



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:46 PM UTC

PDB ID : 4DYU / pdb_00004dyu
Title : The crystal structure of DNA starvation/stationary phase protection protein Dps from *Yersinia pestis* KIM 10
Authors : Tan, K.; Gu, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-02-29
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

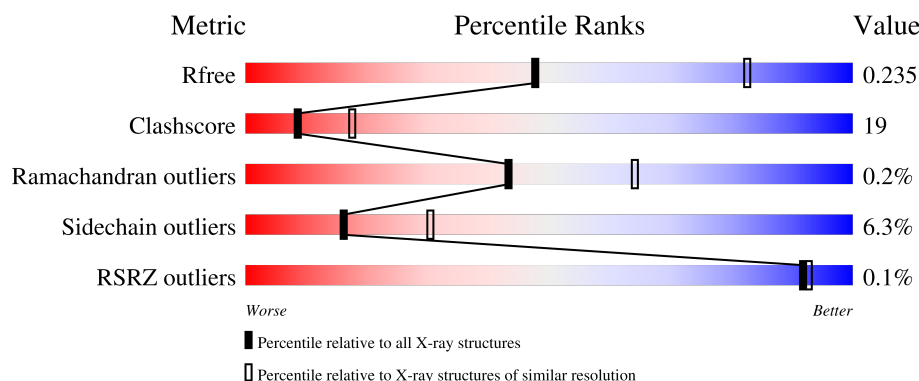
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of 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 $\leq 5\%$. 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	170	
1	B	170	
1	C	170	
1	D	170	
1	E	170	

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Mol	Chain	Length	Quality of chain
1	F	170	
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
3	SO4	B	202	-	-	X	-
3	SO4	D	202	-	-	X	-
3	SO4	F	202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15159 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 DNA protection during starvation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	B	154	Total	C	N	O	S	0	0	0
			1231	778	215	234	4			
1	C	154	Total	C	N	O	S	0	0	0
			1231	778	215	234	4			
1	D	156	Total	C	N	O	S	0	0	0
			1246	786	217	239	4			
1	E	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	F	154	Total	C	N	O	S	0	0	0
			1231	778	215	234	4			
1	G	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	H	157	Total	C	N	O	S	0	0	0
			1253	791	218	240	4			
1	I	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	J	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	K	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			
1	L	155	Total	C	N	O	S	0	0	0
			1240	783	216	237	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q7CJ65
A	-1	ASN	-	expression tag	UNP Q7CJ65
A	0	ALA	-	expression tag	UNP Q7CJ65
B	-2	SER	-	expression tag	UNP Q7CJ65
B	-1	ASN	-	expression tag	UNP Q7CJ65

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q7CJ65
C	-2	SER	-	expression tag	UNP Q7CJ65
C	-1	ASN	-	expression tag	UNP Q7CJ65
C	0	ALA	-	expression tag	UNP Q7CJ65
D	-2	SER	-	expression tag	UNP Q7CJ65
D	-1	ASN	-	expression tag	UNP Q7CJ65
D	0	ALA	-	expression tag	UNP Q7CJ65
E	-2	SER	-	expression tag	UNP Q7CJ65
E	-1	ASN	-	expression tag	UNP Q7CJ65
E	0	ALA	-	expression tag	UNP Q7CJ65
F	-2	SER	-	expression tag	UNP Q7CJ65
F	-1	ASN	-	expression tag	UNP Q7CJ65
F	0	ALA	-	expression tag	UNP Q7CJ65
G	-2	SER	-	expression tag	UNP Q7CJ65
G	-1	ASN	-	expression tag	UNP Q7CJ65
G	0	ALA	-	expression tag	UNP Q7CJ65
H	-2	SER	-	expression tag	UNP Q7CJ65
H	-1	ASN	-	expression tag	UNP Q7CJ65
H	0	ALA	-	expression tag	UNP Q7CJ65
I	-2	SER	-	expression tag	UNP Q7CJ65
I	-1	ASN	-	expression tag	UNP Q7CJ65
I	0	ALA	-	expression tag	UNP Q7CJ65
J	-2	SER	-	expression tag	UNP Q7CJ65
J	-1	ASN	-	expression tag	UNP Q7CJ65
J	0	ALA	-	expression tag	UNP Q7CJ65
K	-2	SER	-	expression tag	UNP Q7CJ65
K	-1	ASN	-	expression tag	UNP Q7CJ65
K	0	ALA	-	expression tag	UNP Q7CJ65
L	-2	SER	-	expression tag	UNP Q7CJ65
L	-1	ASN	-	expression tag	UNP Q7CJ65
L	0	ALA	-	expression tag	UNP Q7CJ65

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Zn 2	0	0
2	F	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	J	1	Total 1	Zn 1	0	0
2	K	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	20	Total	O	0	0
			20	20		
4	C	18	Total	O	0	0
			18	18		
4	D	24	Total	O	0	0
			24	24		
4	E	15	Total	O	0	0
			15	15		
4	F	22	Total	O	0	0
			22	22		
4	G	14	Total	O	0	0
			14	14		
4	H	19	Total	O	0	0
			19	19		
4	I	16	Total	O	0	0
			16	16		
4	J	13	Total	O	0	0
			13	13		

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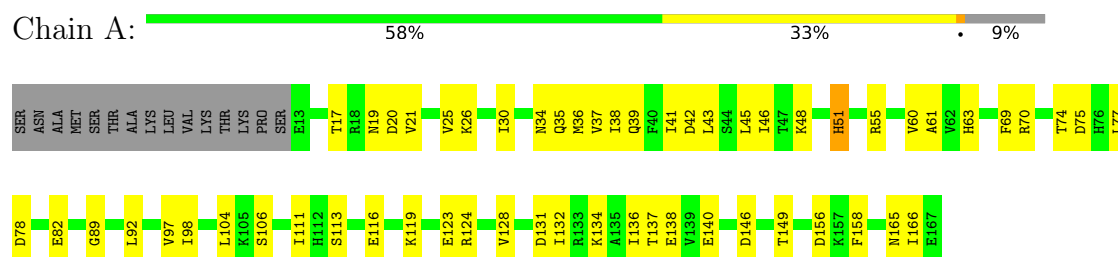
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	21	Total	O	0	0
			21	21		
4	L	10	Total	O	0	0
			10	10		

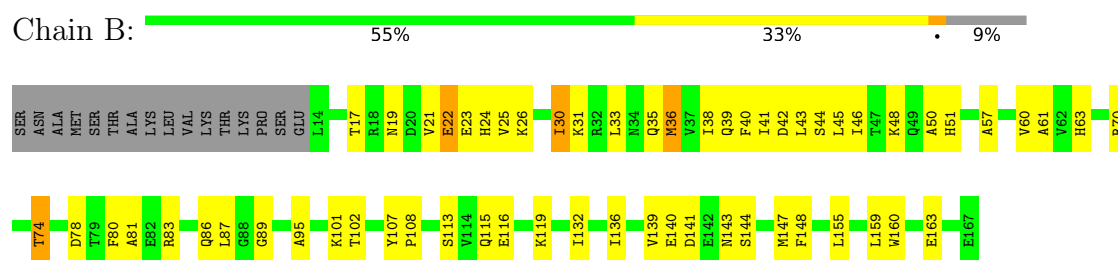
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

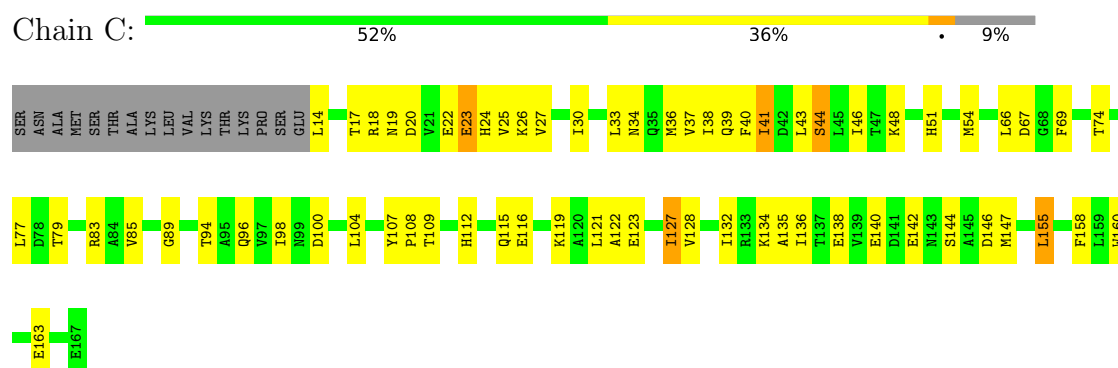
- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein

