



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:43 am BST

PDB ID : 2IDE
Title : Crystal Structure of the molybdenum cofactor biosynthesis protein C (TTHA1789) from *Thermus Thermophilus* HB8
Authors : Jeyakanthan, J.; Kanaugia, S.P.; Vasuki Ranjani, C.; Sekar, K.; Baba, S.; Ebihara, A.; Kuramitsu, S.; Shinkai, A.; Shiro, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-09-15
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

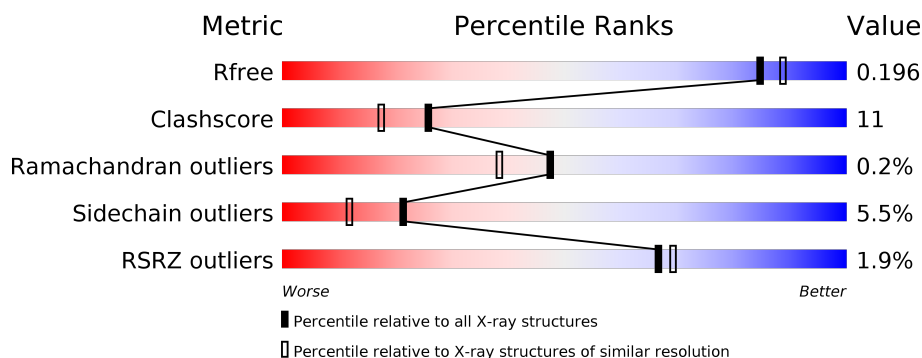
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	157	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	157	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 6%</div> </div> </div>
1	C	157	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• • 6%</div> </div> </div>
1	D	157	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	E	157	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	F	157	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	157	<div><div>%</div><div><div></div><div>76%</div><div>17%</div><div>• 6%</div></div></div>
1	H	157	<div><div>3%</div><div><div></div><div>76%</div><div>15%</div><div>• 6%</div></div></div>
1	I	157	<div><div>%</div><div><div></div><div>76%</div><div>17%</div><div>• 6%</div></div></div>
1	J	157	<div><div>2%</div><div><div></div><div>76%</div><div>16%</div><div>• 6%</div></div></div>
1	K	157	<div><div>2%</div><div><div></div><div>71%</div><div>18%</div><div>• • 6%</div></div></div>
1	L	157	<div><div>%</div><div><div></div><div>75%</div><div>17%</div><div>• 6%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14850 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 Molybdenum cofactor biosynthesis protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1104	696	195	207	6			
1	B	148	Total	C	N	O	S	0	0	0
			1105	697	195	207	6			
1	C	147	Total	C	N	O	S	0	0	0
			1096	692	194	204	6			
1	D	147	Total	C	N	O	S	0	0	0
			1096	692	194	204	6			
1	E	147	Total	C	N	O	S	0	0	0
			1096	692	194	204	6			
1	F	146	Total	C	N	O	S	0	0	0
			1092	690	193	203	6			
1	G	147	Total	C	N	O	S	0	0	0
			1096	692	194	204	6			
1	H	148	Total	C	N	O	S	0	0	0
			1105	697	195	207	6			
1	I	147	Total	C	N	O	S	0	0	0
			1101	695	194	206	6			
1	J	148	Total	C	N	O	S	0	0	0
			1105	697	195	207	6			
1	K	148	Total	C	N	O	S	0	0	0
			1105	697	195	207	6			
1	L	148	Total	C	N	O	S	0	0	0
			1105	697	195	207	6			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

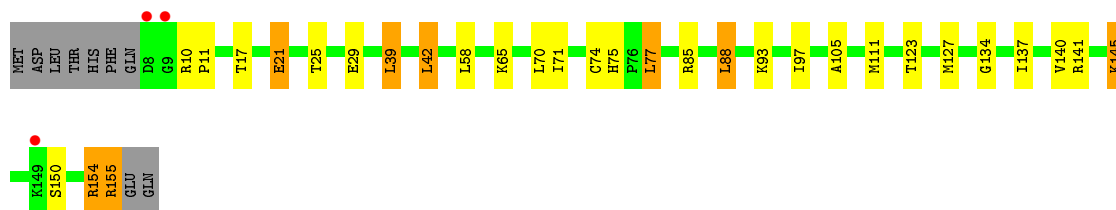
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total 142	O 142	0	0
3	B	130	Total 130	O 130	0	0
3	C	117	Total 117	O 117	0	0
3	D	130	Total 130	O 130	0	0
3	E	110	Total 110	O 110	0	0
3	F	134	Total 134	O 134	0	0
3	G	141	Total 141	O 141	0	0
3	H	138	Total 138	O 138	0	0
3	I	135	Total 135	O 135	0	0
3	J	124	Total 124	O 124	0	0
3	K	135	Total 135	O 135	0	0
3	L	148	Total 148	O 148	0	0

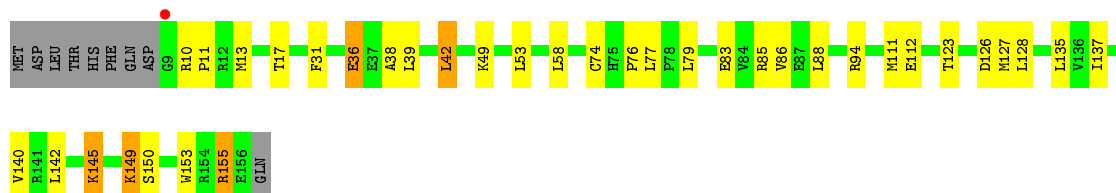
3 Residue-property plots [i](#)

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

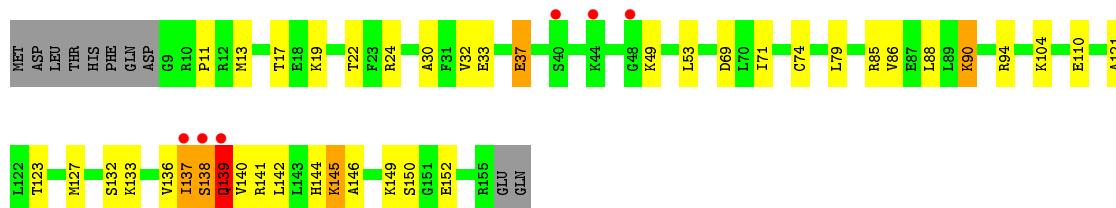
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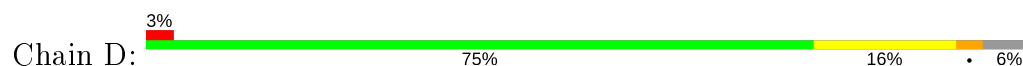
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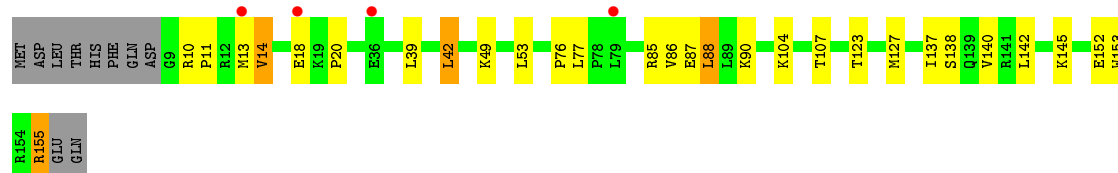


