



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:55 am BST

PDB ID : 6JD2
Title : Crystal structure of Sulfolobus solfataricus ketol-acid reductoisomerase (Sso-KARI) in complex with Mg²⁺ at pH8.5
Authors : Chen, C.Y.; Chang, Y.C.; Lin, K.F.; Huang, C.H.; Lin, B.L.; Ko, T.P.; Hsieh, D.L.; Tsai, M.D.
Deposited on : 2019-01-30
Resolution : 2.53 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

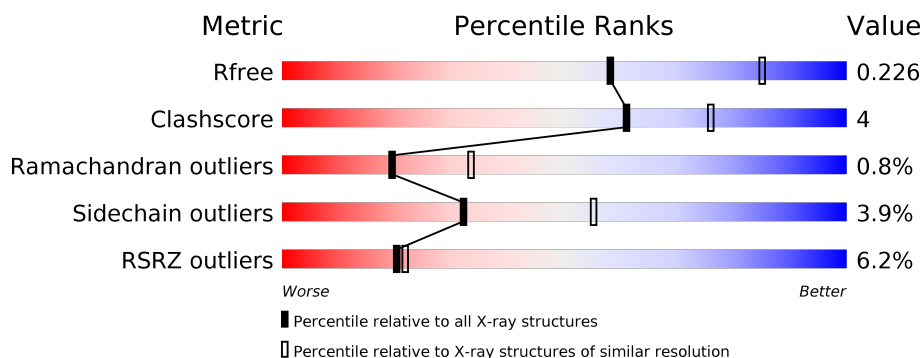
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	333	<div> <div>11%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	333	<div> <div>14%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	C	333	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	D	333	<div> <div>6%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	E	333	<div> <div>12%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	F	333	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	333	<div><div></div><div>6%</div><div>87%</div><div>11%</div><div>..</div></div>
1	H	333	<div><div></div><div>3%</div><div>86%</div><div>11%</div><div>..</div></div>
1	I	333	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>
1	J	333	<div><div></div><div>2%</div><div>86%</div><div>11%</div><div>..</div></div>
1	K	333	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>
1	L	333	<div><div></div><div>5%</div><div>86%</div><div>12%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31683 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 Putative ketol-acid reductoisomerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2572	1663	422	477	10			
1	B	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	C	327	Total	C	N	O	S	0	0	0
			2571	1661	421	479	10			
1	D	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	E	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	F	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	G	328	Total	C	N	O	S	0	0	0
			2580	1667	423	480	10			
1	H	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	I	326	Total	C	N	O	S	0	0	0
			2563	1657	420	476	10			
1	J	329	Total	C	N	O	S	0	0	0
			2587	1672	424	481	10			
1	K	328	Total	C	N	O	S	0	0	0
			2579	1668	423	478	10			
1	L	329	Total	C	N	O	S	0	0	0
			2588	1674	425	479	10			

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	35	Total O 35 35	0	0
4	C	76	Total O 76 76	0	0
4	D	52	Total O 52 52	0	0
4	E	38	Total O 38 38	0	0
4	F	71	Total O 71 71	0	0
4	G	60	Total O 60 60	0	0
4	H	86	Total O 86 86	0	0

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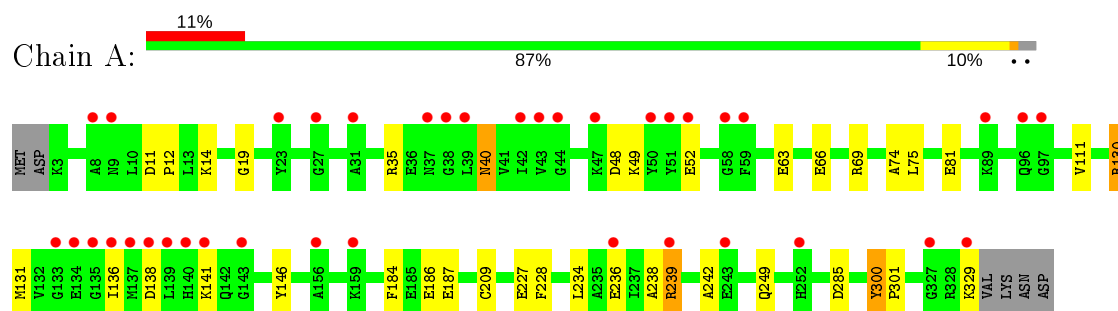
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	67	Total 67	O 67	0	0
4	J	92	Total 92	O 92	0	0
4	K	74	Total 74	O 74	0	0
4	L	71	Total 71	O 71	0	0

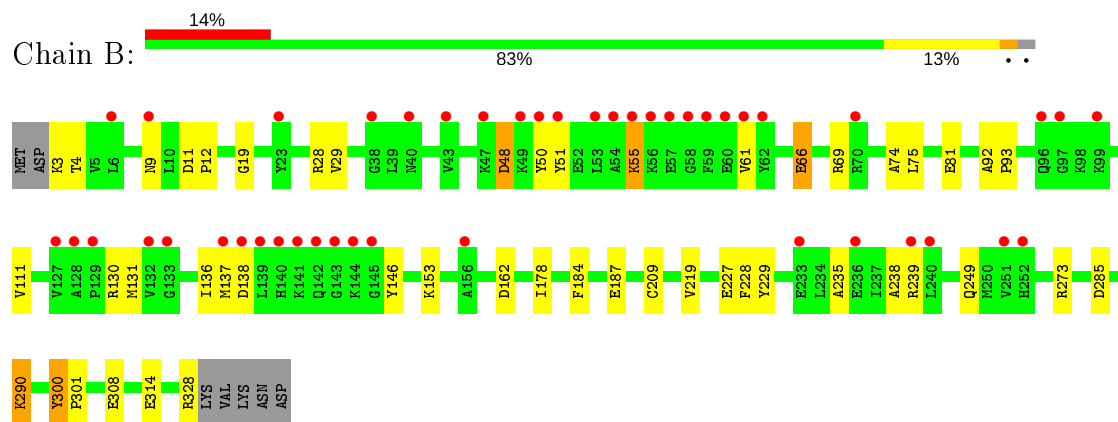
3 Residue-property plots [i](#)

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.