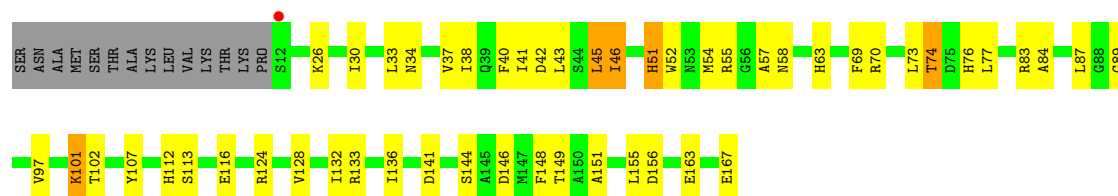


- Molecule 1: DNA protection during starvation protein



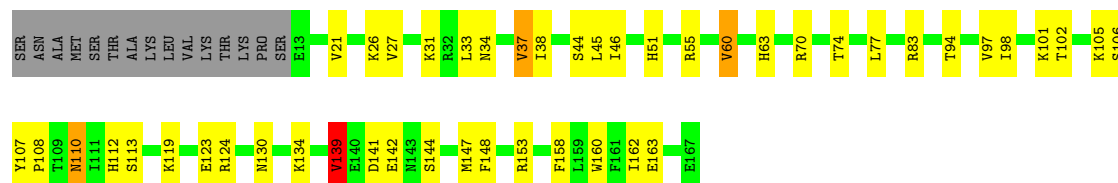
- Molecule 1: DNA protection during starvation protein





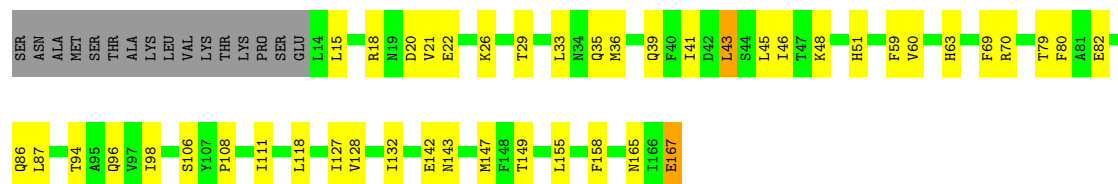
- Molecule 1: DNA protection during starvation protein

Chain E: 64% 25% 9%



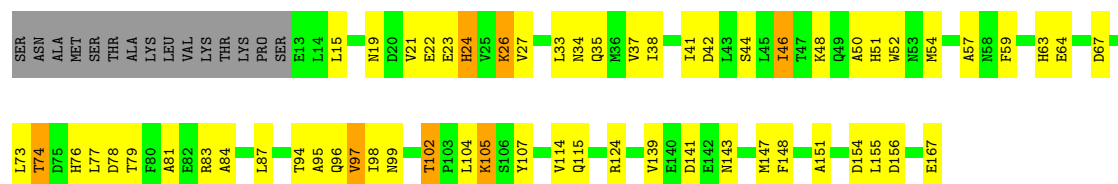
- Molecule 1: DNA protection during starvation protein

Chain F: 64% 25% 9%



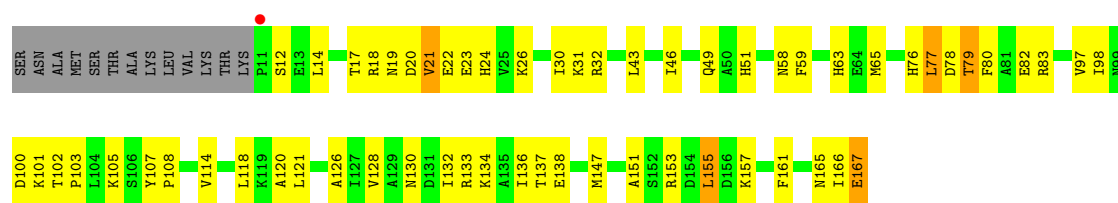
- Molecule 1: DNA protection during starvation protein

Chain G: 56% 31% 9%



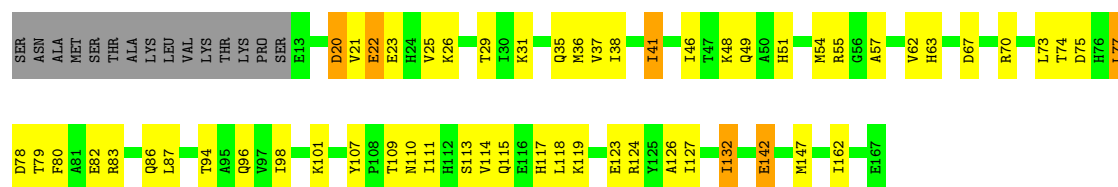
- Molecule 1: DNA protection during starvation protein

Chain H: 57% 32% 8%



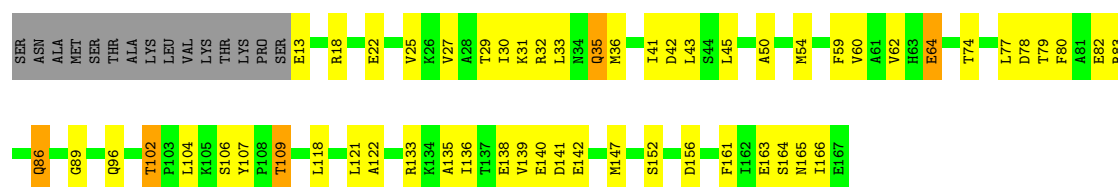
- Molecule 1: DNA protection during starvation protein

Chain I: 



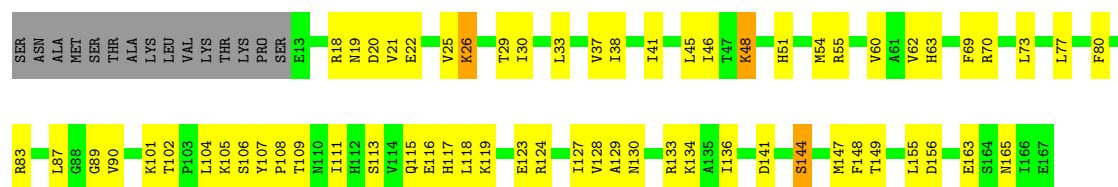
- Molecule 1: DNA protection during starvation protein

Chain J: 



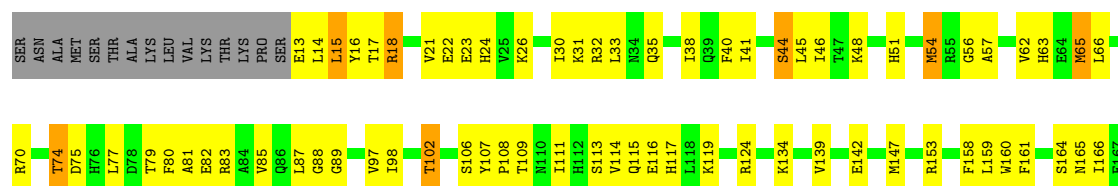
- Molecule 1: DNA protection during starvation protein

Chain K: 



- Molecule 1: DNA protection during starvation protein

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.41Å 105.10Å 191.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.75 46.19 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.19-2.75) 99.6 (46.19-2.75)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.179 , 0.269 (Not available) , 0.235	Depositor DCC
R_{free} test set	2834 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15159	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.56	0/1261	0.89	1/1707 (0.1%)
1	B	0.56	0/1252	0.89	0/1695
1	C	0.52	0/1252	0.85	0/1695
1	D	0.55	0/1267	0.90	1/1715 (0.1%)
1	E	0.57	0/1261	0.88	4/1707 (0.2%)
1	F	0.57	0/1252	0.83	0/1695
1	G	0.59	0/1261	0.93	2/1707 (0.1%)
1	H	0.53	0/1275	0.89	1/1726 (0.1%)
1	I	0.60	0/1261	0.85	1/1707 (0.1%)
1	J	0.54	0/1261	0.84	2/1707 (0.1%)
1	K	0.54	0/1261	0.89	0/1707
1	L	0.53	0/1261	0.87	0/1707
All	All	0.55	0/15125	0.88	12/20475 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	102	THR	CA-C-N	7.09	127.69	120.04
1	G	102	THR	C-N-CA	7.09	127.69	120.04
1	A	138	GLU	N-CA-C	6.23	118.15	111.36
1	E	60	VAL	N-CA-C	5.58	115.78	110.42
1	I	62	VAL	N-CA-C	-5.47	105.39	110.53
1	H	103	PRO	N-CA-C	-5.35	107.66	114.35
1	E	45	LEU	N-CA-C	-5.13	105.69	111.28
1	J	107	TYR	CA-C-N	5.11	125.12	119.90
1	J	107	TYR	C-N-CA	5.11	125.12	119.90
1	E	139	VAL	N-CA-C	5.06	115.57	108.89
1	D	102	THR	N-CA-C	5.03	116.17	109.93
1	E	37	VAL	CB-CA-C	-5.03	105.43	112.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1240	0	1228	46	0
1	B	1231	0	1222	51	0
1	C	1231	0	1222	64	0
1	D	1246	0	1233	35	0
1	E	1240	0	1228	36	0
1	F	1231	0	1222	43	0
1	G	1240	0	1228	51	0
1	H	1253	0	1241	58	0
1	I	1240	0	1228	58	0
1	J	1240	0	1228	51	0
1	K	1240	0	1228	58	0
1	L	1240	0	1228	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	2	0
3	D	10	0	0	3	0
3	E	5	0	0	1	0
3	F	5	0	0	2	0
3	G	5	0	0	1	0
3	H	5	0	0	1	0
3	J	10	0	0	1	0
3	K	5	0	0	0	0
4	A	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	1	0
4	C	18	0	0	1	0
4	D	24	0	0	0	0
4	E	15	0	0	0	0
4	F	22	0	0	1	0
4	G	14	0	0	0	0
4	H	19	0	0	0	0
4	I	16	0	0	1	0
4	J	13	0	0	1	0
4	K	21	0	0	2	0
4	L	10	0	0	0	0
All	All	15159	0	14736	562	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 19.