- Molecule 1: Molybdenum cofactor biosynthesis protein C

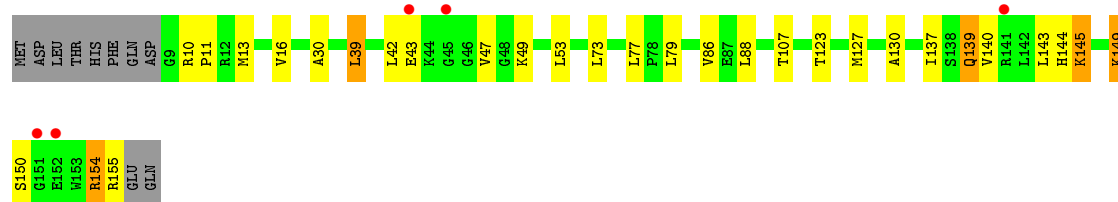


- Molecule 1: Molybdenum cofactor biosynthesis protein C

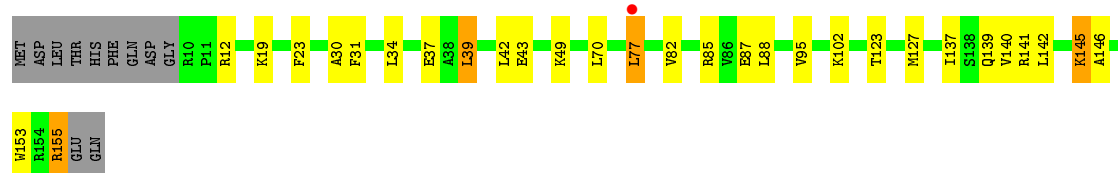
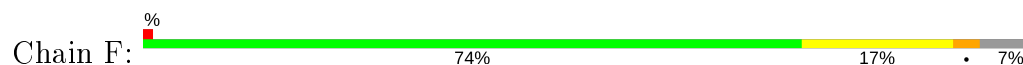




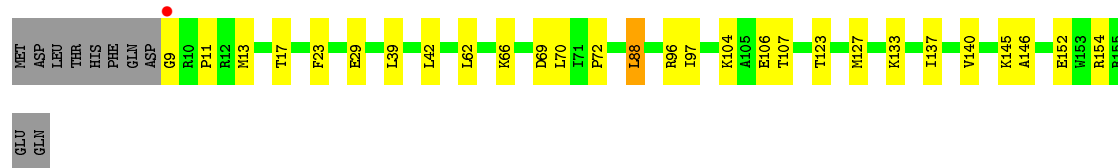
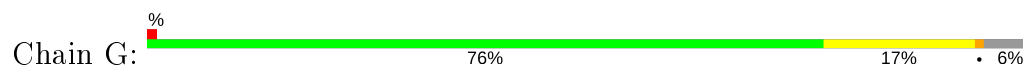
- Molecule 1: Molybdenum cofactor biosynthesis protein C



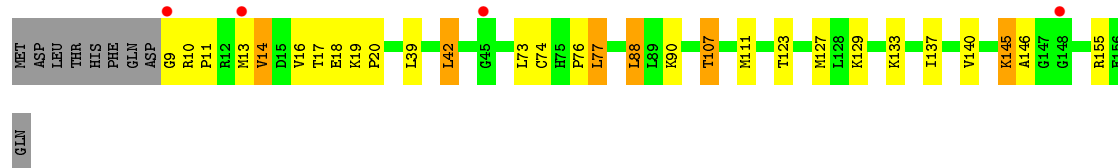
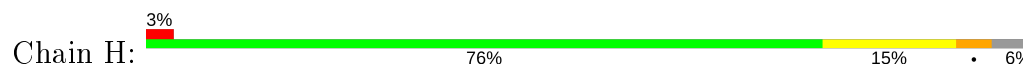
- Molecule 1: Molybdenum cofactor biosynthesis protein C



- Molecule 1: Molybdenum cofactor biosynthesis protein C

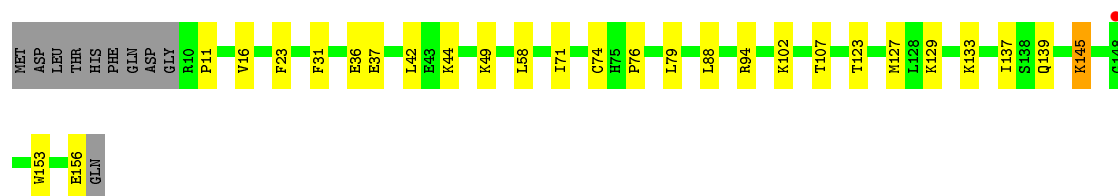


- Molecule 1: Molybdenum cofactor biosynthesis protein C

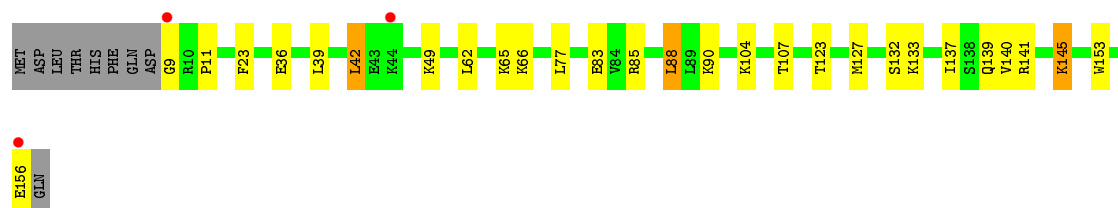
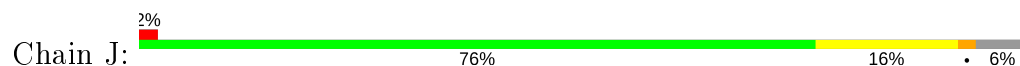