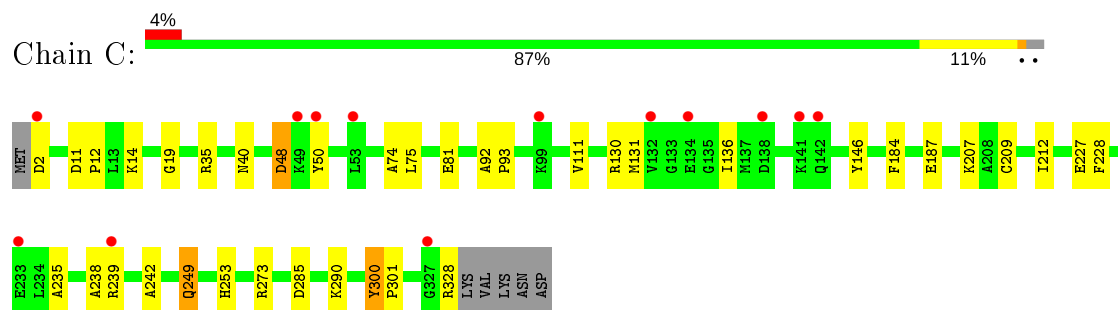
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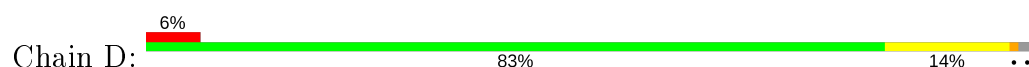
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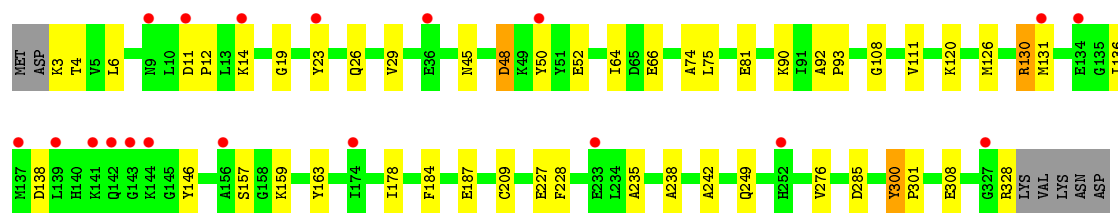


- Molecule 1: Putative ketol-acid reductoisomerase 2

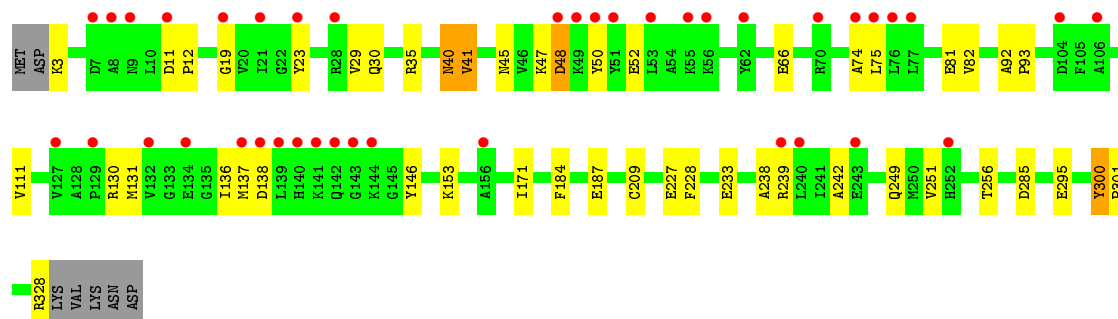
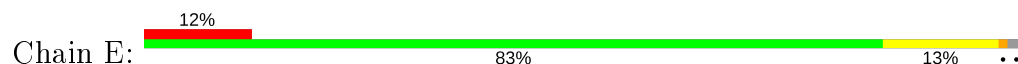


- Molecule 1: Putative ketol-acid reductoisomerase 2

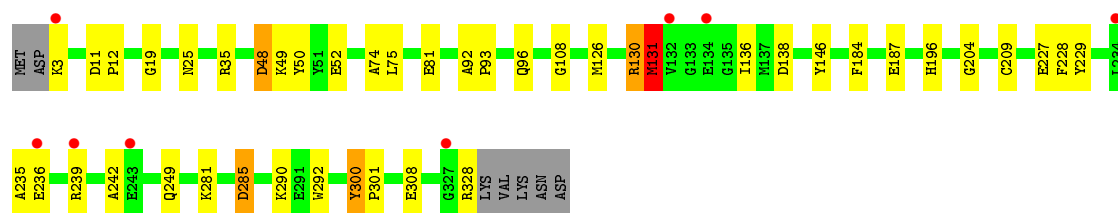
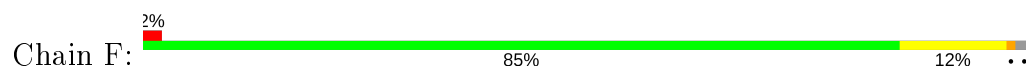




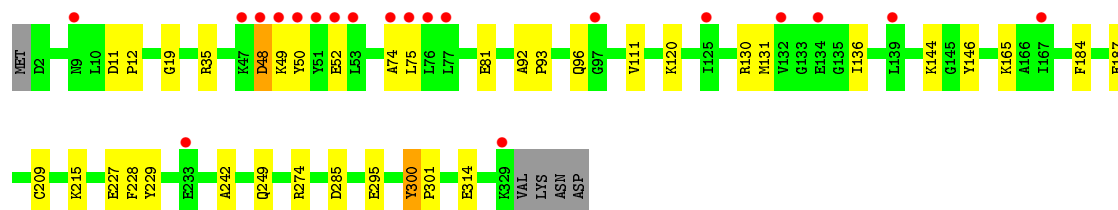
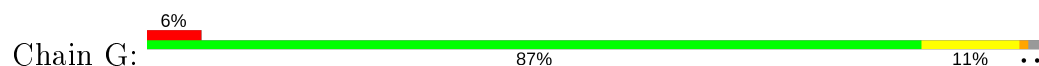
• Molecule 1: Putative ketol-acid reductoisomerase 2



