J:45:ILE:HB	2.40	0.41
1:A:33:GLU:CD	1:A:45:ILE:HB	2.40	0.41
1:A:3:ILE:N	1:A:3:ILE:HD12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:HG22	1:C:101:GLY:N	2.36	0.41
1:C:3:ILE:HD13	1:C:53:VAL:HG12	2.01	0.41
1:D:99:VAL:O	1:D:100:ILE:HD13	2.20	0.41
1:F:8:VAL:CG1	1:F:15:LEU:HD13	2.48	0.41
1:F:33:GLU:CB	1:F:45:ILE:HD12	2.51	0.41
1:A:53:VAL:HG21	1:A:86:VAL:HG11	2.02	0.41
1:A:53:VAL:HG23	1:A:57:ASP:HB2	2.01	0.41
1:F:4:GLY:O	1:F:30:ILE:HA	2.20	0.41
1:F:110:LYS:O	1:F:114:ILE:HG13	2.21	0.41
1:H:75:ILE:CD1	1:H:115:GLN:HG2	2.50	0.41
1:H:17:ARG:NH1	1:H:62:GLU:OE1	2.54	0.41
1:L:66:ARG:HA	1:L:66:ARG:HD3	1.76	0.41
1:B:8:VAL:O	1:B:34:LYS:HA	2.21	0.41
1:F:19:LEU:O	1:F:23:LYS:HG3	2.20	0.41
1:F:5:TYR:CZ	1:F:46:LEU:HB2	2.56	0.41
1:G:63:SER:OG	1:G:66:ARG:HG2	2.20	0.41
1:H:92:SER:C	1:H:94:PRO:HD3	2.40	0.41
1:K:60:ILE:HG22	1:K:89:MSE:HB3	2.03	0.41
1:E:40:ILE:HG23	1:E:73:GLU:OE1	2.21	0.41
1:J:32:THR:O	1:J:45:ILE:HD13	2.19	0.41
1:B:66:ARG:NE	1:B:66:ARG:HA	2.36	0.41
1:C:6:ALA:HB2	1:C:22:LEU:HD12	2.02	0.41
1:B:109:MSE:CE	1:D:112:LEU:HB3	2.49	0.41
1:K:116:ILE:O	1:K:120:VAL:HG23	2.20	0.41
1:A:18:GLN:O	1:A:22:LEU:HG	2.21	0.41
1:A:39:SER:HA	1:A:73:GLU:OE2	2.21	0.41
1:B:102:ASN:ND2	1:B:105:LEU:HD13	2.36	0.41
1:C:4:GLY:O	1:C:30:ILE:HA	2.21	0.41
1:D:59:PHE:O	1:D:88:LEU:HA	2.21	0.41
1:E:109:MSE:HE1	1:G:113:VAL:CG2	2.51	0.41
1:I:70:ASN:O	1:I:74:VAL:HG23	2.20	0.41
1:J:109:MSE:HB3	1:J:109:MSE:HE2	2.01	0.41
1:I:93:LEU:HD21	1:L:99:VAL:O	2.20	0.41
1:E:111:ASP:O	1:E:115:GLN:HG3	2.21	0.41
1:I:74:VAL:O	1:I:78:VAL:HG23	2.21	0.41
1:J:5:TYR:O	1:J:61:VAL:HG12	2.21	0.41
1:J:84:LYS:HB3	1:J:86:VAL:HG23	2.03	0.41
1:I:116:ILE:HG21	1:L:100:ILE:HD13	2.03	0.41
1:L:39:SER:HA	1:L:73:GLU:OE2	2.21	0.41
1:A:116:ILE:O	1:A:120:VAL:HG23	2.21	0.40
1:F:9:SER:HB3	2:F:201:SO4:O2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:ILE:N	1:I:3:ILE:HD12	2.35	0.40
1:I:71:TYR:O	1:I:75:ILE:HG12	2.21	0.40
1:J:40:ILE:HG22	1:J:43:ARG:HH21	1.85	0.40
1:B:112:LEU:O	1:B:116:ILE:HG13	2.21	0.40
1:I:116:ILE:CG2	1:L:105:LEU:HD23	2.51	0.40
1:A:93:LEU:HA	1:A:94:PRO:HD3	1.86	0.40
1:C:110:LYS:O	1:C:114:ILE:HG13	2.20	0.40
1:B:109:MSE:HE3	1:D:112:LEU:CG	2.51	0.40
1:E:112:LEU:HD22	1:E:116:ILE:HD11	2.02	0.40
1:I:113:VAL:O	1:I:117:LEU:HG	2.20	0.40
1:J:60:ILE:HA	1:J:89:MSE:O	2.22	0.40
1:J:89:MSE:HE3	1:J:94:PRO:CB	2.41	0.40
1:A:39:SER:OG	1:A:41:GLU:HG3	2.21	0.40
1:B:95:MSE:HE2	1:D:101:GLY:HA2	2.04	0.40
1:C:105:LEU:HG	1:D:119:MSE:CE	2.52	0.40
1:E:6:ALA:HB2	1:E:22:LEU:HD12	2.01	0.40
1:F:13:GLN:N	1:F:13:GLN:OE1	2.54	0.40
1:G:1:MSE:HG3	1:G:28:GLU:OE2	2.21	0.40
1:D:39:SER:O	1:D:43:ARG:NH1	2.55	0.40
1:D:98:GLU:HG2	1:H:2:ILE:HG13	2.04	0.40
1:F:103:PRO:O	1:F:107:LYS:HG3	2.21	0.40
1:G:53:VAL:HG21	1:G:59:PHE:HD1	1.87	0.40
1:I:58:ARG:HG2	1:I:60:ILE:HG23	2.04	0.40
1:J:58:ARG:NH2	1:J:96:MSE:HE2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	124/128 (97%)	119 (96%)	4 (3%)	1 (1%)	24 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	C	123/128 (96%)	119 (97%)	4 (3%)	0	100	100
1	D	123/128 (96%)	119 (97%)	4 (3%)	0	100	100
1	E	123/128 (96%)	120 (98%)	3 (2%)	0	100	100
1	F	123/128 (96%)	120 (98%)	3 (2%)	0	100	100
1	G	118/128 (92%)	114 (97%)	4 (3%)	0	100	100
1	H	123/128 (96%)	121 (98%)	2 (2%)	0	100	100
1	I	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
1	J	123/128 (96%)	120 (98%)	3 (2%)	0	100	100
1	K	124/128 (97%)	118 (95%)	5 (4%)	1 (1%)	24	63
1	L	123/128 (96%)	120 (98%)	3 (2%)	0	100	100
All	All	1476/1536 (96%)	1432 (97%)	42 (3%)	2 (0%)	56	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	PRO
1	K	94	PRO