All (562) 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:L:65:MET:HE2	1:L:161:PHE:CD2	1.91	1.05
1:F:80:PHE:HD1	1:F:147:MET:HE2	1.19	1.02
1:E:60:VAL:HB	1:L:65:MET:HE3	1.49	0.94
1:A:30:ILE:HD13	1:A:89:GLY:HA3	1.53	0.90
1:A:92:LEU:CD2	1:C:109:THR:HG21	2.03	0.88
1:F:80:PHE:CD1	1:F:147:MET:HE2	2.09	0.87
1:G:102:THR:HG22	1:G:104:LEU:H	1.40	0.87
1:A:17:THR:HG22	1:A:19:ASN:H	1.38	0.86
1:L:80:PHE:HA	1:L:147:MET:HE1	1.58	0.85
1:C:144:SER:HA	1:C:147:MET:HE3	1.58	0.85
1:H:65:MET:HE2	1:H:161:PHE:HD2	1.43	0.82
1:K:41:ILE:HG12	1:K:77:LEU:HD11	1.61	0.82
1:J:32:ARG:NH1	1:J:36:MET:HE1	1.93	0.82
1:H:98:ILE:O	1:H:102:THR:HG23	1.78	0.82
1:C:36:MET:HE2	1:C:132:ILE:HB	1.63	0.81
1:J:32:ARG:NH2	1:J:138:GLU:OE2	2.13	0.80
1:H:80:PHE:HD1	1:H:147:MET:CE	1.93	0.80
1:H:65:MET:HE2	1:H:161:PHE:CD2	2.16	0.79
1:C:23:GLU:HG3	1:C:24:HIS:N	1.97	0.79
1:F:80:PHE:HD1	1:F:147:MET:CE	1.92	0.79
1:K:119:LYS:O	1:K:123:GLU:HG2	1.84	0.78
1:L:65:MET:HE2	1:L:161:PHE:HD2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HG21	1:L:142:GLU:HG2	1.66	0.77
1:J:102:THR:HG22	1:J:104:LEU:H	1.50	0.76
1:I:41:ILE:HG12	1:I:77:LEU:HD11	1.67	0.76
1:F:79:THR:HG22	1:F:147:MET:HE3	1.67	0.76
1:F:36:MET:HE2	1:F:132:ILE:HB	1.66	0.76
1:C:33:LEU:O	1:C:37:VAL:HG23	1.86	0.75
1:K:51:HIS:CE1	1:K:63:HIS:CE1	2.75	0.75
1:C:144:SER:HA	1:C:147:MET:CE	2.17	0.74
1:H:79:THR:HG23	1:H:147:MET:HE3	1.70	0.74
1:J:60:VAL:O	1:J:64:GLU:HG2	1.88	0.74
1:C:20:ASP:OD2	1:H:134:LYS:NZ	2.22	0.73
1:G:124:ARG:HG3	1:G:124:ARG:HH11	1.53	0.73
1:C:83:ARG:HG2	1:C:147:MET:HE1	1.71	0.73
1:A:156:ASP:OD2	1:I:83:ARG:NH1	2.22	0.73
1:J:83:ARG:NH2	1:J:141:ASP:OD1	2.21	0.73
1:A:92:LEU:HD23	1:C:109:THR:HG21	1.70	0.72
1:G:105:LYS:NZ	3:G:201:SO4:O1	2.22	0.72
1:I:23:GLU:O	1:I:26:LYS:HB2	1.89	0.72
1:L:80:PHE:HD1	1:L:147:MET:CE	2.02	0.71
1:B:113:SER:OG	1:B:116:GLU:HG3	1.91	0.71
1:I:80:PHE:HA	1:I:147:MET:HE1	1.71	0.71
1:I:80:PHE:HD1	1:I:147:MET:HE2	1.55	0.71
1:F:143:ASN:O	1:F:147:MET:HG2	1.91	0.71
1:B:107:TYR:CG	1:B:108:PRO:HD2	2.26	0.70
1:J:42:ASP:OD2	1:J:102:THR:HG21	1.91	0.70
1:K:21:VAL:HG11	1:K:87:LEU:HD22	1.72	0.70
1:E:70:ARG:NH2	3:E:203:SO4:O2	2.23	0.70
1:F:36:MET:CE	1:F:132:ILE:HB	2.21	0.70
1:H:65:MET:HE2	1:H:161:PHE:HB3	1.74	0.70
1:K:128:VAL:HG12	1:K:155:LEU:HD21	1.72	0.70
1:L:31:LYS:O	1:L:35:GLN:HG3	1.92	0.70
1:J:118:LEU:HB3	1:J:166:ILE:HD11	1.73	0.69
1:C:134:LYS:O	1:C:138:GLU:HG3	1.93	0.69
1:H:97:VAL:O	1:H:101:LYS:HB2	1.93	0.69
1:L:18:ARG:HG2	1:L:18:ARG:HH11	1.58	0.69
1:G:139:VAL:HG12	1:G:141:ASP:H	1.58	0.69
1:D:30:ILE:HD13	1:D:89:GLY:HA3	1.73	0.69
1:H:80:PHE:HA	1:H:147:MET:HE1	1.75	0.69
1:J:30:ILE:HD13	1:J:89:GLY:HA3	1.75	0.69
1:L:108:PRO:HD3	1:L:124:ARG:NH2	2.08	0.69
1:E:107:TYR:CD2	1:E:108:PRO:HD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:MET:HG2	1:G:114:VAL:HG22	1.74	0.68
1:B:80:PHE:CD1	1:B:147:MET:HE3	2.28	0.68
1:D:132:ILE:O	1:D:136:ILE:HG13	1.93	0.68
1:L:18:ARG:HH11	1:L:18:ARG:CG	2.07	0.68
1:A:70:ARG:O	1:A:74:THR:HG23	1.93	0.68
1:A:134:LYS:NZ	1:I:20:ASP:OD1	2.23	0.68
1:C:136:ILE:HG21	1:J:142:GLU:HG2	1.76	0.68
1:E:46:ILE:HD13	1:E:124:ARG:HD3	1.76	0.68
1:H:78:ASP:O	1:H:82:GLU:HG3	1.94	0.68
3:D:202:SO4:O1	1:I:57:ALA:HB1	1.94	0.67
1:H:80:PHE:HD1	1:H:147:MET:HE2	1.60	0.67
1:L:98:ILE:O	1:L:102:THR:OG1	2.11	0.67
1:E:60:VAL:CB	1:L:65:MET:HE3	2.24	0.67
1:F:21:VAL:O	1:F:26:LYS:HE3	1.95	0.67
1:J:106:SER:HB2	3:J:203:SO4:O4	1.95	0.67
1:K:129:ALA:HA	1:K:155:LEU:HD23	1.76	0.66
1:C:48:LYS:O	1:C:51:HIS:HB3	1.96	0.66
1:I:109:THR:HG23	1:K:90:VAL:HG11	1.78	0.66
1:E:119:LYS:O	1:E:123:GLU:HG2	1.95	0.66
1:C:146:ASP:OD2	1:H:153:ARG:NH1	2.28	0.66
1:D:33:LEU:O	1:D:37:VAL:HG23	1.95	0.66
1:K:37:VAL:O	1:K:41:ILE:HG13	1.96	0.65
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.96	0.65
1:D:37:VAL:O	1:D:41:ILE:HG13	1.96	0.65
1:B:80:PHE:HD1	1:B:147:MET:HE3	1.60	0.65
1:D:167:GLU:HG2	1:I:57:ALA:HB2	1.78	0.65
1:F:79:THR:O	1:F:147:MET:HE1	1.97	0.65
1:H:20:ASP:O	1:H:21:VAL:C	2.39	0.65
1:I:46:ILE:HD13	1:I:124:ARG:HD3	1.79	0.65
1:A:92:LEU:HD21	1:C:109:THR:HG21	1.76	0.65
1:F:80:PHE:HA	1:F:147:MET:HE1	1.79	0.65
1:I:51:HIS:O	1:I:63:HIS:HD2	1.80	0.65
1:J:83:ARG:HH21	1:J:141:ASP:CG	2.04	0.65
1:I:94:THR:O	1:I:98:ILE:HG12	1.97	0.64
1:L:107:TYR:HA	1:L:124:ARG:HH21	1.62	0.64
1:C:46:ILE:HG23	1:C:107:TYR:CD1	2.32	0.64
1:J:32:ARG:NH1	1:J:36:MET:CE	2.60	0.64
1:K:26:LYS:HG2	1:K:87:LEU:O	1.97	0.64
1:G:94:THR:HG22	1:G:96:GLN:OE1	1.97	0.64
1:E:83:ARG:HH21	1:E:141:ASP:CG	2.06	0.63
1:L:54:MET:HG2	1:L:114:VAL:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLN:O	1:B:119:LYS:HG3	1.99	0.63
1:I:54:MET:HG2	1:I:114:VAL:HG22	1.79	0.63
1:J:32:ARG:HH12	1:J:36:MET:HE1	1.62	0.63
1:B:33:LEU:HD21	1:B:147:MET:HE1	1.80	0.62
1:H:43:LEU:HG	1:H:128:VAL:HG21	1.81	0.62
1:I:36:MET:HE3	1:I:132:ILE:HA	1.81	0.62
1:J:25:VAL:HG13	1:J:140:GLU:HG3	1.81	0.62
1:B:115:GLN:HG2	4:B:314:HOH:O	1.99	0.62
1:G:42:ASP:OD2	1:G:102:THR:HG21	2.00	0.62
1:F:79:THR:HG22	1:F:147:MET:CE	2.29	0.62
1:I:31:LYS:O	1:I:35:GLN:HG3	2.00	0.62
1:J:96:GLN:HG2	1:L:106:SER:OG	2.00	0.62
1:I:75:ASP:HB2	4:I:305:HOH:O	2.00	0.61
1:I:118:LEU:HD22	1:I:162:ILE:HG23	1.81	0.61
1:A:82:GLU:HG2	1:E:160:TRP:CH2	2.35	0.61
1:L:77:LEU:HA	1:L:80:PHE:CD2	2.36	0.61
1:H:83:ARG:NH1	1:J:156:ASP:OD2	2.33	0.61
1:F:96:GLN:OE1	1:F:96:GLN:N	2.27	0.60
1:G:22:GLU:HB3	1:G:24:HIS:CE1	2.36	0.60
1:G:41:ILE:O	1:G:44:SER:HB2	2.02	0.60
1:H:80:PHE:HA	1:H:147:MET:CE	2.32	0.60
1:C:79:THR:CG2	1:C:147:MET:HG2	2.32	0.60
1:G:19:ASN:O	1:G:26:LYS:NZ	2.34	0.60
1:I:79:THR:OG1	1:I:147:MET:HE3	2.01	0.60
1:C:18:ARG:HB3	1:H:126:ALA:HB1	1.83	0.60
1:C:123:GLU:O	1:C:127:ILE:HG23	2.02	0.60
1:A:104:LEU:HD13	1:A:124:ARG:HB3	1.83	0.60
1:C:79:THR:HG22	1:C:147:MET:HG2	1.84	0.60
1:A:60:VAL:CG2	1:H:65:MET:HE3	2.32	0.59
1:G:33:LEU:O	1:G:37:VAL:HG23	2.02	0.59
1:K:80:PHE:CE1	1:K:147:MET:HG2	2.36	0.59
1:I:80:PHE:HD1	1:I:147:MET:CE	2.15	0.59
1:H:14:LEU:HD13	1:H:26:LYS:HD3	1.84	0.59
1:H:80:PHE:HZ	1:H:151:ALA:HB2	1.66	0.59
1:K:19:ASN:OD1	1:K:21:VAL:HG12	2.03	0.59
1:C:40:PHE:O	1:C:44:SER:N	2.35	0.59
1:D:51:HIS:CE1	1:D:63:HIS:CE1	2.91	0.59
1:F:106:SER:HB2	3:F:202:SO4:O4	2.02	0.59
1:H:51:HIS:CE1	1:H:63:HIS:CE1	2.91	0.59