- Molecule 1: Molybdenum cofactor biosynthesis protein C

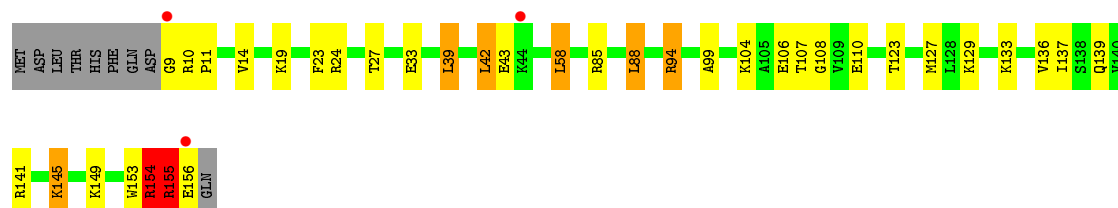




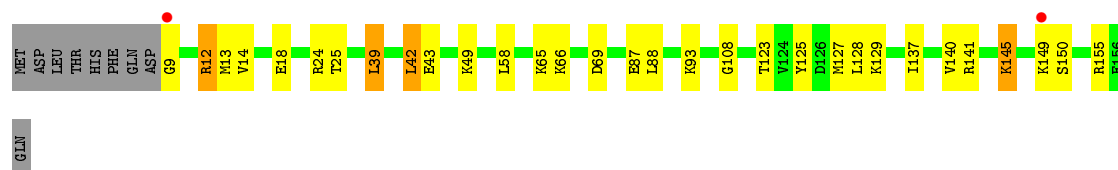
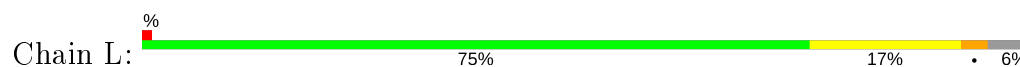
• Molecule 1: Molybdenum cofactor biosynthesis protein C



• Molecule 1: Molybdenum cofactor biosynthesis protein C



• Molecule 1: Molybdenum cofactor biosynthesis protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.81Å 109.84Å 115.19Å 90.00° 104.86° 90.00°	Depositor
Resolution (Å)	49.66 – 1.90 49.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.66-1.90) 98.7 (49.66-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.226 0.196 , 0.196	Depositor DCC
R_{free} test set	6132 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14850	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6183e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.28	0/1116	0.71	1/1506 (0.1%)
1	B	0.28	0/1117	0.63	0/1507
1	C	0.31	0/1108	0.72	3/1495 (0.2%)
1	D	0.30	0/1108	0.63	0/1495
1	E	0.33	0/1108	0.67	2/1495 (0.1%)
1	F	0.29	0/1104	0.63	0/1490
1	G	0.30	0/1108	0.64	0/1495
1	H	0.31	0/1117	0.64	0/1507
1	I	0.33	0/1113	0.67	0/1502
1	J	0.30	0/1117	0.64	0/1507
1	K	0.30	0/1117	0.68	2/1507 (0.1%)
1	L	0.32	0/1117	0.66	0/1507
All	All	0.30	0/13350	0.66	8/18013 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	K	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	SER	N-CA-C	-7.37	91.11	111.00
1	A	155	ARG	NE-CZ-NH2	-7.17	116.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ILE	N-CA-C	-7.14	91.73	111.00
1	K	155	ARG	N-CA-CB	-6.10	99.62	110.60
1	C	139	GLN	N-CA-C	5.98	127.15	111.00
1	K	154	ARG	CB-CA-C	-5.46	99.47	110.40
1	E	154	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	E	154	ARG	NE-CZ-NH2	5.13	122.86	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	149	LYS	Peptide
1	K	154	ARG	Peptide

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	1104	0	1170	27	0
1	B	1105	0	1172	30	0
1	C	1096	0	1166	41	0
1	D	1096	0	1166	25	0
1	E	1096	0	1166	29	0
1	F	1092	0	1163	29	0
1	G	1096	0	1166	21	0
1	H	1105	0	1172	24	0
1	I	1101	0	1169	29	0
1	J	1105	0	1172	31	0
1	K	1105	0	1172	38	0
1	L	1105	0	1172	29	0
2	A	10	0	0	0	0
2	C	10	0	0	0	0
2	E	10	0	0	1	0
2	G	10	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	1	0
2	J	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	5	0	0	1	0
3	A	142	0	0	2	0
3	B	130	0	0	0	0
3	C	117	0	0	7	0
3	D	130	0	0	3	0
3	E	110	0	0	2	0
3	F	134	0	0	4	0
3	G	141	0	0	3	0
3	H	138	0	0	3	0
3	I	135	0	0	8	0
3	J	124	0	0	6	0
3	K	135	0	0	4	0
3	L	148	0	0	10	0
All	All	14850	0	14026	287	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 11.