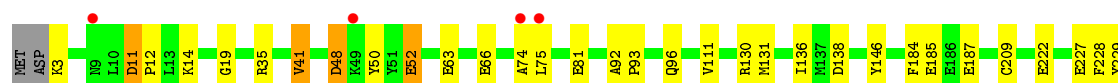
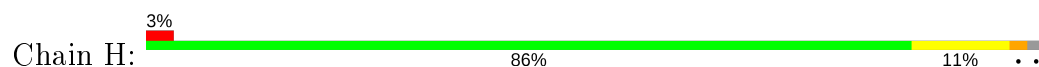
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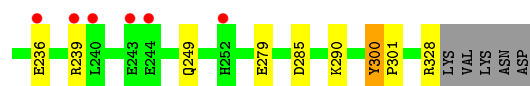


• Molecule 1: Putative ketol-acid reductoisomerase 2

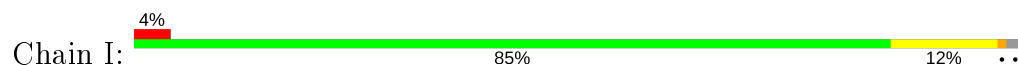


• Molecule 1: Putative ketol-acid reductoisomerase 2

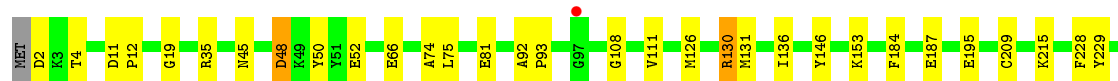
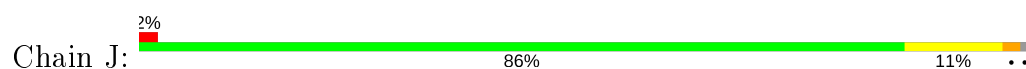




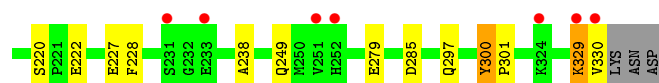
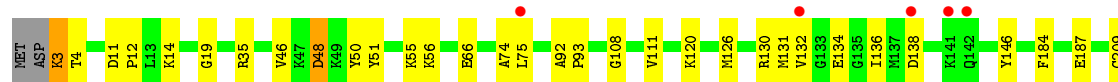
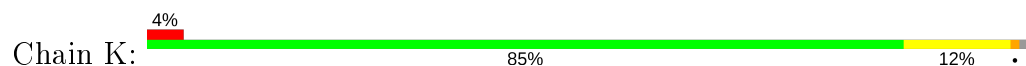
- Molecule 1: Putative ketol-acid reductoisomerase 2



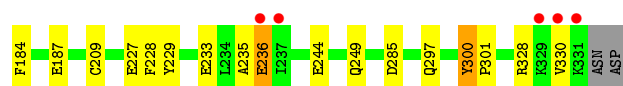
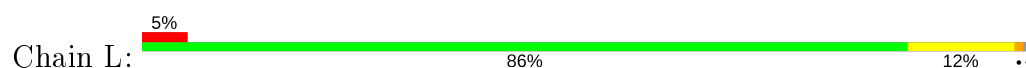
- Molecule 1: Putative ketol-acid reductoisomerase 2



- Molecule 1: Putative ketol-acid reductoisomerase 2



- Molecule 1: Putative ketol-acid reductoisomerase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.56Å 179.87Å 187.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.53 30.06 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.53) 98.8 (30.06-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.54Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.188 , 0.226 0.191 , 0.226	Depositor DCC
R_{free} test set	8361 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31683	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	0/2625	0.85	3/3544 (0.1%)
1	B	0.73	1/2616 (0.0%)	0.85	1/3533 (0.0%)
1	C	0.73	0/2624	0.89	5/3544 (0.1%)
1	D	0.76	1/2616 (0.0%)	0.84	2/3533 (0.1%)
1	E	0.74	0/2616	0.85	1/3533 (0.0%)
1	F	0.74	0/2616	0.88	3/3533 (0.1%)
1	G	0.77	1/2633 (0.0%)	0.92	5/3555 (0.1%)
1	H	0.76	0/2616	0.88	2/3533 (0.1%)
1	I	0.76	1/2616 (0.0%)	0.91	4/3533 (0.1%)
1	J	0.77	2/2640 (0.1%)	0.87	2/3565 (0.1%)
1	K	0.78	1/2632 (0.0%)	0.90	5/3554 (0.1%)
1	L	0.73	0/2641	0.85	3/3565 (0.1%)
All	All	0.75	7/31491 (0.0%)	0.87	36/42525 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	222	GLU	CD-OE1	7.17	1.33	1.25
1	I	314	GLU	CD-OE1	7.08	1.33	1.25
1	B	314	GLU	CD-OE2	6.65	1.32	1.25
1	G	314	GLU	CD-OE1	6.28	1.32	1.25
1	J	195	GLU	CD-OE1	5.20	1.31	1.25
1	D	308	GLU	CD-OE1	5.07	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	314	GLU	CD-OE2	5.05	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	35	ARG	NE-CZ-NH2	-13.35	113.62	120.30
1	I	35	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	G	35	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	F	285	ASP	CB-CA-C	-10.91	88.58	110.40
1	G	35	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	C	285	ASP	CB-CA-C	-10.77	88.87	110.40
1	B	285	ASP	CB-CA-C	-10.71	88.99	110.40
1	I	285	ASP	CB-CA-C	-10.69	89.01	110.40
1	E	285	ASP	CB-CA-C	-10.64	89.12	110.40
1	K	285	ASP	CB-CA-C	-10.64	89.12	110.40
1	G	285	ASP	CB-CA-C	-10.60	89.20	110.40
1	L	285	ASP	CB-CA-C	-10.42	89.55	110.40
1	A	285	ASP	CB-CA-C	-10.41	89.57	110.40
1	D	285	ASP	CB-CA-C	-10.38	89.63	110.40
1	G	274	ARG	NE-CZ-NH2	7.57	124.09	120.30
1	K	35	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	C	35	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	H	285	ASP	CB-CA-C	7.13	124.65	110.40
1	J	285	ASP	CB-CA-C	6.81	124.02	110.40
1	F	130	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	G	35	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	130	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	K	35	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	273	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	H	222	GLU	CB-CG-CD	5.86	130.02	114.20
1	I	35	ARG	CG-CD-NE	-5.81	99.61	111.80
1	L	35	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	K	222	GLU	CG-CD-OE1	5.58	129.45	118.30
1	C	35	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	C	273	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	K	222	GLU	CB-CG-CD	5.44	128.89	114.20
1	J	35	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	A	35	ARG	CG-CD-NE	5.42	123.19	111.80
1	L	35	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	F	35	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	D	130	ARG	NE-CZ-NH1	5.13	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	285	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2572	0	2600	19	0
1	B	2563	0	2587	34	0
1	C	2571	0	2591	24	0
1	D	2563	0	2587	38	0
1	E	2563	0	2587	29	0
1	F	2563	0	2587	29	0
1	G	2580	0	2604	15	0
1	H	2563	0	2587	20	0
1	I	2563	0	2587	29	0
1	J	2587	0	2613	24	0
1	K	2579	0	2609	28	0
1	L	2588	0	2622	27	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
2	H	4	0	6	1	0
2	I	4	0	6	0	0
2	J	4	0	6	0	0
2	K	4	0	6	1	0
2	L	4	0	6	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	34	0	0	0	0
4	B	35	0	0	1	0
4	C	76	0	0	1	0
4	D	52	0	0	0	0
4	E	38	0	0	2	0
4	F	71	0	0	2	0
4	G	60	0	0	1	0
4	H	86	0	0	2	0
4	I	67	0	0	6	0
4	J	92	0	0	0	0
4	K	74	0	0	1	0
4	L	71	0	0	1	0
All	All	31683	0	31233	278	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 4.