1:H:128:VAL:HG12	1:H:155:LEU:HD21	1.83	0.59
1:I:21:VAL:O	1:I:22:GLU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:ILE:HD13	1:K:124:ARG:HD3	1.83	0.59
1:K:55:ARG:O	1:K:113:SER:HA	2.03	0.59
1:F:82:GLU:O	1:F:86:GLN:HG3	2.02	0.59
1:G:76:HIS:NE2	1:G:154:ASP:OD2	2.25	0.59
1:H:51:HIS:CE1	1:H:63:HIS:NE2	2.71	0.59
1:C:94:THR:O	1:C:98:ILE:HG12	2.03	0.58
1:F:21:VAL:HG12	1:F:26:LYS:HG3	1.86	0.58
1:F:127:ILE:HA	4:F:320:HOH:O	2.02	0.58
1:K:80:PHE:CD1	1:K:147:MET:HG2	2.38	0.58
1:F:94:THR:O	1:F:98:ILE:HG12	2.03	0.58
1:L:48:LYS:O	1:L:51:HIS:HB3	2.04	0.58
1:B:60:VAL:HB	1:F:165:ASN:HD21	1.67	0.58
1:F:142:GLU:OE1	1:F:142:GLU:N	2.20	0.58
1:A:106:SER:HB2	4:A:315:HOH:O	2.02	0.58
1:F:80:PHE:CD1	1:F:147:MET:CE	2.81	0.58
1:G:26:LYS:HG2	1:G:87:LEU:HD22	1.85	0.58
1:J:135:ALA:HA	1:J:138:GLU:HG2	1.86	0.58
1:E:33:LEU:CD2	1:E:147:MET:HE1	2.34	0.58
1:E:130:ASN:O	1:E:134:LYS:HD3	2.04	0.58
1:C:128:VAL:HG12	1:C:155:LEU:HD21	1.86	0.57
1:K:130:ASN:HA	1:K:133:ARG:NH1	2.19	0.57
1:A:60:VAL:HG21	1:H:65:MET:HE3	1.85	0.57
1:H:76:HIS:O	1:H:79:THR:HG22	2.04	0.57
1:D:124:ARG:NH2	3:D:203:SO4:O2	2.31	0.57
1:I:80:PHE:CD1	1:I:147:MET:HE2	2.39	0.57
1:H:65:MET:CE	1:H:161:PHE:HB3	2.34	0.57
1:F:51:HIS:CE1	1:F:63:HIS:CE1	2.92	0.57
1:J:161:PHE:O	1:J:165:ASN:ND2	2.38	0.57
1:E:98:ILE:O	1:E:102:THR:HG22	2.04	0.57
1:L:62:VAL:O	1:L:66:LEU:HG	2.05	0.57
1:A:17:THR:HG23	1:E:163:GLU:OE1	2.04	0.57
1:C:23:GLU:HG3	1:C:24:HIS:H	1.68	0.57
1:G:79:THR:HG21	1:L:153:ARG:NH2	2.20	0.56
1:F:18:ARG:NH1	1:K:163:GLU:HG2	2.20	0.56
1:H:107:TYR:CE1	1:H:120:ALA:HB1	2.39	0.56
1:K:30:ILE:HD13	1:K:89:GLY:HA3	1.87	0.56
1:I:31:LYS:HE2	1:I:35:GLN:HE21	1.70	0.56
1:C:14:LEU:HD11	1:C:27:VAL:HG23	1.87	0.56
1:E:33:LEU:HD21	1:E:147:MET:HE1	1.87	0.56
1:B:43:LEU:O	1:B:46:ILE:HG12	2.06	0.56
1:H:32:ARG:NH1	1:H:138:GLU:OE1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:305:HOH:O	1:L:46:ILE:HD11	2.05	0.56
1:A:25:VAL:HG13	1:A:140:GLU:HB2	1.87	0.56
1:C:96:GLN:CD	1:C:96:GLN:H	2.14	0.56
1:G:124:ARG:HG3	1:G:124:ARG:NH1	2.21	0.56
1:C:79:THR:HG22	1:C:147:MET:SD	2.46	0.55
1:D:34:ASN:O	1:D:38:ILE:HG13	2.06	0.55
1:D:163:GLU:OE2	1:K:18:ARG:NH1	2.36	0.55
1:E:34:ASN:O	1:E:38:ILE:HG13	2.06	0.55
1:K:48:LYS:HD3	1:K:70:ARG:HD2	1.89	0.55
1:I:111:ILE:HG13	1:I:117:HIS:CE1	2.41	0.55
1:I:51:HIS:CE1	1:I:63:HIS:NE2	2.75	0.55
1:A:35:GLN:O	1:A:39:GLN:HG2	2.07	0.55
1:B:30:ILE:HD12	1:B:89:GLY:HA3	1.87	0.55
1:G:143:ASN:O	1:G:147:MET:HE3	2.07	0.54
1:I:46:ILE:O	1:I:49:GLN:HB3	2.07	0.54
1:L:81:ALA:O	1:L:85:VAL:HG23	2.07	0.54
1:L:15:LEU:HD12	1:L:88:GLY:O	2.07	0.54
1:B:22:GLU:OE1	1:B:24:HIS:HB2	2.08	0.54
1:L:80:PHE:HA	1:L:147:MET:CE	2.35	0.54
1:A:119:LYS:O	1:A:123:GLU:HG2	2.07	0.54
1:I:46:ILE:HG23	1:I:107:TYR:CD1	2.43	0.54
1:C:30:ILE:HD13	1:C:89:GLY:HA3	1.89	0.54
1:L:51:HIS:O	1:L:63:HIS:HD2	1.90	0.53
1:L:79:THR:HG22	1:L:147:MET:HE3	1.90	0.53
1:F:80:PHE:HA	1:F:147:MET:CE	2.37	0.53
1:G:79:THR:HG21	1:L:153:ARG:HH21	1.73	0.53
1:J:102:THR:CG2	1:J:104:LEU:HB2	2.38	0.53
1:B:160:TRP:CH2	1:L:82:GLU:HG2	2.44	0.53
1:C:34:ASN:O	1:C:38:ILE:HG13	2.07	0.53
1:D:54:MET:HA	1:D:112:HIS:O	2.08	0.53
1:A:20:ASP:OD2	1:E:134:LYS:NZ	2.41	0.53
1:B:26:LYS:HD3	1:B:87:LEU:O	2.09	0.53
1:H:80:PHE:CD1	1:H:147:MET:HE2	2.42	0.53
1:B:74:THR:HG21	3:B:202:SO4:O3	2.08	0.53
1:E:33:LEU:O	1:E:37:VAL:HG23	2.09	0.53
1:H:80:PHE:HZ	1:H:151:ALA:CB	2.21	0.53
1:D:113:SER:HB3	1:D:116:GLU:HB2	1.90	0.53
1:L:111:ILE:HG13	1:L:117:HIS:CE1	2.43	0.53
1:C:109:THR:O	1:C:109:THR:HG22	2.09	0.53
1:E:55:ARG:O	1:E:113:SER:HA	2.08	0.53
1:I:118:LEU:CD2	1:I:162:ILE:HG23	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:SD	1:A:132:ILE:HD12	2.50	0.52
1:I:55:ARG:O	1:I:113:SER:HA	2.09	0.52
1:F:79:THR:C	1:F:147:MET:HE1	2.35	0.52
1:K:128:VAL:HG12	1:K:155:LEU:CD2	2.37	0.52
1:A:136:ILE:HD11	1:A:149:THR:HA	1.91	0.52
1:J:41:ILE:O	1:J:45:LEU:HD13	2.09	0.52
1:B:57:ALA:HB2	1:F:167:GLU:HG3	1.91	0.52
1:D:30:ILE:HD13	1:D:89:GLY:CA	2.40	0.52
1:K:54:MET:HE2	1:K:63:HIS:HB2	1.91	0.52
1:A:43:LEU:HD11	1:A:128:VAL:HG21	1.90	0.52
1:G:102:THR:HG22	1:G:104:LEU:N	2.19	0.52
1:I:73:LEU:O	1:I:77:LEU:HB2	2.10	0.52
1:L:16:TYR:CG	1:L:17:THR:N	2.77	0.52
1:L:80:PHE:HD1	1:L:147:MET:HE3	1.74	0.52
1:C:142:GLU:H	1:C:142:GLU:CD	2.16	0.52
1:H:107:TYR:CD1	1:H:108:PRO:HD2	2.45	0.51
1:K:141:ASP:OD2	1:K:144:SER:HB3	2.09	0.51
1:L:160:TRP:CD1	1:L:164:SER:HG	2.28	0.51
1:H:65:MET:HE1	1:H:165:ASN:HD21	1.75	0.51
1:I:37:VAL:O	1:I:41:ILE:HG13	2.10	0.51
1:B:36:MET:HG3	1:B:132:ILE:HD12	1.92	0.51
1:H:107:TYR:CG	1:H:108:PRO:HD2	2.45	0.51
1:J:29:THR:HG22	1:J:33:LEU:HD12	1.92	0.51
1:J:136:ILE:HD11	1:J:152:SER:HB2	1.92	0.51
1:D:136:ILE:HG12	1:D:148:PHE:HB3	1.93	0.51
1:K:123:GLU:O	1:K:127:ILE:HG13	2.09	0.51
1:C:100:ASP:OD2	1:C:100:ASP:N	2.41	0.51
1:A:30:ILE:CD1	1:A:89:GLY:HA3	2.34	0.51
1:H:128:VAL:HG12	1:H:155:LEU:CD2	2.41	0.51
1:G:139:VAL:HG21	1:G:148:PHE:HE2	1.76	0.51
1:I:94:THR:HG21	4:K:303:HOH:O	2.11	0.51
1:C:142:GLU:OE1	1:C:142:GLU:N	2.37	0.51
1:H:17:THR:C	1:H:19:ASN:H	2.18	0.51
1:K:128:VAL:CG1	1:K:155:LEU:HD21	2.38	0.51
1:B:70:ARG:HH21	1:D:70:ARG:HH21	1.59	0.50
1:C:135:ALA:O	1:C:136:ILE:C	2.52	0.50
1:K:111:ILE:HB	1:K:116:GLU:HB3	1.92	0.50
1:B:35:GLN:O	1:B:39:GLN:HG2	2.11	0.50
1:C:41:ILE:HG13	1:C:77:LEU:HD22	1.93	0.50
1:D:146:ASP:HB2	1:F:149:THR:HG21	1.93	0.50
1:L:13:GLU:O	1:L:14:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:HIS:CD2	1:G:63:HIS:CD2	2.99	0.50
1:J:96:GLN:H	1:J:96:GLN:CD	2.19	0.50
1:H:65:MET:HE1	1:H:165:ASN:ND2	2.26	0.50
1:A:61:ALA:HB1	1:K:60:VAL:HG13	1.93	0.50
1:C:96:GLN:O	1:C:100:ASP:OD2	2.30	0.50
1:G:21:VAL:O	1:G:26:LYS:HE2	2.11	0.50
1:C:20:ASP:OD1	1:H:133:ARG:NH1	2.44	0.50
1:L:21:VAL:O	1:L:26:LYS:HE3	2.11	0.50
1:K:107:TYR:CG	1:K:108:PRO:HD2	2.47	0.50
1:I:51:HIS:CD2	1:I:63:HIS:O	2.65	0.49
1:K:41:ILE:HG12	1:K:77:LEU:CD1	2.39	0.49
1:A:165:ASN:HD21	1:K:60:VAL:HB	1.77	0.49
1:I:82:GLU:O	1:I:86:GLN:HG3	2.11	0.49
1:J:121:LEU:O	1:J:122:ALA:C	2.56	0.49
1:E:139:VAL:HG11	1:E:144:SER:HB2	1.95	0.49
1:J:32:ARG:O	1:J:35:GLN:HG2	2.12	0.49
1:L:51:HIS:O	1:L:63:HIS:CD2	2.65	0.49
1:H:114:VAL:O	1:H:118:LEU:HG	2.13	0.49
1:L:74:THR:HG22	1:L:75:ASP:N	2.28	0.49
1:C:79:THR:HG22	1:C:147:MET:CG	2.42	0.49