All (287) 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:B:149:LYS:H	1:B:149:LYS:HD3	1.25	1.00
1:C:90:LYS:H	1:C:90:LYS:HD3	1.28	0.96
1:G:17:THR:O	1:J:104:LYS:HE2	1.70	0.92
1:C:121:ALA:HB1	1:C:137:ILE:HD12	1.49	0.92
1:A:10:ARG:CZ	1:D:85:ARG:HD3	2.07	0.85
1:G:133:LYS:HE2	1:L:145:LYS:HE2	1.57	0.83
1:J:132:SER:HB3	3:J:2233:HOH:O	1.79	0.82
1:D:142:LEU:O	1:D:155:ARG:NH1	2.12	0.81
1:I:58:LEU:HD23	1:K:58:LEU:HD12	1.66	0.78
1:G:96:ARG:HD3	3:G:2309:HOH:O	1.85	0.77
1:H:145:LYS:HE2	1:K:133:LYS:HE2	1.68	0.75
1:L:69:ASP:HB2	3:L:193:HOH:O	1.85	0.75
1:K:154:ARG:O	1:K:154:ARG:HG2	1.85	0.74
1:E:47:VAL:HG21	1:E:130:ALA:HB3	1.70	0.73
1:I:145:LYS:HE2	1:J:133:LYS:HE2	1.70	0.73
1:C:90:LYS:N	1:C:90:LYS:HD3	2.05	0.72
1:K:23:PHE:CE1	1:K:104:LYS:HD3	2.24	0.72
1:B:76:PRO:HG2	1:C:79:LEU:H	1.55	0.72
1:G:9:GLY:HA2	3:G:2229:HOH:O	1.89	0.71
1:K:149:LYS:H	1:K:149:LYS:HD2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2234:HOH:O	1:J:66:LYS:HE3	1.90	0.70
1:C:30:ALA:HA	1:C:139:GLN:O	1.91	0.70
1:C:149:LYS:HB3	3:C:2273:HOH:O	1.90	0.69
1:L:12:ARG:HG2	1:L:12:ARG:HH11	1.55	0.69
1:F:31:PHE:HZ	3:F:171:HOH:O	1.77	0.68
1:I:16:VAL:HG11	1:I:107:THR:CG2	2.24	0.68
1:K:154:ARG:HH11	1:K:154:ARG:HG3	1.60	0.67
1:K:33:GLU:OE2	1:K:94:ARG:HD2	1.96	0.66
3:H:2241:HOH:O	1:L:12:ARG:HB2	1.96	0.65
1:A:17:THR:O	1:D:104:LYS:HE2	1.95	0.65
1:D:138:SER:HB3	3:D:275:HOH:O	1.96	0.65
1:J:139:GLN:HE21	1:J:141:ARG:HH11	1.43	0.65
1:B:83:GLU:OE2	1:F:12:ARG:HD3	1.98	0.64
1:C:69:ASP:HB2	3:C:2214:HOH:O	1.97	0.64
1:K:141:ARG:HD2	1:K:156:GLU:HG3	1.80	0.64
1:K:154:ARG:O	1:K:154:ARG:CG	2.45	0.63
1:A:141:ARG:CZ	1:A:155:ARG:HH22	2.12	0.62
1:E:155:ARG:O	1:E:155:ARG:HG2	2.00	0.62
1:C:137:ILE:HB	1:D:140:VAL:HB	1.82	0.61
1:F:39:LEU:O	1:F:43:GLU:HG3	1.99	0.61
1:K:154:ARG:O	1:K:155:ARG:HB3	2.01	0.60
1:E:144:HIS:HD2	1:E:154:ARG:HG2	1.66	0.60
1:I:36:GLU:HG3	3:I:2235:HOH:O	2.01	0.60
1:G:23:PHE:HE1	1:G:104:LYS:HD3	1.67	0.60
1:H:9:GLY:N	3:H:2230:HOH:O	2.34	0.60
1:L:39:LEU:O	1:L:43:GLU:HG3	2.01	0.59
1:L:93:LYS:HD2	3:L:197:HOH:O	2.02	0.59
1:K:154:ARG:HG3	1:K:154:ARG:NH1	2.19	0.58
1:C:110:GLU:OE2	1:C:145:LYS:HE3	2.03	0.58
1:A:39:LEU:HD12	1:A:93:LYS:HD3	1.85	0.58
1:D:76:PRO:HG2	1:E:79:LEU:H	1.69	0.58
1:B:11:PRO:HA	1:E:49:LYS:O	2.05	0.57
1:H:145:LYS:C	1:H:145:LYS:HD2	2.25	0.57
1:K:149:LYS:H	1:K:149:LYS:CD	2.17	0.57
1:B:140:VAL:HB	1:E:137:ILE:HB	1.86	0.57
1:I:37:GLU:HG3	3:I:2314:HOH:O	2.04	0.57
1:G:140:VAL:HB	1:L:137:ILE:HB	1.86	0.57
1:A:85:ARG:HE	1:E:10:ARG:NH1	2.03	0.57
1:I:31:PHE:HB3	1:I:94:ARG:HD2	1.87	0.56
1:K:141:ARG:CD	1:K:156:GLU:HG3	2.34	0.56
1:A:141:ARG:CZ	1:A:155:ARG:NH2	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:LYS:HD3	3:L:185:HOH:O	2.06	0.56
1:J:23:PHE:HE2	1:J:104:LYS:HD3	1.70	0.56
1:H:42:LEU:HD13	1:H:88:LEU:HG	1.87	0.56
1:C:136:VAL:HG12	1:C:137:ILE:O	2.05	0.55
1:K:19:LYS:HD2	1:K:149:LYS:CE	2.36	0.55
1:A:75:HIS:O	1:A:77:LEU:HD13	2.06	0.55
1:I:139:GLN:HA	1:J:137:ILE:O	2.06	0.55
1:K:19:LYS:HD2	1:K:149:LYS:HE2	1.89	0.55
1:B:31:PHE:CD2	1:B:94:ARG:HD2	2.41	0.55
1:F:102:LYS:HE2	3:F:237:HOH:O	2.06	0.55
1:E:155:ARG:CG	1:E:155:ARG:O	2.55	0.54
1:D:18:GLU:HB3	1:H:18:GLU:HB3	1.89	0.54
1:J:123:THR:O	1:J:127:MET:HG2	2.08	0.54
1:L:25:THR:HG22	3:L:212:HOH:O	2.08	0.53
1:I:133:LYS:NZ	1:J:145:LYS:HE2	2.23	0.53
1:I:156:GLU:N	3:I:2323:HOH:O	2.38	0.53
1:L:155:ARG:HD3	3:L:200:HOH:O	2.08	0.53
1:A:21:GLU:HG3	1:A:105:ALA:HA	1.90	0.52
1:C:145:LYS:HG2	1:C:146:ALA:N	2.23	0.52
1:C:19:LYS:HE3	1:C:149:LYS:HD2	1.90	0.52
1:J:139:GLN:HE21	1:J:141:ARG:NH1	2.07	0.52
1:B:49:LYS:O	1:E:11:PRO:HA	2.09	0.52
1:H:145:LYS:HD2	1:H:146:ALA:N	2.25	0.52
1:L:42:LEU:HG	1:L:128:LEU:HD11	1.92	0.52
1:B:123:THR:O	1:B:127:MET:HG2	2.10	0.52
1:G:137:ILE:HB	1:L:140:VAL:HB	1.91	0.52
1:I:49:LYS:O	1:J:11:PRO:HA	2.11	0.51
1:L:12:ARG:HG2	1:L:12:ARG:NH1	2.25	0.51
1:L:149:LYS:HG2	1:L:150:SER:H	1.75	0.51
1:C:11:PRO:HA	1:D:49:LYS:O	2.10	0.51
1:D:42:LEU:HD13	1:D:88:LEU:HG	1.92	0.51
1:C:37:GLU:HG3	1:C:132:SER:OG	2.11	0.51
1:K:145:LYS:HE3	1:K:153:TRP:HB3	1.92	0.50
1:K:24:ARG:HD3	1:K:108:GLY:HA2	1.94	0.50
3:H:2337:HOH:O	1:K:9:GLY:HA2	2.11	0.50
1:A:145:LYS:NZ	1:A:150:SER:OG	2.45	0.50
1:C:133:LYS:HG2	1:D:145:LYS:HZ3	1.76	0.50
1:C:144:HIS:HD2	3:C:2226:HOH:O	1.94	0.50
1:H:88:LEU:HD13	1:H:90:LYS:HG2	1.94	0.50
1:G:106:GLU:OE2	1:J:104:LYS:HE3	2.12	0.50
1:J:85:ARG:HD2	3:J:2269:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:CD	1:C:145:LYS:HE2	2.33	0.49
1:D:77:LEU:HD11	1:D:107:THR:HG23	1.93	0.49
1:K:42:LEU:HD13	1:K:88:LEU:HG	1.94	0.49