All (278) 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:233:GLU:OE1	4:E:601:HOH:O	1.65	1.14
1:G:165:LYS:NZ	4:G:601:HOH:O	1.94	0.99
1:D:159:LYS:HG3	1:D:163:TYR:CE2	2.07	0.88
1:G:242:ALA:O	1:H:328:ARG:NH1	2.14	0.81
1:A:138:ASP:O	1:A:141:LYS:HG2	1.82	0.80
1:K:227:GLU:OE2	1:L:130:ARG:NH1	2.14	0.80
1:F:131:MET:HA	1:F:131:MET:CE	2.15	0.76
1:B:51:TYR:CE1	1:B:61:VAL:HG12	2.20	0.76
1:B:55:LYS:HE3	1:B:55:LYS:HA	1.69	0.74
1:C:290:LYS:HE2	1:E:295:GLU:OE1	1.87	0.74
1:B:136:ILE:HG23	1:B:146:TYR:CE2	2.24	0.72
1:J:249:GLN:OE1	1:J:253:HIS:HE1	1.72	0.72
1:C:136:ILE:HG23	1:C:146:TYR:CE2	2.26	0.71
1:L:120:LYS:HE2	1:L:120:LYS:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLU:OE2	1:D:130:ARG:NH1	2.23	0.71
1:E:136:ILE:HG23	1:E:146:TYR:CE2	2.25	0.71
1:G:227:GLU:OE2	1:H:130:ARG:NH1	2.24	0.71
1:I:66:GLU:OE1	1:I:70:ARG:NH2	2.24	0.70
1:H:35:ARG:HB2	1:H:41:VAL:HG21	1.75	0.68
1:D:126:MET:HE3	1:D:184:PHE:HA	1.77	0.67
1:I:297:GLN:OE1	4:I:601:HOH:O	2.13	0.66
1:G:130:ARG:NH1	1:H:227:GLU:OE2	2.28	0.66
1:D:4:THR:HG23	1:D:178:ILE:CG1	2.26	0.65
1:E:35:ARG:HB2	1:E:41:VAL:HG21	1.78	0.65
1:D:157:SER:OG	1:D:159:LYS:HG2	1.97	0.65
1:F:131:MET:HE2	1:F:131:MET:HA	1.79	0.63
1:J:126:MET:CE	1:J:184:PHE:HA	2.28	0.63
4:I:601:HOH:O	1:K:297:GLN:OE1	2.16	0.62
1:B:4:THR:HG23	1:B:178:ILE:CG1	2.29	0.62
1:I:120:LYS:HE2	1:I:120:LYS:O	1.99	0.62
1:F:290:LYS:HE2	1:G:295:GLU:OE1	1.98	0.62
1:L:3:LYS:HA	1:L:3:LYS:HE2	1.79	0.62
1:I:328:ARG:NH1	1:J:242:ALA:O	2.33	0.62
1:D:126:MET:CE	1:D:184:PHE:HA	2.29	0.62
1:I:126:MET:CE	1:I:184:PHE:HA	2.30	0.61
1:L:126:MET:CE	1:L:184:PHE:HA	2.30	0.61
1:F:126:MET:CE	1:F:184:PHE:HA	2.30	0.61
1:D:4:THR:HG23	1:D:178:ILE:HG13	1.82	0.61
1:D:26:GLN:O	1:D:29:VAL:HG22	2.00	0.60
1:C:249:GLN:OE1	1:C:253:HIS:HE1	1.84	0.60
1:D:159:LYS:HG3	1:D:163:TYR:HE2	1.63	0.60
1:F:281:LYS:HE2	4:F:558:HOH:O	2.00	0.60
1:E:47:LYS:HG3	1:E:47:LYS:O	2.00	0.60
1:K:126:MET:CE	1:K:184:PHE:HA	2.30	0.60
1:L:130:ARG:NH2	1:L:187:GLU:OE2	2.34	0.60
1:J:126:MET:HE1	1:J:184:PHE:HA	1.83	0.60
1:K:130:ARG:NH1	1:L:227:GLU:OE2	2.35	0.60
1:A:130:ARG:NH2	1:A:187:GLU:OE2	2.35	0.59
1:E:130:ARG:NH2	1:E:187:GLU:OE2	2.36	0.59
1:G:130:ARG:NH2	1:G:187:GLU:OE2	2.37	0.58
1:J:130:ARG:NH2	1:J:187:GLU:OE2	2.37	0.58
1:C:130:ARG:NH2	1:C:187:GLU:OE2	2.37	0.58
1:C:212:ILE:HD12	1:D:276:VAL:CG1	2.34	0.57
1:B:51:TYR:CD1	1:B:61:VAL:CG1	2.88	0.57
1:A:130:ARG:NH1	1:B:227:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:NH2	1:B:187:GLU:OE2	2.38	0.56
1:D:130:ARG:NH2	1:D:187:GLU:OE2	2.37	0.56
1:I:130:ARG:NH2	1:I:187:GLU:OE2	2.38	0.56
1:H:52:GLU:HG3	4:H:549:HOH:O	2.05	0.56
1:A:227:GLU:OE2	1:B:130:ARG:NH1	2.39	0.56
1:F:130:ARG:NH2	1:F:187:GLU:OE2	2.38	0.56
1:J:108:GLY:CA	1:J:126:MET:CE	2.83	0.56
1:I:11:ASP:O	4:I:602:HOH:O	2.18	0.55
1:K:130:ARG:NH2	1:K:187:GLU:OE2	2.37	0.55
1:L:126:MET:HE1	1:L:184:PHE:HA	1.88	0.55
1:H:130:ARG:NH2	1:H:187:GLU:OE2	2.38	0.55
1:K:126:MET:HE1	1:K:184:PHE:HA	1.88	0.55
1:F:126:MET:HE3	1:F:184:PHE:HA	1.89	0.55
1:B:51:TYR:CD1	1:B:61:VAL:HG12	2.41	0.54
1:D:108:GLY:CA	1:D:126:MET:CE	2.86	0.54
1:A:11:ASP:HA	1:A:14:LYS:HG3	1.90	0.53
1:C:328:ARG:NH1	1:D:242:ALA:O	2.41	0.53
1:I:126:MET:HE3	1:I:184:PHE:HA	1.89	0.53
1:E:242:ALA:O	1:F:328:ARG:NH1	2.43	0.52
1:B:4:THR:HG23	1:B:178:ILE:HG13	1.90	0.52
1:J:136:ILE:HG23	1:J:146:TYR:CE1	2.44	0.52
1:E:227:GLU:OE2	1:F:130:ARG:NH1	2.43	0.52
1:K:108:GLY:CA	1:K:126:MET:CE	2.87	0.52
1:I:196:HIS:HE1	4:I:610:HOH:O	1.91	0.52
1:H:136:ILE:HG23	1:H:146:TYR:CE1	2.45	0.52
1:I:249:GLN:NE2	1:I:253:HIS:NE2	2.58	0.52
1:D:11:ASP:HA	1:D:14:LYS:HG3	1.91	0.52
1:B:4:THR:CG2	1:B:178:ILE:HG13	2.40	0.52
1:B:4:THR:CG2	1:B:178:ILE:HD11	2.40	0.51
1:H:63:GLU:OE2	4:H:501:HOH:O	2.19	0.51
1:F:108:GLY:CA	1:F:126:MET:CE	2.88	0.51
1:I:195:GLU:HG2	4:I:657:HOH:O	2.09	0.51
1:B:290:LYS:HE3	1:I:295:GLU:OE1	2.11	0.51
1:H:279:GLU:OE2	2:H:402:BME:S2	2.63	0.51
1:K:136:ILE:HG23	1:K:146:TYR:CE1	2.45	0.51
1:L:108:GLY:CA	1:L:126:MET:CE	2.88	0.51
1:F:136:ILE:HG23	1:F:146:TYR:CE1	2.44	0.51
1:L:136:ILE:HG23	1:L:146:TYR:CE1	2.46	0.51
1:B:51:TYR:CE1	1:B:61:VAL:CG1	2.91	0.51
1:I:136:ILE:HG23	1:I:146:TYR:CE1	2.45	0.51