1:E:105:LYS:O	1:E:106:SER:C	2.55	0.49
1:F:43:LEU:HD22	1:F:128:VAL:HG21	1.95	0.49
1:L:65:MET:HE1	1:L:165:ASN:HD21	1.78	0.49
1:B:33:LEU:CD2	1:B:147:MET:HE1	2.41	0.49
1:F:106:SER:HB2	3:F:202:SO4:S	2.52	0.49
1:D:136:ILE:CD1	1:D:149:THR:HA	2.43	0.49
1:H:51:HIS:O	1:H:63:HIS:HD2	1.95	0.49
1:D:69:PHE:O	1:D:73:LEU:HG	2.12	0.49
1:F:35:GLN:O	1:F:39:GLN:HG3	2.13	0.49
1:E:21:VAL:HG12	1:E:26:LYS:HG3	1.95	0.48
1:E:144:SER:HA	1:E:147:MET:HE2	1.94	0.48
1:G:50:ALA:O	1:G:54:MET:HB2	2.12	0.48
1:B:159:LEU:O	1:B:163:GLU:HG3	2.13	0.48
1:C:54:MET:HA	1:C:112:HIS:O	2.13	0.48
1:H:130:ASN:OD1	1:H:133:ARG:NH2	2.44	0.48
1:G:139:VAL:HG21	1:G:148:PHE:CE2	2.48	0.48
1:G:33:LEU:HD11	1:G:83:ARG:HG3	1.94	0.48
1:L:80:PHE:CD1	1:L:147:MET:CE	2.90	0.48
3:B:202:SO4:O1	1:D:74:THR:HG21	2.13	0.48
1:E:139:VAL:HG21	1:E:148:PHE:HE2	1.78	0.48
1:G:46:ILE:HG12	1:G:107:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:MET:HE1	1:I:63:HIS:HB2	1.95	0.48
1:C:18:ARG:HB3	1:H:126:ALA:CB	2.44	0.48
1:I:51:HIS:HD2	1:I:63:HIS:O	1.97	0.48
1:B:36:MET:HB3	1:B:80:PHE:CD2	2.49	0.48
1:C:26:LYS:O	1:C:30:ILE:HG13	2.14	0.48
1:I:31:LYS:HE2	1:I:35:GLN:NE2	2.29	0.47
1:K:33:LEU:HD23	1:K:148:PHE:CZ	2.48	0.47
1:L:65:MET:HE1	1:L:165:ASN:ND2	2.28	0.47
1:A:30:ILE:HD13	1:A:89:GLY:CA	2.34	0.47
1:A:41:ILE:O	1:A:45:LEU:HG	2.14	0.47
1:A:41:ILE:HG21	1:A:98:ILE:HD11	1.96	0.47
1:K:21:VAL:HG13	1:K:26:LYS:HD2	1.94	0.47
1:I:36:MET:CE	1:I:132:ILE:HA	2.44	0.47
1:J:32:ARG:CZ	1:J:135:ALA:HB2	2.44	0.47
1:J:78:ASP:OD1	1:L:48:LYS:NZ	2.48	0.47
1:B:26:LYS:O	1:B:30:ILE:HG23	2.15	0.47
1:H:59:PHE:HB3	1:K:165:ASN:OD1	2.14	0.47
1:I:70:ARG:NH2	1:K:70:ARG:HH21	2.13	0.47
1:J:79:THR:HG22	1:J:147:MET:SD	2.55	0.47
1:G:96:GLN:H	1:G:96:GLN:CD	2.22	0.47
1:C:69:PHE:CE2	1:C:158:PHE:HB3	2.49	0.47
1:C:163:GLU:OE2	1:J:18:ARG:HG3	2.15	0.47
1:F:39:GLN:O	1:F:43:LEU:HB2	2.14	0.47
1:J:77:LEU:HD12	1:J:78:ASP:N	2.29	0.47
1:A:55:ARG:HH21	1:C:85:VAL:HG13	1.79	0.47
1:B:139:VAL:HG11	1:B:148:PHE:HE2	1.80	0.47
1:C:39:GLN:O	1:C:43:LEU:HB2	2.15	0.47
1:L:18:ARG:CG	1:L:18:ARG:NH1	2.71	0.47
1:E:110:ASN:O	1:E:112:HIS:ND1	2.47	0.47
1:A:51:HIS:CE1	1:A:63:HIS:CE1	3.03	0.47
1:A:119:LYS:CG	1:A:166:ILE:HD13	2.45	0.47
1:B:42:ASP:O	1:B:46:ILE:HG23	2.15	0.47
1:L:40:PHE:O	1:L:44:SER:HB2	2.15	0.47
1:D:26:LYS:HG2	1:D:87:LEU:HB3	1.97	0.46
1:J:82:GLU:O	1:J:86:GLN:HG3	2.14	0.46
1:J:102:THR:HG22	1:J:104:LEU:HB2	1.97	0.46
1:K:83:ARG:HH21	1:K:141:ASP:CG	2.23	0.46
1:L:33:LEU:HD11	1:L:83:ARG:HG3	1.96	0.46
1:B:81:ALA:CB	1:D:52:TRP:CE2	2.98	0.46
1:D:83:ARG:HH21	1:D:141:ASP:CG	2.24	0.46
1:G:104:LEU:N	1:G:104:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:PHE:O	1:K:73:LEU:HG	2.15	0.46
1:C:89:GLY:HA2	4:C:305:HOH:O	2.15	0.46
1:H:18:ARG:NH1	1:J:163:GLU:HG2	2.30	0.46
1:I:25:VAL:O	1:I:29:THR:OG1	2.28	0.46
1:K:46:ILE:HG23	1:K:107:TYR:CD1	2.51	0.46
1:D:33:LEU:HD13	1:D:84:ALA:N	2.30	0.46
1:F:36:MET:HE2	1:F:132:ILE:HD12	1.98	0.46
1:A:51:HIS:ND1	1:A:63:HIS:O	2.35	0.46
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.77	0.46
1:E:112:HIS:CD2	1:G:15:LEU:HD11	2.51	0.46
1:I:26:LYS:HD3	1:I:87:LEU:O	2.16	0.46
1:B:83:ARG:O	1:B:86:GLN:HB2	2.16	0.46
1:I:51:HIS:O	1:I:63:HIS:CD2	2.66	0.46
1:B:60:VAL:HG13	1:B:61:ALA:N	2.30	0.46
1:B:95:ALA:N	1:D:45:LEU:HD23	2.30	0.46
1:C:115:GLN:O	1:C:116:GLU:C	2.57	0.46
1:F:70:ARG:NH1	3:H:202:SO4:O1	2.42	0.46
1:L:51:HIS:CE1	1:L:63:HIS:CE1	3.04	0.46
3:D:202:SO4:O4	1:G:57:ALA:HB1	2.15	0.46
1:I:118:LEU:HA	1:I:118:LEU:HD23	1.78	0.46
1:E:51:HIS:CE1	1:E:63:HIS:CE1	3.04	0.45
1:G:48:LYS:HG3	1:G:52:TRP:CZ2	2.50	0.45
1:A:38:ILE:CD1	1:A:97:VAL:HG12	2.46	0.45
1:C:40:PHE:O	1:C:44:SER:HB2	2.16	0.45
1:H:19:ASN:O	1:H:26:LYS:NZ	2.48	0.45
1:K:136:ILE:HD11	1:K:149:THR:HA	1.98	0.45
1:L:54:MET:HG2	1:L:114:VAL:HG22	1.98	0.45
1:A:42:ASP:O	1:A:46:ILE:HD13	2.15	0.45
1:B:48:LYS:HA	1:B:51:HIS:HB3	1.99	0.45
1:D:76:HIS:CE1	1:D:151:ALA:HA	2.52	0.45
1:D:136:ILE:HD13	1:D:149:THR:HA	1.98	0.45
1:K:115:GLN:NE2	4:K:307:HOH:O	2.32	0.45
1:C:160:TRP:CH2	1:J:82:GLU:HG2	2.51	0.45
1:K:29:THR:O	1:K:30:ILE:C	2.59	0.45
1:D:40:PHE:HB3	1:D:77:LEU:HB3	1.99	0.45
1:E:60:VAL:HB	1:L:65:MET:CE	2.32	0.45
1:H:107:TYR:CE1	1:H:120:ALA:CB	2.99	0.45
1:J:29:THR:HG22	1:J:33:LEU:CD1	2.46	0.45
1:F:48:LYS:O	1:F:51:HIS:HB3	2.17	0.45
1:J:77:LEU:HD12	1:J:77:LEU:C	2.42	0.45
1:F:26:LYS:HD3	1:F:87:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:THR:HG21	1:L:147:MET:HG2	1.99	0.45
1:K:33:LEU:HD11	1:K:83:ARG:HG3	1.98	0.45
1:K:45:LEU:O	1:K:46:ILE:C	2.60	0.45
1:L:40:PHE:HB3	1:L:77:LEU:HB3	1.98	0.45
1:F:20:ASP:OD2	1:K:134:LYS:NZ	2.49	0.45
1:I:48:LYS:O	1:I:51:HIS:HB3	2.15	0.45
1:I:70:ARG:HH21	1:K:70:ARG:HH21	1.64	0.45
1:J:54:MET:SD	1:J:62:VAL:HG12	2.57	0.45
1:L:113:SER:OG	1:L:116:GLU:HG3	2.17	0.45
1:A:136:ILE:HG21	1:I:142:GLU:HG3	1.98	0.44
1:L:108:PRO:HB2	1:L:111:ILE:HG23	1.98	0.44
1:A:92:LEU:HD23	1:C:109:THR:CG2	2.44	0.44
1:C:119:LYS:O	1:C:123:GLU:HG2	2.18	0.44
1:I:75:ASP:O	1:I:79:THR:HG23	2.18	0.44
1:J:50:ALA:O	1:J:54:MET:HG3	2.16	0.44
1:J:32:ARG:NH2	1:J:135:ALA:HB2	2.32	0.44
1:A:51:HIS:CD2	1:A:51:HIS:C	2.95	0.44
1:I:115:GLN:O	1:I:119:LYS:HG3	2.17	0.44
1:B:50:ALA:HB2	1:B:107:TYR:OH	2.17	0.44
1:E:27:VAL:O	1:E:31:LYS:HG3	2.17	0.44
1:G:98:ILE:O	1:G:99:ASN:C	2.59	0.44
1:B:40:PHE:CZ	1:B:155:LEU:HD22	2.53	0.44
1:J:102:THR:HG22	1:J:104:LEU:N	2.27	0.44
1:C:123:GLU:O	1:C:127:ILE:CG2	2.65	0.44
1:I:80:PHE:HA	1:I:147:MET:CE	2.44	0.44
1:K:54:MET:HE1	1:K:62:VAL:HG12	1.99	0.44
1:K:105:LYS:O	1:K:106:SER:C	2.61	0.44
1:A:119:LYS:HG2	1:A:166:ILE:HD13	1.99	0.44
1:B:83:ARG:NH1	1:B:143:ASN:HD22	2.16	0.44
1:G:46:ILE:HG12	1:G:107:TYR:HB2	1.98	0.44
1:I:54:MET:CE	1:I:63:HIS:HB2	2.48	0.44
1:J:136:ILE:HD11	1:J:152:SER:CB	2.48	0.44
1:L:119:LYS:HG2	1:L:166:ILE:HD13	1.99	0.44
1:G:74:THR:O	1:G:77:LEU:HB3	2.18	0.44
1:H:20:ASP:O	1:H:21:VAL:O	2.36	0.44
1:B:38:ILE:HD13	1:B:101:LYS:HB2	2.00	0.43
1:D:57:ALA:O	1:D:58:ASN:HB3	2.17	0.43
1:G:124:ARG:NH1	1:G:124:ARG:CG	2.81	0.43
1:I:38:ILE:HD13	1:I:101:LYS:HB2	2.00	0.43
1:I:94:THR:HG22	1:I:96:GLN:H	1.82	0.43
1:B:25:VAL:HG13	1:B:140:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:VAL:HG12	1:C:140:GLU:HG3	2.00	0.43