1:A:137:ILE:O	1:F:139:GLN:HA	2.12	0.49
1:E:149:LYS:HE2	1:L:18:GLU:OE2	2.12	0.49
1:A:134:GLY:O	1:F:155:ARG:NH2	2.39	0.49
1:B:13:MET:HE3	1:C:79:LEU:O	2.13	0.49
1:C:139:GLN:HA	1:D:137:ILE:O	2.12	0.49
1:E:16:VAL:HG11	1:E:107:THR:CG2	2.43	0.49
1:A:11:PRO:HA	1:F:49:LYS:O	2.13	0.49
1:A:42:LEU:HD13	1:A:88:LEU:HG	1.95	0.49
1:D:18:GLU:HB2	3:D:159:HOH:O	2.13	0.49
1:I:137:ILE:HB	1:J:140:VAL:HB	1.95	0.49
1:C:49:LYS:O	1:D:11:PRO:HA	2.13	0.48
1:L:12:ARG:HH11	1:L:12:ARG:CG	2.26	0.48
1:B:127:MET:SD	1:E:73:LEU:HD12	2.54	0.48
1:J:90:LYS:HE3	3:J:2237:HOH:O	2.13	0.48
1:A:65:LYS:HD3	1:E:13:MET:CE	2.43	0.48
1:F:145:LYS:C	1:F:145:LYS:HD2	2.33	0.48
1:C:139:GLN:HB2	3:C:2295:HOH:O	2.13	0.48
1:C:13:MET:HB2	1:F:82:VAL:HB	1.96	0.48
1:K:149:LYS:HD2	1:K:149:LYS:N	2.23	0.48
1:D:20:PRO:HB3	1:I:23:PHE:CG	2.48	0.48
1:A:25:THR:HG22	3:A:2245:HOH:O	2.14	0.48
1:B:38:ALA:HB2	1:B:135:LEU:HD21	1.95	0.48
1:F:142:LEU:O	1:F:155:ARG:HG3	2.13	0.47
1:C:110:GLU:OE2	1:C:145:LYS:CE	2.63	0.47
1:G:23:PHE:HD1	1:G:104:LYS:HG2	1.78	0.47
1:I:145:LYS:C	1:I:145:LYS:HD2	2.34	0.47
1:J:42:LEU:HD13	1:J:88:LEU:HG	1.95	0.47
1:I:16:VAL:HG21	1:I:107:THR:HG23	1.95	0.47
1:A:85:ARG:HG2	1:E:10:ARG:NH1	2.30	0.47
1:A:70:LEU:HD11	1:F:70:LEU:HD21	1.95	0.47
1:G:13:MET:HE1	1:J:65:LYS:HD3	1.97	0.47
1:I:145:LYS:HG3	1:I:153:TRP:HB3	1.96	0.47
3:I:2307:HOH:O	1:J:107:THR:HG23	2.14	0.47
1:C:144:HIS:HE1	1:C:152:GLU:OE2	1.98	0.47
1:C:32:VAL:HG22	1:C:137:ILE:CD1	2.45	0.47
1:E:47:VAL:O	1:E:47:VAL:HG22	2.14	0.47
1:D:123:THR:O	1:D:127:MET:HG2	2.14	0.47
1:F:19:LYS:HE3	3:F:268:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:PRO:HA	1:J:49:LYS:O	2.15	0.47
1:B:74:CYS:SG	1:B:111:MET:HG3	2.55	0.47
1:B:137:ILE:O	1:E:139:GLN:HA	2.15	0.47
1:H:73:LEU:HD12	1:K:127:MET:SD	2.55	0.47
1:F:141:ARG:HD2	1:F:155:ARG:HD2	1.97	0.47
1:A:140:VAL:HB	1:F:137:ILE:HB	1.96	0.46
1:K:19:LYS:HB2	1:K:106:GLU:HB3	1.97	0.46
1:A:39:LEU:CD1	1:A:93:LYS:HD3	2.45	0.46
1:H:137:ILE:O	1:K:139:GLN:HA	2.15	0.46
1:C:32:VAL:HG22	1:C:137:ILE:HD13	1.97	0.46
1:D:145:LYS:HG2	1:D:153:TRP:HB3	1.97	0.46
1:A:123:THR:O	1:A:127:MET:HG2	2.16	0.46
1:A:137:ILE:HB	1:F:140:VAL:HB	1.98	0.46
1:H:76:PRO:HG2	1:I:79:LEU:H	1.81	0.46
1:I:16:VAL:HG11	1:I:107:THR:HG22	1.96	0.46
1:B:77:LEU:CD1	1:B:79:LEU:HD23	2.46	0.46
1:C:33:GLU:OE2	1:C:94:ARG:HD2	2.15	0.46
1:H:77:LEU:HD23	1:H:77:LEU:H	1.80	0.46
1:G:11:PRO:HA	1:L:49:LYS:O	2.16	0.46
1:B:17:THR:O	1:C:104:LYS:HD3	2.16	0.45
1:L:141:ARG:CZ	3:L:200:HOH:O	2.64	0.45
1:A:29:GLU:HA	1:A:97:ILE:O	2.17	0.45
1:A:71:ILE:HB	1:A:74:CYS:SG	2.57	0.45
3:I:2307:HOH:O	1:J:77:LEU:HD11	2.17	0.45
1:J:145:LYS:C	1:J:145:LYS:HD2	2.36	0.45
1:K:149:LYS:HE3	3:K:2312:HOH:O	2.17	0.45
1:A:154:ARG:NH2	3:A:2295:HOH:O	2.49	0.45
1:E:155:ARG:NH2	3:E:2278:HOH:O	2.48	0.45
1:F:77:LEU:HD23	1:F:77:LEU:H	1.82	0.45
1:H:13:MET:O	1:H:14:VAL:C	2.55	0.45
1:F:145:LYS:HG3	1:F:153:TRP:HB3	1.98	0.45
1:H:140:VAL:HB	1:K:137:ILE:HB	1.99	0.45
1:F:145:LYS:HD2	1:F:146:ALA:N	2.32	0.45
1:H:10:ARG:HA	1:H:11:PRO:HD3	1.83	0.44
1:J:156:GLU:HG3	3:J:2320:HOH:O	2.16	0.44
1:L:87:GLU:HB3	3:L:190:HOH:O	2.17	0.44
1:B:79:LEU:HD21	1:B:112:GLU:HG2	2.00	0.44
1:D:90:LYS:NZ	3:D:182:HOH:O	2.47	0.44
1:B:36:GLU:H	1:B:36:GLU:CD	2.20	0.44
3:C:2308:HOH:O	1:D:107:THR:HG23	2.17	0.44
1:F:37:GLU:N	1:F:37:GLU:OE1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:PHE:CE1	1:G:104:LYS:HD3	2.50	0.44
1:K:145:LYS:HD2	1:K:145:LYS:C	2.38	0.44
1:C:37:GLU:H	1:C:37:GLU:HG2	1.47	0.43
1:G:23:PHE:CD1	1:G:104:LYS:HG2	2.52	0.43
1:K:39:LEU:O	1:K:43:GLU:HG3	2.18	0.43
1:C:22:THR:O	1:C:24:ARG:HG2	2.18	0.43
1:E:53:LEU:HD22	1:E:86:VAL:HG12	2.00	0.43
1:F:155:ARG:HH11	1:F:155:ARG:CG	2.28	0.43
1:B:137:ILE:HB	1:E:140:VAL:HB	1.99	0.43
1:B:142:LEU:O	1:B:155:ARG:HG3	2.17	0.43
1:F:123:THR:O	1:F:127:MET:HG2	2.19	0.43
1:I:156:GLU:O	1:I:156:GLU:HG2	2.17	0.43
1:L:125:TYR:O	1:L:129:LYS:HB2	2.18	0.43
1:F:87:GLU:HG2	3:F:163:HOH:O	2.18	0.43
1:F:155:ARG:NH1	1:F:155:ARG:CG	2.81	0.43
1:E:39:LEU:O	1:E:43:GLU:HG3	2.19	0.43
1:E:30:ALA:HA	1:E:139:GLN:O	2.19	0.43
1:A:74:CYS:SG	1:A:111:MET:HG3	2.58	0.43
1:B:149:LYS:HG2	1:B:150:SER:H	1.83	0.43
1:C:71:ILE:HB	1:C:74:CYS:HB2	2.00	0.43
1:K:149:LYS:NZ	3:K:2245:HOH:O	2.51	0.43
1:E:149:LYS:HE2	1:L:18:GLU:CD	2.40	0.43
1:B:145:LYS:C	1:B:145:LYS:HD2	2.39	0.43
1:G:13:MET:CE	1:J:65:LYS:HD3	2.48	0.43
1:G:145:LYS:HG3	1:G:146:ALA:N	2.33	0.42
1:H:16:VAL:HG11	1:H:107:THR:HG23	2.01	0.42
1:I:58:LEU:HD23	1:K:58:LEU:CD1	2.44	0.42
1:I:76:PRO:HD3	1:L:65:LYS:HD3	2.00	0.42
1:A:85:ARG:NE	1:E:10:ARG:NH1	2.66	0.42