1:J:320:LYS:HG3	1:J:330:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ILE:HD12	1:D:276:VAL:HG12	1.92	0.51
1:F:196:HIS:HE1	4:F:510:HOH:O	1.94	0.51
1:I:108:GLY:CA	1:I:126:MET:CE	2.88	0.51
1:C:207:LYS:HE3	4:C:641:HOH:O	2.11	0.50
1:C:249:GLN:OE1	1:C:253:HIS:CE1	2.64	0.50
1:D:136:ILE:HG23	1:D:146:TYR:CE1	2.46	0.50
1:L:328:ARG:O	1:L:330:VAL:HG23	2.12	0.50
1:G:136:ILE:HG23	1:G:146:TYR:CE1	2.47	0.50
1:J:108:GLY:CA	1:J:126:MET:HE2	2.41	0.50
1:J:75:LEU:N	1:J:75:LEU:HD12	2.27	0.50
1:D:4:THR:CG2	1:D:178:ILE:HG13	2.42	0.50
1:E:3:LYS:HA	1:E:3:LYS:HE2	1.93	0.50
1:K:75:LEU:HD12	1:K:75:LEU:N	2.27	0.49
1:A:136:ILE:HG23	1:A:146:TYR:CE1	2.46	0.49
1:D:75:LEU:N	1:D:75:LEU:HD12	2.28	0.49
1:K:3:LYS:HE2	1:K:4:THR:H	1.78	0.49
1:A:238:ALA:HB3	1:B:235:ALA:HA	1.94	0.49
1:K:132:VAL:HB	1:L:236:GLU:OE2	2.12	0.49
1:I:75:LEU:HD12	1:I:75:LEU:N	2.28	0.49
1:B:51:TYR:CD1	1:B:61:VAL:HG11	2.48	0.49
1:D:64:ILE:HD12	1:D:90:LYS:HE2	1.95	0.49
1:I:227:GLU:OE1	1:J:130:ARG:NH1	2.46	0.49
1:H:35:ARG:HB2	1:H:41:VAL:CG2	2.41	0.48
1:B:300:TYR:N	1:B:301:PRO:CD	2.77	0.48
1:G:75:LEU:HD12	1:G:75:LEU:N	2.28	0.48
1:D:4:THR:CG2	1:D:178:ILE:HD11	2.42	0.48
1:H:236:GLU:OE2	1:H:239:ARG:NH2	2.45	0.48
1:E:256:THR:HG1	1:F:292:TRP:HE1	1.62	0.48
1:F:75:LEU:N	1:F:75:LEU:HD12	2.29	0.48
1:G:209:CYS:HB3	1:G:228:PHE:CZ	2.49	0.48
1:H:11:ASP:N	1:H:12:PRO:CD	2.77	0.48
1:I:11:ASP:N	1:I:12:PRO:CD	2.77	0.48
1:J:209:CYS:HB3	1:J:228:PHE:CZ	2.49	0.48
1:G:11:ASP:N	1:G:12:PRO:CD	2.77	0.48
1:J:108:GLY:N	1:J:126:MET:HE2	2.28	0.48
1:L:300:TYR:N	1:L:301:PRO:CD	2.76	0.48
1:B:4:THR:HG23	1:B:178:ILE:HD11	1.96	0.48
1:D:23:TYR:H	1:D:45:ASN:ND2	2.12	0.48
1:H:209:CYS:HB3	1:H:228:PHE:CZ	2.49	0.48
1:I:233:GLU:HB2	4:I:627:HOH:O	2.13	0.48
1:C:209:CYS:HB3	1:C:228:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:TYR:H	1:E:45:ASN:ND2	2.12	0.47
1:F:11:ASP:N	1:F:12:PRO:CD	2.77	0.47
1:H:300:TYR:N	1:H:301:PRO:CD	2.77	0.47
1:K:209:CYS:HB3	1:K:228:PHE:CZ	2.48	0.47
1:B:209:CYS:HB3	1:B:228:PHE:CZ	2.50	0.47
1:C:11:ASP:N	1:C:12:PRO:CD	2.77	0.47
1:L:75:LEU:N	1:L:75:LEU:HD12	2.28	0.47
1:D:300:TYR:N	1:D:301:PRO:CD	2.77	0.47
1:E:11:ASP:N	1:E:12:PRO:CD	2.77	0.47
1:B:11:ASP:N	1:B:12:PRO:CD	2.78	0.47
1:C:300:TYR:N	1:C:301:PRO:CD	2.78	0.47
1:K:300:TYR:N	1:K:301:PRO:CD	2.77	0.47
1:I:126:MET:HE1	1:I:184:PHE:HA	1.96	0.47
1:J:300:TYR:N	1:J:301:PRO:CD	2.78	0.47
1:B:75:LEU:N	1:B:75:LEU:HD12	2.30	0.47
1:D:11:ASP:N	1:D:12:PRO:CD	2.78	0.47
1:E:300:TYR:N	1:E:301:PRO:CD	2.78	0.47
1:H:75:LEU:N	1:H:75:LEU:HD12	2.29	0.47
1:K:11:ASP:N	1:K:12:PRO:CD	2.77	0.47
1:A:238:ALA:CB	1:B:235:ALA:HA	2.45	0.47
1:C:75:LEU:HD12	1:C:75:LEU:N	2.30	0.47
1:F:126:MET:HE1	1:F:184:PHE:HA	1.96	0.47
1:I:209:CYS:HB3	1:I:228:PHE:CZ	2.49	0.47
1:J:11:ASP:N	1:J:12:PRO:CD	2.78	0.47
1:L:209:CYS:HB3	1:L:228:PHE:CZ	2.49	0.47
1:A:11:ASP:N	1:A:12:PRO:CD	2.78	0.47
1:A:300:TYR:N	1:A:301:PRO:CD	2.78	0.47
1:D:209:CYS:HB3	1:D:228:PHE:CZ	2.50	0.47
1:F:131:MET:HE3	1:F:131:MET:HA	1.95	0.47
1:F:209:CYS:HB3	1:F:228:PHE:CZ	2.50	0.47
1:F:300:TYR:N	1:F:301:PRO:CD	2.78	0.47
1:G:300:TYR:N	1:G:301:PRO:CD	2.77	0.47
1:L:120:LYS:HE2	1:L:120:LYS:N	2.28	0.47
1:L:11:ASP:N	1:L:12:PRO:CD	2.78	0.47
1:E:209:CYS:HB3	1:E:228:PHE:CZ	2.49	0.47
1:A:209:CYS:HB3	1:A:228:PHE:CZ	2.49	0.46
1:B:29:VAL:HG22	1:B:137:MET:HG3	1.98	0.46
1:I:300:TYR:N	1:I:301:PRO:CD	2.78	0.46
1:A:75:LEU:N	1:A:75:LEU:HD12	2.30	0.46
1:B:66:GLU:HG2	1:B:69:ARG:HH12	1.81	0.46
1:E:75:LEU:N	1:E:75:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:GLY:HA3	1:J:126:MET:CE	2.45	0.46
1:C:238:ALA:HB3	1:D:235:ALA:HA	1.97	0.46
1:D:108:GLY:HA3	1:D:126:MET:HE1	1.97	0.46
1:E:35:ARG:HB2	1:E:41:VAL:CG2	2.43	0.46
1:A:40:ASN:ND2	1:A:40:ASN:N	2.63	0.46
1:L:126:MET:HE3	1:L:184:PHE:HA	1.98	0.46
1:E:29:VAL:HG22	1:E:137:MET:HG3	1.98	0.46
1:H:96:GLN:HB2	1:H:96:GLN:HE21	1.38	0.46
1:G:19:GLY:O	1:G:74:ALA:HA	2.16	0.45
1:K:126:MET:HE3	1:K:184:PHE:HA	1.98	0.45
1:E:40:ASN:ND2	1:E:40:ASN:N	2.64	0.45
1:I:19:GLY:O	1:I:74:ALA:HA	2.16	0.45
1:L:297:GLN:OE1	4:L:501:HOH:O	2.21	0.45
1:C:130:ARG:NH1	1:D:227:GLU:OE2	2.49	0.45
1:K:19:GLY:O	1:K:74:ALA:HA	2.16	0.45
1:C:290:LYS:CE	1:E:295:GLU:OE1	2.62	0.45
1:B:19:GLY:O	1:B:74:ALA:HA	2.17	0.45
1:A:236:GLU:OE2	1:A:239:ARG:NH2	2.44	0.45