1:L:15:LEU:HD12	1:L:88:GLY:C	2.43	0.43
1:G:35:GLN:HA	1:G:38:ILE:HD12	2.00	0.43
1:G:73:LEU:O	1:G:77:LEU:HB2	2.18	0.43
1:H:22:GLU:OE1	1:H:24:HIS:HB2	2.19	0.43
1:J:133:ARG:HA	1:J:136:ILE:HD12	2.00	0.43
1:A:43:LEU:CD1	1:A:128:VAL:HG21	2.47	0.43
1:A:111:ILE:HG22	1:A:116:GLU:OE2	2.19	0.43
1:F:108:PRO:HG2	1:F:111:ILE:HD13	2.00	0.43
1:B:163:GLU:OE2	1:L:18:ARG:NH1	2.51	0.43
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.86	0.43
1:E:158:PHE:O	1:E:162:ILE:HG13	2.19	0.43
1:I:123:GLU:O	1:I:127:ILE:HG12	2.19	0.43
1:J:13:GLU:N	1:J:13:GLU:CD	2.76	0.43
1:J:77:LEU:HA	1:J:80:PHE:CD2	2.53	0.43
1:K:38:ILE:HD13	1:K:101:LYS:HB2	1.98	0.43
1:K:133:ARG:NH2	1:K:156:ASP:OD1	2.49	0.43
1:C:46:ILE:HG23	1:C:107:TYR:CE1	2.53	0.43
1:D:33:LEU:HD11	1:D:83:ARG:HG3	2.01	0.43
1:F:69:PHE:CE1	1:F:158:PHE:CD1	3.06	0.43
1:G:81:ALA:O	1:G:84:ALA:HB3	2.18	0.43
1:H:46:ILE:HA	1:H:49:GLN:HB3	2.00	0.43
1:C:104:LEU:HD23	1:C:127:ILE:HD11	1.99	0.43
1:E:51:HIS:CE1	1:E:63:HIS:NE2	2.87	0.43
1:H:12:SER:C	1:H:14:LEU:H	2.27	0.43
1:I:70:ARG:HE	1:I:74:THR:HG21	1.84	0.43
1:D:43:LEU:HG	1:D:128:VAL:HG21	2.00	0.43
1:G:26:LYS:HD3	1:G:87:LEU:O	2.18	0.43
1:G:48:LYS:NZ	1:G:67:ASP:OD1	2.51	0.43
1:H:77:LEU:C	1:H:77:LEU:HD12	2.44	0.43
1:K:130:ASN:HA	1:K:133:ARG:HH12	1.83	0.43
1:L:44:SER:OG	1:L:70:ARG:HD2	2.19	0.43
1:B:143:ASN:O	1:B:147:MET:HB2	2.19	0.42
1:C:33:LEU:HD13	1:C:83:ARG:HB3	2.01	0.42
1:C:36:MET:HE2	1:C:132:ILE:CB	2.40	0.42
1:C:107:TYR:CG	1:C:108:PRO:HD2	2.54	0.42
1:J:102:THR:HG21	1:J:104:LEU:HB2	2.01	0.42
1:L:83:ARG:O	1:L:87:LEU:HG	2.19	0.42
1:B:43:LEU:HD12	1:B:46:ILE:HD11	2.01	0.42
1:F:51:HIS:NE2	1:F:63:HIS:CE1	2.87	0.42
1:G:51:HIS:HD2	1:G:63:HIS:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:MET:HE3	1:G:147:MET:HB2	1.82	0.42
1:I:54:MET:HE1	1:I:63:HIS:N	2.34	0.42
1:J:133:ARG:NH2	1:J:156:ASP:OD1	2.46	0.42
1:L:40:PHE:CB	1:L:77:LEU:HB3	2.49	0.42
1:C:158:PHE:CD1	1:C:158:PHE:N	2.86	0.42
1:D:46:ILE:HG12	1:D:107:TYR:HB2	2.01	0.42
1:K:21:VAL:HG11	1:K:87:LEU:CD2	2.47	0.42
1:B:22:GLU:O	1:B:23:GLU:C	2.62	0.42
1:B:139:VAL:HG11	1:B:148:PHE:CE2	2.54	0.42
1:B:51:HIS:ND1	1:B:63:HIS:O	2.53	0.42
1:F:29:THR:HG22	1:F:33:LEU:CD1	2.50	0.42
1:H:30:ILE:O	1:H:31:LYS:C	2.62	0.42
1:L:107:TYR:O	1:L:108:PRO:C	2.62	0.42
1:J:32:ARG:HD2	1:J:35:GLN:OE1	2.20	0.42
1:C:121:LEU:O	1:C:122:ALA:C	2.62	0.42
1:G:54:MET:HE3	1:G:59:PHE:CD1	2.55	0.42
1:K:147:MET:HE3	1:K:147:MET:HB2	1.68	0.42
1:E:107:TYR:CG	1:E:108:PRO:HD2	2.54	0.42
1:H:80:PHE:CD1	1:H:147:MET:CE	2.85	0.42
1:K:45:LEU:O	1:K:48:LYS:N	2.52	0.42
1:E:55:ARG:CZ	1:G:15:LEU:HD13	2.49	0.42
1:K:102:THR:HG23	1:K:102:THR:O	2.20	0.42
1:K:117:HIS:O	1:K:118:LEU:C	2.62	0.42
1:B:48:LYS:O	1:B:51:HIS:HB3	2.20	0.42
1:D:133:ARG:HH21	1:D:156:ASP:CG	2.28	0.42
1:K:18:ARG:O	1:K:19:ASN:C	2.63	0.42
1:B:41:ILE:O	1:B:45:LEU:HG	2.19	0.41
1:B:102:THR:O	1:B:102:THR:HG23	2.19	0.41
1:C:23:GLU:O	1:C:24:HIS:C	2.62	0.41
1:J:54:MET:HE2	1:J:54:MET:HB2	1.83	0.41
1:J:109:THR:O	1:J:109:THR:CG2	2.67	0.41
1:J:118:LEU:CB	1:J:166:ILE:HD11	2.46	0.41
1:H:80:PHE:CZ	1:H:151:ALA:HB2	2.51	0.41
1:I:126:ALA:O	1:I:127:ILE:C	2.63	0.41
1:K:20:ASP:O	1:K:21:VAL:C	2.63	0.41
1:L:56:GLY:O	1:L:57:ALA:C	2.62	0.41
1:G:76:HIS:CE1	1:G:151:ALA:HA	2.55	0.41
1:H:22:GLU:OE2	1:H:23:GLU:N	2.53	0.41
1:E:94:THR:O	1:E:97:VAL:N	2.54	0.41
1:F:41:ILE:O	1:F:45:LEU:HG	2.19	0.41
1:G:34:ASN:O	1:G:38:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:O	1:A:70:ARG:C	2.63	0.41
1:C:79:THR:HG21	1:C:147:MET:HG2	2.02	0.41
1:E:60:VAL:CG2	1:L:65:MET:HE3	2.50	0.41
1:F:59:PHE:O	1:F:60:VAL:C	2.62	0.41
1:L:22:GLU:OE2	1:L:24:HIS:NE2	2.50	0.41
1:L:41:ILE:O	1:L:45:LEU:HG	2.21	0.41
1:L:134:LYS:HA	1:L:134:LYS:HD3	1.51	0.41
1:A:124:ARG:O	1:A:128:VAL:HG23	2.20	0.41
1:B:141:ASP:HB3	1:B:144:SER:HB2	2.02	0.41
1:E:139:VAL:CG1	1:E:141:ASP:H	2.33	0.41
1:G:115:GLN:OE1	1:G:167:GLU:N	2.54	0.41
1:H:132:ILE:O	1:H:136:ILE:HG13	2.20	0.41
1:A:21:VAL:O	1:A:26:LYS:HE3	2.21	0.41
1:A:48:LYS:HG3	1:A:70:ARG:NH1	2.35	0.41
1:F:155:LEU:HD23	1:F:155:LEU:HA	1.84	0.41
1:A:34:ASN:O	1:A:38:ILE:HG12	2.21	0.41
1:C:17:THR:C	1:C:19:ASN:N	2.78	0.41
1:G:26:LYS:CD	1:G:87:LEU:O	2.69	0.41
1:D:97:VAL:O	1:D:101:LYS:HB2	2.21	0.41
1:F:118:LEU:HD23	1:F:118:LEU:HA	1.87	0.41
1:G:51:HIS:O	1:G:63:HIS:HD2	2.03	0.41
1:B:19:ASN:ND2	1:G:156:ASP:OD2	2.50	0.41
1:D:38:ILE:HD13	1:D:101:LYS:HB3	2.02	0.41
1:E:97:VAL:O	1:E:101:LYS:HB2	2.21	0.41
1:L:158:PHE:O	1:L:159:LEU:C	2.64	0.41
1:A:146:ASP:OD2	1:E:153:ARG:NH1	2.48	0.40
1:B:51:HIS:O	1:B:63:HIS:ND1	2.53	0.40
1:K:46:ILE:HG23	1:K:107:TYR:CE1	2.57	0.40
1:L:107:TYR:CD2	1:L:108:PRO:HD2	2.57	0.40
1:A:69:PHE:CE1	1:A:158:PHE:CD1	3.09	0.40
1:C:66:LEU:N	1:C:66:LEU:HD23	2.35	0.40
1:D:42:ASP:O	1:D:46:ILE:HB	2.21	0.40
1:G:94:THR:O	1:G:95:ALA:C	2.64	0.40
1:H:166:ILE:O	1:H:167:GLU:C	2.63	0.40
1:I:48:LYS:HD3	1:I:48:LYS:HA	2.00	0.40
1:I:70:ARG:HE	1:I:74:THR:CG2	2.34	0.40
1:J:135:ALA:HA	1:J:138:GLU:CG	2.50	0.40
1:B:83:ARG:HH12	1:B:143:ASN:HD22	1.69	0.40
1:B:107:TYR:CD1	1:B:108:PRO:HD2	2.57	0.40
1:H:100:ASP:O	1:H:101:LYS:HD3	2.21	0.40
1:K:54:MET:HE1	1:K:62:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:LEU:HD12	1:K:104:LEU:HA	1.84	0.40
1:C:147:MET:HE3	1:C:147:MET:HB2	1.92	0.40
1:G:97:VAL:O	1:G:98:ILE:C	2.64	0.40
1:H:121:LEU:HA	1:H:121:LEU:HD23	1.76	0.40
1:I:48:LYS:NZ	1:I:67:ASP:OD1	2.48	0.40
1:L:30:ILE:HD13	1:L:89:GLY:HA3	2.02	0.40
1:L:111:ILE:CG1	1:L:117:HIS:CE1	3.04	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	153/170 (90%)	150 (98%)	3 (2%)	0	100	100
1	B	152/170 (89%)	146 (96%)	6 (4%)	0	100	100
1	C	152/170 (89%)	144 (95%)	8 (5%)	0	100	100
1	D	154/170 (91%)	145 (94%)	9 (6%)	0	100	100
1	E	153/170 (90%)	144 (94%)	9 (6%)	0	100	100
1	F	152/170 (89%)	147 (97%)	5 (3%)	0	100	100
1	G	153/170 (90%)	143 (94%)	10 (6%)	0	100	100
1	H	155/170 (91%)	144 (93%)	10 (6%)	1 (1%)	21	38
1	I	153/170 (90%)	145 (95%)	8 (5%)	0	100	100
1	J	153/170 (90%)	140 (92%)	11 (7%)	2 (1%)	9	18
1	K	153/170 (90%)	142 (93%)	11 (7%)	0	100	100
1	L	153/170 (90%)	141 (92%)	12 (8%)	0	100	100
All	All	1836/2040 (90%)	1731 (94%)	102 (6%)	3 (0%)	43	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	21	VAL
1	J	86	GLN
1	J	59	PHE