1:H:19:LYS:HB3	1:H:20:PRO:HD2	2.01	0.42
1:I:123:THR:O	1:I:127:MET:HG2	2.20	0.42
1:A:10:ARG:HA	1:A:11:PRO:HD3	1.89	0.42
1:C:137:ILE:HG22	1:C:138:SER:O	2.19	0.42
1:I:129:LYS:HB3	1:I:129:LYS:HE2	1.89	0.42
1:K:123:THR:O	1:K:127:MET:HG2	2.19	0.42
1:C:133:LYS:HD3	1:D:145:LYS:HE2	2.01	0.42
1:F:77:LEU:N	1:F:77:LEU:CD2	2.82	0.42
1:C:139:GLN:C	3:C:2295:HOH:O	2.57	0.42
1:K:23:PHE:HE1	1:K:104:LYS:HD3	1.81	0.42
1:B:53:LEU:HD22	1:B:86:VAL:HG12	2.02	0.42
1:I:44:LYS:HE3	3:I:2341:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ARG:HA	1:D:11:PRO:HD3	1.88	0.42
1:F:34:LEU:HD11	1:F:95:VAL:HG23	2.02	0.42
1:L:9:GLY:N	3:L:288:HOH:O	2.53	0.42
1:B:145:LYS:NZ	1:B:150:SER:OG	2.44	0.42
1:D:53:LEU:HD22	1:D:86:VAL:HG12	2.01	0.42
1:F:85:ARG:NH1	1:F:85:ARG:HG3	2.34	0.42
1:J:145:LYS:HG3	1:J:153:TRP:HB3	2.02	0.42
1:C:17:THR:HG21	1:F:23:PHE:CD1	2.54	0.42
1:C:53:LEU:HD22	1:C:86:VAL:HG12	2.00	0.42
1:G:70:LEU:HD23	1:L:66:LYS:HD2	2.02	0.42
1:G:62:LEU:O	1:G:66:LYS:HE2	2.20	0.41
1:E:154:ARG:HD2	3:E:2277:HOH:O	2.20	0.41
1:H:155:ARG:NH2	1:K:136:VAL:CG2	2.83	0.41
1:I:129:LYS:NZ	2:I:2210:PO4:O2	2.48	0.41
1:I:71:ILE:HB	1:I:74:CYS:HB2	2.02	0.41
1:K:129:LYS:HE2	1:K:129:LYS:HB3	1.90	0.41
1:B:149:LYS:H	1:B:149:LYS:CD	2.05	0.41
1:C:123:THR:O	1:C:127:MET:HG2	2.19	0.41
1:B:10:ARG:CZ	1:C:85:ARG:HG2	2.50	0.41
1:H:123:THR:O	1:H:127:MET:HG2	2.19	0.41
1:C:140:VAL:HB	1:D:137:ILE:HB	2.02	0.41
1:E:123:THR:O	1:E:127:MET:HG2	2.20	0.41
1:I:102:LYS:HE2	3:I:2273:HOH:O	2.20	0.41
1:I:133:LYS:HZ3	1:J:145:LYS:HE2	1.84	0.41
1:L:149:LYS:NZ	3:L:194:HOH:O	2.54	0.41
1:B:42:LEU:HG	1:B:128:LEU:HD11	2.03	0.41
1:K:10:ARG:HA	1:K:11:PRO:HD3	1.91	0.41
1:H:129:LYS:NZ	2:K:2211:PO4:O2	2.46	0.41
1:B:38:ALA:CB	1:B:135:LEU:HD21	2.51	0.41
1:E:145:LYS:NZ	1:E:150:SER:O	2.45	0.41
1:E:47:VAL:HG21	1:E:130:ALA:CB	2.47	0.41
1:H:17:THR:HG21	1:I:23:PHE:CE1	2.55	0.41
1:E:143:LEU:O	1:E:154:ARG:HA	2.21	0.41
1:F:30:ALA:HA	1:F:139:GLN:O	2.21	0.41
1:C:17:THR:HG21	1:F:23:PHE:CE1	2.55	0.41
1:G:29:GLU:HA	1:G:97:ILE:O	2.21	0.41
1:J:77:LEU:HD21	1:J:107:THR:HG22	2.02	0.41
1:L:24:ARG:HD3	1:L:108:GLY:HA2	2.02	0.41
1:L:13:MET:O	1:L:14:VAL:C	2.59	0.41
1:K:145:LYS:HD3	3:K:2240:HOH:O	2.21	0.41
1:G:123:THR:O	1:G:127:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:GLY:N	3:J:2323:HOH:O	2.53	0.41
1:K:27:THR:HA	1:K:99:ALA:O	2.20	0.41
1:G:42:LEU:CD2	1:G:88:LEU:HG	2.50	0.40
1:K:149:LYS:HD3	3:K:2252:HOH:O	2.22	0.40
1:L:25:THR:HG21	3:L:244:HOH:O	2.20	0.40
1:D:13:MET:O	1:D:14:VAL:C	2.60	0.40
1:H:77:LEU:CD2	1:H:77:LEU:N	2.84	0.40
1:B:145:LYS:HG3	1:B:153:TRP:HB3	2.02	0.40
1:C:141:ARG:HG2	3:C:2295:HOH:O	2.21	0.40
1:D:77:LEU:HD21	1:D:107:THR:HG22	2.03	0.40
1:E:144:HIS:CD2	1:E:154:ARG:HG2	2.51	0.40
1:H:74:CYS:SG	1:H:111:MET:HG3	2.62	0.40
1:L:123:THR:O	1:L:127:MET:HG2	2.21	0.40
1:J:139:GLN:NE2	1:J:141:ARG:HH11	2.14	0.40
3:G:2233:HOH:O	1:J:83:GLU:HG3	2.20	0.40
1:H:133:LYS:HE3	1:K:110:GLU:OE2	2.21	0.40
1:B:126:ASP:OD1	2:E:2205:PO4:O4	2.40	0.40
1:B:149:LYS:HD3	1:B:149:LYS:N	2.09	0.40
1:H:129:LYS:HE2	1:H:129:LYS:HB3	1.87	0.40
1:J:36:GLU:HG3	3:J:2216:HOH:O	2.21	0.40
1:G:72:PRO:HA	1:J:62:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/157 (93%)	141 (97%)	5 (3%)	0	100	100
1	B	146/157 (93%)	140 (96%)	6 (4%)	0	100	100
1	C	145/157 (92%)	137 (94%)	8 (6%)	0	100	100
1	D	145/157 (92%)	142 (98%)	2 (1%)	1 (1%)	22	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	145/157 (92%)	139 (96%)	6 (4%)	0	100	100
1	F	144/157 (92%)	141 (98%)	3 (2%)	0	100	100
1	G	145/157 (92%)	140 (97%)	5 (3%)	0	100	100
1	H	146/157 (93%)	144 (99%)	1 (1%)	1 (1%)	22	12
1	I	145/157 (92%)	142 (98%)	3 (2%)	0	100	100
1	J	146/157 (93%)	144 (99%)	2 (1%)	0	100	100
1	K	146/157 (93%)	142 (97%)	3 (2%)	1 (1%)	22	12
1	L	146/157 (93%)	142 (97%)	4 (3%)	0	100	100
All	All	1745/1884 (93%)	1694 (97%)	48 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	VAL
1	H	14	VAL
1	K	14	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/124 (93%)	107 (93%)	8 (7%)	15	7
1	B	115/124 (93%)	106 (92%)	9 (8%)	12	5
1	C	114/124 (92%)	107 (94%)	7 (6%)	18	9
1	D	114/124 (92%)	108 (95%)	6 (5%)	22	13
1	E	114/124 (92%)	108 (95%)	6 (5%)	22	13
1	F	114/124 (92%)	108 (95%)	6 (5%)	22	13
1	G	114/124 (92%)	108 (95%)	6 (5%)	22	13
1	H	115/124 (93%)	109 (95%)	6 (5%)	23	14
1	I	115/124 (93%)	112 (97%)	3 (3%)	46	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	115/124 (93%)	111 (96%)	4 (4%)	36	27
1	K	115/124 (93%)	106 (92%)	9 (8%)	12	5
1	L	115/124 (93%)	109 (95%)	6 (5%)	23	14
All	All	1375/1488 (92%)	1299 (94%)	76 (6%)	21	12