### 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	116/111 (104%)	115 (99%)	1 (1%)	84	94
1	B	117/111 (105%)	117 (100%)	0	100	100
1	C	115/111 (104%)	115 (100%)	0	100	100
1	D	115/111 (104%)	115 (100%)	0	100	100
1	E	115/111 (104%)	115 (100%)	0	100	100
1	F	115/111 (104%)	115 (100%)	0	100	100
1	G	112/111 (101%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	115/111 (104%)	115 (100%)	0	100	100
1	I	116/111 (104%)	114 (98%)	2 (2%)	68	89
1	J	115/111 (104%)	114 (99%)	1 (1%)	84	94
1	K	116/111 (104%)	115 (99%)	1 (1%)	84	94
1	L	115/111 (104%)	114 (99%)	1 (1%)	84	94
All	All	1382/1332 (104%)	1376 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	I	70	ASN
1	I	87	GLN
1	J	109	MSE
1	K	109	MSE
1	L	119	MSE

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

Mol	Chain	Res	Type
1	A	13	GLN
1	B	18	GLN
1	C	115	GLN
1	D	42	ASN
1	E	115	GLN
1	I	70	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

21 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	201	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	201	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	B	202	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	C	201	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	C	202	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	201	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	E	201	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	F	201	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	G	201	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	H	201	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	H	202	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	H	203	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	I	201	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	I	202	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	I	203	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	I	204	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	J	201	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	J	202	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	K	201	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	L	201	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	L	202	-	4,4,4	0.26	0	6,6,6	0.07	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	201	-	-	0/0/0/0	0/0/0/0
2	SO4	B	201	-	-	0/0/0/0	0/0/0/0
2	SO4	B	202	-	-	0/0/0/0	0/0/0/0
2	SO4	C	201	-	-	0/0/0/0	0/0/0/0
2	SO4	C	202	-	-	0/0/0/0	0/0/0/0
2	SO4	D	201	-	-	0/0/0/0	0/0/0/0
2	SO4	E	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	201	-	-	0/0/0/0	0/0/0/0
2	SO4	G	201	-	-	0/0/0/0	0/0/0/0
2	SO4	H	201	-	-	0/0/0/0	0/0/0/0
2	SO4	H	202	-	-	0/0/0/0	0/0/0/0
2	SO4	H	203	-	-	0/0/0/0	0/0/0/0
2	SO4	I	201	-	-	0/0/0/0	0/0/0/0
2	SO4	I	202	-	-	0/0/0/0	0/0/0/0
2	SO4	I	203	-	-	0/0/0/0	0/0/0/0
2	SO4	I	204	-	-	0/0/0/0	0/0/0/0
2	SO4	J	201	-	-	0/0/0/0	0/0/0/0
2	SO4	J	202	-	-	0/0/0/0	0/0/0/0
2	SO4	K	201	-	-	0/0/0/0	0/0/0/0
2	SO4	L	201	-	-	0/0/0/0	0/0/0/0
2	SO4	L	202	-	-	0/0/0/0	0/0/0/0