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	133/146 (91%)	125 (94%)	8 (6%)	17	32
1	B	132/146 (90%)	124 (94%)	8 (6%)	17	31
1	C	132/146 (90%)	124 (94%)	8 (6%)	17	31
1	D	134/146 (92%)	127 (95%)	7 (5%)	21	39
1	E	133/146 (91%)	127 (96%)	6 (4%)	24	46
1	F	132/146 (90%)	127 (96%)	5 (4%)	29	52
1	G	133/146 (91%)	122 (92%)	11 (8%)	10	19
1	H	135/146 (92%)	127 (94%)	8 (6%)	18	33
1	I	133/146 (91%)	125 (94%)	8 (6%)	17	32
1	J	133/146 (91%)	122 (92%)	11 (8%)	10	19
1	K	133/146 (91%)	127 (96%)	6 (4%)	24	46
1	L	133/146 (91%)	119 (90%)	14 (10%)	6	13
All	All	1596/1752 (91%)	1496 (94%)	100 (6%)	16	30

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	51	HIS
1	A	75	ASP
1	A	77	LEU
1	A	78	ASP
1	A	113	SER
1	A	131	ASP
1	A	137	THR

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Mol	Chain	Res	Type
1	B	17	THR
1	B	22	GLU
1	B	30	ILE
1	B	31	LYS
1	B	36	MET
1	B	44	SER
1	B	74	THR
1	B	78	ASP
1	C	22	GLU
1	C	23	GLU
1	C	41	ILE
1	C	44	SER
1	C	67	ASP
1	C	74	THR
1	C	127	ILE
1	C	155	LEU
1	D	45	LEU
1	D	46	ILE
1	D	51	HIS
1	D	55	ARG
1	D	74	THR
1	D	101	LYS
1	D	144	SER
1	E	44	SER
1	E	74	THR
1	E	77	LEU
1	E	110	ASN
1	E	139	VAL
1	E	142	GLU
1	F	15	LEU
1	F	22	GLU
1	F	43	LEU
1	F	46	ILE
1	F	167	GLU
1	G	23	GLU
1	G	24	HIS
1	G	26	LYS
1	G	27	VAL
1	G	46	ILE
1	G	64	GLU
1	G	74	THR
1	G	78	ASP