1:F:19:GLY:O	1:F:74:ALA:HA	2.16	0.45
1:D:19:GLY:O	1:D:74:ALA:HA	2.17	0.45
1:H:19:GLY:O	1:H:74:ALA:HA	2.16	0.45
1:J:108:GLY:HA3	1:J:126:MET:HE1	1.99	0.45
1:C:242:ALA:O	1:D:328:ARG:NH1	2.50	0.45
1:E:328:ARG:NH1	1:F:242:ALA:O	2.50	0.44
1:C:19:GLY:O	1:C:74:ALA:HA	2.17	0.44
1:L:19:GLY:O	1:L:74:ALA:HA	2.18	0.44
1:L:108:GLY:CA	1:L:126:MET:HE2	2.48	0.44
1:D:4:THR:HG23	1:D:178:ILE:HD11	1.99	0.44
1:E:130:ARG:NH1	1:F:227:GLU:OE1	2.50	0.44
1:K:108:GLY:CA	1:K:126:MET:HE2	2.47	0.44
1:A:19:GLY:O	1:A:74:ALA:HA	2.17	0.44
1:E:30:GLN:HE21	1:E:171:ILE:HG21	1.83	0.44
1:E:19:GLY:O	1:E:74:ALA:HA	2.18	0.43
1:A:234:LEU:HG	1:B:238:ALA:CB	2.48	0.43
1:J:19:GLY:O	1:J:74:ALA:HA	2.18	0.43
1:K:238:ALA:HB3	1:L:235:ALA:HA	1.99	0.43
1:A:242:ALA:O	1:B:328:ARG:NH1	2.51	0.43
1:C:238:ALA:CB	1:D:235:ALA:HA	2.48	0.43
1:J:45:ASN:ND2	1:J:48:ASP:OD1	2.52	0.43
1:B:4:THR:HG23	1:B:178:ILE:CD1	2.49	0.42
1:L:108:GLY:N	1:L:126:MET:HE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:THR:HG23	1:D:178:ILE:CD1	2.50	0.42
1:F:92:ALA:N	1:F:93:PRO:CD	2.83	0.42
1:F:48:ASP:HB2	1:F:50:TYR:H	1.85	0.42
1:I:108:GLY:CA	1:I:126:MET:HE2	2.50	0.42
1:B:273:ARG:HD3	4:B:519:HOH:O	2.19	0.42
1:D:108:GLY:HA3	1:D:126:MET:CE	2.50	0.42
1:J:111:VAL:HB	1:J:184:PHE:CD2	2.55	0.42
1:C:92:ALA:N	1:C:93:PRO:CD	2.83	0.42
1:E:92:ALA:N	1:E:93:PRO:CD	2.83	0.42
1:F:108:GLY:CA	1:F:126:MET:HE2	2.50	0.42
1:L:29:VAL:HG22	1:L:137:MET:HG2	2.00	0.42
1:H:92:ALA:N	1:H:93:PRO:CD	2.83	0.42
1:K:279:GLU:OE2	2:K:500:BME:S2	2.71	0.42
1:B:66:GLU:HG2	1:B:69:ARG:NH1	2.35	0.41
1:B:92:ALA:N	1:B:93:PRO:CD	2.83	0.41
1:D:108:GLY:CA	1:D:126:MET:HE2	2.50	0.41
1:D:92:ALA:N	1:D:93:PRO:CD	2.83	0.41
4:E:608:HOH:O	1:F:204:GLY:HA3	2.19	0.41
1:G:92:ALA:N	1:G:93:PRO:CD	2.83	0.41
1:J:92:ALA:N	1:J:93:PRO:CD	2.84	0.41
1:L:111:VAL:HB	1:L:184:PHE:CD2	2.56	0.41
1:L:233:GLU:O	1:L:236:GLU:HG3	2.20	0.41
1:A:186:GLU:HG3	1:B:219:VAL:HG22	2.02	0.41
1:I:48:ASP:HB2	1:I:50:TYR:H	1.86	0.41
1:J:48:ASP:HB2	1:J:50:TYR:H	1.86	0.41
1:B:111:VAL:HB	1:B:184:PHE:CD2	2.56	0.41
1:C:235:ALA:HA	1:D:238:ALA:HB3	2.02	0.41
1:E:82:VAL:HG22	1:E:82:VAL:O	2.20	0.41
1:G:48:ASP:HB2	1:G:50:TYR:H	1.85	0.41
1:G:111:VAL:HB	1:G:184:PHE:CD2	2.56	0.41
1:K:220:SER:CB	4:K:602:HOH:O	2.68	0.41
1:K:48:ASP:HB2	1:K:50:TYR:H	1.85	0.41
1:E:48:ASP:HB2	1:E:50:TYR:H	1.86	0.41
1:I:92:ALA:N	1:I:93:PRO:CD	2.84	0.41
1:K:108:GLY:HA3	1:K:126:MET:CE	2.51	0.41
1:K:92:ALA:N	1:K:93:PRO:CD	2.83	0.41
1:A:111:VAL:HB	1:A:184:PHE:CD2	2.56	0.41
1:E:238:ALA:HB3	1:F:235:ALA:HA	2.02	0.41
1:H:48:ASP:HB2	1:H:50:TYR:H	1.86	0.41
1:I:238:ALA:HB3	1:J:235:ALA:HA	2.03	0.41
1:K:108:GLY:HA3	1:K:126:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:HB2	1:B:50:TYR:H	1.86	0.41
1:F:108:GLY:N	1:F:126:MET:HE2	2.36	0.41
1:K:111:VAL:HB	1:K:184:PHE:CD2	2.56	0.41
1:C:111:VAL:HB	1:C:184:PHE:CD2	2.56	0.40
1:K:329:LYS:HD2	1:L:244:GLU:HG2	2.02	0.40
1:D:111:VAL:HB	1:D:184:PHE:CD2	2.56	0.40
1:I:108:GLY:HA3	1:I:126:MET:HE1	2.02	0.40
1:C:48:ASP:HB2	1:C:50:TYR:H	1.86	0.40
1:K:51:TYR:CZ	1:K:55:LYS:HE3	2.56	0.40
1:L:92:ALA:N	1:L:93:PRO:CD	2.84	0.40
1:I:111:VAL:HB	1:I:184:PHE:CD2	2.56	0.40
1:K:108:GLY:N	1:K:126:MET:HE2	2.36	0.40
1:D:48:ASP:HB2	1:D:50:TYR:H	1.87	0.40
1:E:111:VAL:HB	1:E:184:PHE:CD2	2.56	0.40
1:E:47:LYS:CG	1:E:47:LYS:O	2.69	0.40
1:F:108:GLY:HA3	1:F:126:MET:HE1	2.02	0.40
1:H:111:VAL:HB	1:H:184:PHE:CD2	2.56	0.40
1:I:222:GLU:HG3	1:J:4:THR:HG22	2.04	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	325/333 (98%)	312 (96%)	11 (3%)	2 (1%)	25	41
1	B	324/333 (97%)	309 (95%)	12 (4%)	3 (1%)	17	30
1	C	325/333 (98%)	310 (95%)	13 (4%)	2 (1%)	25	41
1	D	324/333 (97%)	309 (95%)	13 (4%)	2 (1%)	25	41
1	E	324/333 (97%)	310 (96%)	12 (4%)	2 (1%)	25	41
1	F	324/333 (97%)	310 (96%)	11 (3%)	3 (1%)	17	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	326/333 (98%)	313 (96%)	10 (3%)	3 (1%)	17	30
1	H	324/333 (97%)	309 (95%)	12 (4%)	3 (1%)	17	30
1	I	324/333 (97%)	309 (95%)	13 (4%)	2 (1%)	25	41
1	J	327/333 (98%)	315 (96%)	9 (3%)	3 (1%)	17	30
1	K	326/333 (98%)	312 (96%)	12 (4%)	2 (1%)	25	41
1	L	327/333 (98%)	315 (96%)	9 (3%)	3 (1%)	17	30
All	All	3900/3996 (98%)	3733 (96%)	137 (4%)	30 (1%)	19	33