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.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	SO4	1	0
2	C	201	SO4	2	0
2	D	201	SO4	4	0
2	E	201	SO4	2	0
2	F	201	SO4	1	0
2	H	201	SO4	4	0
2	K	201	SO4	1	0
2	L	201	SO4	1	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<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	119/128 (92%)	-0.11	3 (2%) 61 37	55, 81, 152, 187	0
1	B	119/128 (92%)	-0.43	0 100 100	40, 60, 89, 120	0
1	C	118/128 (92%)	-0.30	0 100 100	53, 79, 109, 123	0
1	D	118/128 (92%)	0.05	2 (1%) 73 52	49, 97, 177, 231	0
1	E	118/128 (92%)	0.50	12 (10%) 9 3	95, 153, 204, 261	0
1	F	118/128 (92%)	0.36	10 (8%) 13 4	72, 113, 201, 257	0
1	G	115/128 (89%)	-0.19	1 (0%) 85 72	62, 90, 137, 182	0
1	H	118/128 (92%)	-0.40	0 100 100	38, 66, 93, 120	0
1	I	119/128 (92%)	-0.37	0 100 100	46, 63, 101, 145	0
1	J	118/128 (92%)	-0.21	1 (0%) 87 75	46, 74, 106, 149	0
1	K	119/128 (92%)	0.02	3 (2%) 61 37	51, 93, 171, 230	0
1	L	118/128 (92%)	-0.25	0 100 100	44, 65, 114, 147	0
All	All	1417/1536 (92%)	-0.11	32 (2%) 64 40	38, 80, 168, 261	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	ASP	4.0
1	F	9	SER	3.6
1	F	12	ASP	3.5
1	K	38	LYS	3.4
1	F	10	SER	3.4
1	E	19	LEU	3.3
1	E	59	PHE	3.3
1	E	58	ARG	3.2
1	E	92	SER	3.1
1	F	34	LYS	2.9
1	E	91	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	35	GLN	2.6
1	F	59	PHE	2.6
1	A	10	SER	2.5
1	A	101	GLY	2.5
1	F	37	GLY	2.5
1	E	27	ALA	2.4
1	F	28	GLU	2.4
1	E	88	LEU	2.3
1	F	29	LYS	2.3
1	K	10	SER	2.3
1	E	3	ILE	2.3
1	E	62	GLU	2.3
1	F	11	LEU	2.2
1	D	32	THR	2.2
1	J	41	GLU	2.2
1	K	34	LYS	2.2
1	A	100	ILE	2.1
1	G	101	GLY	2.1
1	E	5	TYR	2.1
1	E	23	LYS	2.0
1	F	15	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	H	203	5/5	0.76	0.24	2.71	177,177,177,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	201	5/5	0.76	0.22	-0.33	156,156,156,156	0
2	SO4	B	201	5/5	0.96	0.13	-0.66	76,77,77,77	0
2	SO4	E	201	5/5	0.81	0.16	-0.71	161,161,162,162	0
2	SO4	D	201	5/5	0.82	0.19	-0.81	154,154,155,155	0
2	SO4	G	201	5/5	0.91	0.16	-1.02	147,147,148,148	0
2	SO4	F	201	5/5	0.64	0.20	-1.02	191,191,192,192	0
2	SO4	C	201	5/5	0.96	0.13	-1.13	94,94,94,94	0
2	SO4	K	201	5/5	0.77	0.17	-1.20	173,173,173,173	0
2	SO4	J	201	5/5	0.93	0.13	-1.39	107,107,107,107	0
2	SO4	L	201	5/5	0.95	0.12	-1.62	86,86,90,91	0
2	SO4	I	201	5/5	0.97	0.12	-2.00	91,91,92,92	0
2	SO4	H	201	5/5	0.98	0.12	-3.17	77,77,77,77	0
2	SO4	B	202	5/5	0.94	0.18	-	103,103,103,103	0
2	SO4	I	203	5/5	0.76	0.18	-	130,131,132,133	0
2	SO4	I	202	5/5	0.82	0.14	-	149,149,149,149	0
2	SO4	C	202	5/5	0.91	0.16	-	128,128,128,129	0
2	SO4	L	202	5/5	0.88	0.29	-	162,162,163,163	0
2	SO4	J	202	5/5	0.70	0.23	-	173,175,175,176	0
2	SO4	I	204	5/5	0.87	0.13	-	159,159,159,159	0
2	SO4	H	202	5/5	0.92	0.21	-	110,110,110,111	0

## 6.5 Other polymers

There are no such residues in this entry.