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	39	LEU
1	A	42	LEU
1	A	58	LEU
1	A	77	LEU
1	A	88	LEU
1	A	145	LYS
1	A	154	ARG
1	B	36	GLU
1	B	39	LEU
1	B	42	LEU
1	B	58	LEU
1	B	85	ARG
1	B	88	LEU
1	B	145	LYS
1	B	149	LYS
1	B	155	ARG
1	C	37	GLU
1	C	88	LEU
1	C	90	LYS
1	C	139	GLN
1	C	142	LEU
1	C	145	LYS
1	C	150	SER
1	D	39	LEU
1	D	42	LEU
1	D	87	GLU
1	D	88	LEU
1	D	152	GLU
1	D	155	ARG
1	E	39	LEU
1	E	42	LEU
1	E	77	LEU

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Mol	Chain	Res	Type
1	E	88	LEU
1	E	139	GLN
1	E	145	LYS
1	F	39	LEU
1	F	42	LEU
1	F	77	LEU
1	F	88	LEU
1	F	145	LYS
1	F	155	ARG
1	G	39	LEU
1	G	69	ASP
1	G	88	LEU
1	G	107	THR
1	G	152	GLU
1	G	154	ARG
1	H	39	LEU
1	H	42	LEU
1	H	77	LEU
1	H	88	LEU
1	H	107	THR
1	H	145	LYS
1	I	42	LEU
1	I	88	LEU
1	I	145	LYS
1	J	39	LEU
1	J	42	LEU
1	J	88	LEU
1	J	145	LYS
1	K	39	LEU
1	K	42	LEU
1	K	58	LEU
1	K	85	ARG
1	K	88	LEU
1	K	94	ARG
1	K	107	THR
1	K	145	LYS
1	K	155	ARG
1	L	12	ARG
1	L	39	LEU
1	L	42	LEU
1	L	58	LEU
1	L	88	LEU