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	131	MET
1	K	131	MET
1	A	131	MET
1	B	131	MET
1	C	131	MET
1	D	131	MET
1	E	131	MET
1	F	131	MET
1	G	131	MET
1	I	131	MET
1	J	131	MET
1	L	131	MET
1	J	229	TYR
1	B	229	TYR
1	F	229	TYR
1	G	229	TYR
1	H	229	TYR
1	L	229	TYR
1	D	300	TYR
1	I	300	TYR
1	A	300	TYR
1	B	300	TYR
1	C	300	TYR
1	E	300	TYR
1	F	300	TYR
1	G	300	TYR
1	J	300	TYR
1	K	300	TYR
1	L	300	TYR

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Mol	Chain	Res	Type
1	H	300	TYR

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	266/272 (98%)	255 (96%)	11 (4%)	30	53
1	B	265/272 (97%)	251 (95%)	14 (5%)	22	40
1	C	266/272 (98%)	259 (97%)	7 (3%)	46	70
1	D	265/272 (97%)	256 (97%)	9 (3%)	37	61
1	E	265/272 (97%)	254 (96%)	11 (4%)	30	51
1	F	265/272 (97%)	252 (95%)	13 (5%)	25	45
1	G	267/272 (98%)	258 (97%)	9 (3%)	37	61
1	H	265/272 (97%)	253 (96%)	12 (4%)	27	48
1	I	265/272 (97%)	260 (98%)	5 (2%)	57	79
1	J	268/272 (98%)	257 (96%)	11 (4%)	30	53
1	K	267/272 (98%)	255 (96%)	12 (4%)	27	48
1	L	268/272 (98%)	257 (96%)	11 (4%)	30	53
All	All	3192/3264 (98%)	3067 (96%)	125 (4%)	32	55