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Mol	Chain	Res	Type
1	G	97	VAL
1	G	105	LYS
1	G	155	LEU
1	H	58	ASN
1	H	77	LEU
1	H	79	THR
1	H	105	LYS
1	H	137	THR
1	H	155	LEU
1	H	157	LYS
1	H	167	GLU
1	I	20	ASP
1	I	22	GLU
1	I	41	ILE
1	I	77	LEU
1	I	78	ASP
1	I	110	ASN
1	I	132	ILE
1	I	142	GLU
1	J	22	GLU
1	J	27	VAL
1	J	31	LYS
1	J	35	GLN
1	J	43	LEU
1	J	64	GLU
1	J	74	THR
1	J	102	THR
1	J	109	THR
1	J	139	VAL
1	J	164	SER
1	K	22	GLU
1	K	25	VAL
1	K	26	LYS
1	K	48	LYS
1	K	109	THR
1	K	144	SER
1	L	15	LEU
1	L	18	ARG
1	L	23	GLU
1	L	32	ARG
1	L	38	ILE
1	L	44	SER

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Mol	Chain	Res	Type
1	L	54	MET
1	L	65	MET
1	L	74	THR
1	L	97	VAL
1	L	102	THR
1	L	109	THR
1	L	115	GLN
1	L	139	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	35	GLN
1	B	143	ASN
1	D	51	HIS
1	E	110	ASN
1	F	51	HIS
1	F	53	ASN
1	G	51	HIS
1	G	63	HIS
1	G	143	ASN
1	H	51	HIS
1	H	58	ASN
1	H	63	HIS
1	I	51	HIS
1	I	63	HIS
1	I	112	HIS
1	J	86	GLN
1	L	53	ASN
1	L	63	HIS
1	L	112	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	B	203	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	B	202	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	E	203	-	4,4,4	0.20	0	6,6,6	0.24	0
3	SO4	H	202	-	4,4,4	0.19	0	6,6,6	0.30	0
3	SO4	G	201	-	4,4,4	0.20	0	6,6,6	0.42	0
3	SO4	J	203	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	K	202	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	F	202	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	J	202	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	203	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	D	203	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	D	202	-	4,4,4	0.24	0	6,6,6	0.16	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 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	SO4	2	0
3	E	203	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	202	SO4	1	0
3	G	201	SO4	1	0
3	J	203	SO4	1	0
3	F	202	SO4	2	0
3	D	203	SO4	1	0
3	D	202	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	155/170 (91%)	-0.48	0 100 100	22, 36, 57, 78	0
1	B	154/170 (90%)	-0.51	0 100 100	18, 36, 52, 67	0
1	C	154/170 (90%)	-0.42	0 100 100	23, 40, 61, 74	0
1	D	156/170 (91%)	-0.56	1 (0%) 85 86	15, 33, 54, 97	0
1	E	155/170 (91%)	-0.58	0 100 100	17, 33, 55, 75	0
1	F	154/170 (90%)	-0.57	0 100 100	17, 33, 53, 66	0
1	G	155/170 (91%)	-0.57	0 100 100	15, 34, 57, 82	0
1	H	157/170 (92%)	-0.37	1 (0%) 85 86	17, 38, 59, 108	0
1	I	155/170 (91%)	-0.55	0 100 100	17, 31, 58, 77	0
1	J	155/170 (91%)	-0.53	0 100 100	23, 36, 57, 80	0
1	K	155/170 (91%)	-0.50	0 100 100	20, 34, 51, 69	0
1	L	155/170 (91%)	-0.39	0 100 100	18, 36, 59, 80	0
All	All	1860/2040 (91%)	-0.50	2 (0%) 92 93	15, 35, 57, 108	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	11	PRO	3.1
1	D	12	SER	2.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	H	202	5/5	0.82	0.13	86,92,94,94	0
3	SO4	F	202	5/5	0.84	0.10	79,82,83,84	5
3	SO4	A	203	5/5	0.86	0.16	85,87,91,92	0
3	SO4	D	203	5/5	0.87	0.11	74,78,79,82	5
3	SO4	E	203	5/5	0.91	0.12	80,81,82,84	0
3	SO4	A	202	5/5	0.92	0.10	75,80,83,85	0
3	SO4	K	202	5/5	0.92	0.10	63,68,69,70	0
3	SO4	J	202	5/5	0.93	0.10	77,80,84,85	0
3	SO4	B	203	5/5	0.95	0.15	78,79,82,83	0
2	ZN	F	201	1/1	0.96	0.04	71,71,71,71	0
3	SO4	D	202	5/5	0.96	0.08	60,68,69,71	0
2	ZN	J	201	1/1	0.96	0.07	98,98,98,98	0
3	SO4	B	202	5/5	0.96	0.07	61,65,68,68	0
3	SO4	G	201	5/5	0.97	0.06	29,37,40,55	0
2	ZN	K	201	1/1	0.97	0.05	80,80,80,80	0
2	ZN	A	201	1/1	0.97	0.04	81,81,81,81	0
2	ZN	C	201	1/1	0.97	0.05	73,73,73,73	0
2	ZN	I	201	1/1	0.98	0.05	82,82,82,82	0
2	ZN	E	201	1/1	0.98	0.07	73,73,73,73	0
2	ZN	E	202	1/1	0.98	0.05	72,72,72,72	0
2	ZN	B	201	1/1	0.98	0.05	81,81,81,81	0
3	SO4	J	203	5/5	0.98	0.06	37,43,47,53	0
2	ZN	H	201	1/1	0.98	0.05	81,81,81,81	0
2	ZN	L	201	1/1	0.99	0.05	68,68,68,68	0
2	ZN	D	201	1/1	0.99	0.03	68,68,68,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.