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Mol	Chain	Res	Type
1	L	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	HIS
1	D	139	GLN
1	E	139	GLN
1	I	139	GLN
1	J	139	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	I	2210	-	4,4,4	1.79	2 (50%)	6,6,6	0.44	0
2	PO4	C	2204	-	4,4,4	1.69	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	J	2209	-	4,4,4	1.68	1 (25%)	6,6,6	0.42	0
2	PO4	E	2205	-	4,4,4	1.78	2 (50%)	6,6,6	0.42	0
2	PO4	A	2201	-	4,4,4	1.83	2 (50%)	6,6,6	0.43	0
2	PO4	G	2212	-	4,4,4	1.70	1 (25%)	6,6,6	0.41	0
2	PO4	H	2208	-	4,4,4	1.61	0	6,6,6	0.43	0
2	PO4	A	2206	-	4,4,4	1.82	1 (25%)	6,6,6	0.41	0
2	PO4	G	2207	-	4,4,4	1.65	1 (25%)	6,6,6	0.46	0
2	PO4	E	2202	-	4,4,4	1.80	2 (50%)	6,6,6	0.45	0
2	PO4	K	2211	-	4,4,4	1.67	1 (25%)	6,6,6	0.45	0
2	PO4	C	2203	-	4,4,4	1.66	1 (25%)	6,6,6	0.41	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2206	PO4	P-O3	-2.40	1.47	1.54
2	A	2201	PO4	P-O3	-2.22	1.47	1.54
2	G	2207	PO4	P-O3	-2.22	1.47	1.54
2	E	2205	PO4	P-O2	-2.20	1.48	1.54
2	E	2202	PO4	P-O4	-2.18	1.48	1.54
2	K	2211	PO4	P-O3	-2.18	1.48	1.54
2	I	2210	PO4	P-O2	-2.16	1.48	1.54
2	E	2202	PO4	P-O2	-2.16	1.48	1.54
2	E	2205	PO4	P-O3	-2.15	1.48	1.54
2	G	2212	PO4	P-O3	-2.13	1.48	1.54
2	J	2209	PO4	P-O3	-2.09	1.48	1.54
2	I	2210	PO4	P-O4	-2.05	1.48	1.54
2	A	2201	PO4	P-O4	-2.02	1.48	1.54
2	C	2203	PO4	P-O4	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2210	PO4	1	0
2	E	2205	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2211	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	148/157 (94%)	0.11	3 (2%) 65 68	14, 26, 49, 60	2 (1%)
1	B	148/157 (94%)	0.07	1 (0%) 87 88	13, 24, 41, 51	2 (1%)
1	C	147/157 (93%)	0.20	6 (4%) 37 40	13, 25, 46, 56	1 (0%)
1	D	147/157 (93%)	0.07	4 (2%) 54 57	11, 23, 46, 57	2 (1%)
1	E	147/157 (93%)	0.20	5 (3%) 45 48	14, 26, 45, 64	2 (1%)
1	F	146/157 (92%)	-0.02	1 (0%) 87 88	12, 24, 40, 48	2 (1%)
1	G	147/157 (93%)	-0.06	1 (0%) 87 88	10, 20, 41, 53	2 (1%)
1	H	148/157 (94%)	-0.12	4 (2%) 54 57	9, 19, 38, 53	2 (1%)
1	I	147/157 (93%)	-0.14	1 (0%) 87 88	9, 18, 37, 59	2 (1%)
1	J	148/157 (94%)	-0.18	3 (2%) 65 68	9, 18, 35, 50	2 (1%)
1	K	148/157 (94%)	-0.11	3 (2%) 65 68	9, 19, 39, 52	2 (1%)
1	L	148/157 (94%)	-0.17	2 (1%) 75 77	10, 20, 36, 61	2 (1%)
All	All	1769/1884 (93%)	-0.01	34 (1%) 66 69	9, 22, 43, 64	23 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLU	5.1
1	E	152	GLU	4.4
1	K	9	GLY	3.7
1	A	9	GLY	3.6
1	H	9	GLY	3.4
1	A	8	ASP	3.4
1	I	148	GLY	3.3
1	A	149	LYS	3.2
1	C	138	SER	3.2
1	B	9	GLY	3.1
1	E	45	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	148	GLY	2.8
1	K	156	GLU	2.8
1	H	13	MET	2.7
1	D	13	MET	2.6
1	G	9	GLY	2.6
1	C	40	SER	2.5
1	E	151	GLY	2.4
1	C	48	GLY	2.3
1	J	9	GLY	2.3
1	H	45	GLY	2.3
1	C	139	GLN	2.2
1	L	9	GLY	2.2
1	C	44	LYS	2.2
1	E	141	ARG	2.2
1	J	44	LYS	2.1
1	C	137	ILE	2.1
1	E	43	GLU	2.1
1	D	36	GLU	2.1
1	K	44	LYS	2.1
1	J	156	GLU	2.0
1	D	79	LEU	2.0
1	F	77	LEU	2.0
1	L	149	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	K	2211	5/5	0.89	0.11	33,37,39,39	0
2	PO4	E	2205	5/5	0.92	0.12	29,30,32,33	0
2	PO4	G	2207	5/5	0.94	0.10	30,31,34,36	0
2	PO4	C	2204	5/5	0.94	0.10	32,32,34,36	0
2	PO4	C	2203	5/5	0.95	0.09	26,28,29,32	0
2	PO4	E	2202	5/5	0.96	0.07	31,31,33,34	0
2	PO4	I	2210	5/5	0.96	0.07	27,30,32,33	0
2	PO4	J	2209	5/5	0.96	0.08	22,22,25,26	0
2	PO4	A	2206	5/5	0.97	0.08	29,29,31,32	0
2	PO4	G	2212	5/5	0.97	0.08	34,35,36,36	0
2	PO4	H	2208	5/5	0.97	0.07	24,26,28,28	0
2	PO4	A	2201	5/5	0.97	0.07	29,30,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.