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	48	ASP
1	A	49	LYS
1	A	52	GLU
1	A	63	GLU
1	A	66	GLU
1	A	69	ARG
1	A	81	GLU
1	A	239	ARG

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Mol	Chain	Res	Type
1	A	249	GLN
1	A	329	LYS
1	B	3	LYS
1	B	9	ASN
1	B	28	ARG
1	B	48	ASP
1	B	55	LYS
1	B	66	GLU
1	B	81	GLU
1	B	138	ASP
1	B	153	LYS
1	B	162	ASP
1	B	239	ARG
1	B	249	GLN
1	B	290	LYS
1	B	308	GLU
1	C	2	ASP
1	C	14	LYS
1	C	40	ASN
1	C	48	ASP
1	C	81	GLU
1	C	239	ARG
1	C	249	GLN
1	D	3	LYS
1	D	6	LEU
1	D	48	ASP
1	D	52	GLU
1	D	66	GLU
1	D	81	GLU
1	D	120	LYS
1	D	138	ASP
1	D	249	GLN
1	E	40	ASN
1	E	41	VAL
1	E	48	ASP
1	E	52	GLU
1	E	66	GLU
1	E	81	GLU
1	E	138	ASP
1	E	153	LYS
1	E	239	ARG
1	E	249	GLN

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Mol	Chain	Res	Type
1	E	251	VAL
1	F	3	LYS
1	F	25	ASN
1	F	48	ASP
1	F	49	LYS
1	F	52	GLU
1	F	81	GLU
1	F	96	GLN
1	F	131	MET
1	F	138	ASP
1	F	236	GLU
1	F	239	ARG
1	F	249	GLN
1	F	308	GLU
1	G	48	ASP
1	G	49	LYS
1	G	52	GLU
1	G	81	GLU
1	G	96	GLN
1	G	120	LYS
1	G	144	LYS
1	G	215	LYS
1	G	249	GLN
1	H	3	LYS
1	H	11	ASP
1	H	14	LYS
1	H	41	VAL
1	H	48	ASP
1	H	52	GLU
1	H	66	GLU
1	H	81	GLU
1	H	138	ASP
1	H	185	GLU
1	H	249	GLN
1	H	290	LYS
1	I	48	ASP
1	I	52	GLU
1	I	81	GLU
1	I	120	LYS
1	I	138	ASP
1	J	2	ASP
1	J	48	ASP

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Mol	Chain	Res	Type
1	J	52	GLU
1	J	66	GLU
1	J	81	GLU
1	J	130	ARG
1	J	153	LYS
1	J	215	LYS
1	J	249	GLN
1	J	329	LYS
1	J	330	VAL
1	K	3	LYS
1	K	14	LYS
1	K	46	VAL
1	K	48	ASP
1	K	56	LYS
1	K	66	GLU
1	K	120	LYS
1	K	134	GLU
1	K	138	ASP
1	K	249	GLN
1	K	329	LYS
1	K	330	VAL
1	L	14	LYS
1	L	48	ASP
1	L	52	GLU
1	L	66	GLU
1	L	81	GLU
1	L	99	LYS
1	L	120	LYS
1	L	138	ASP
1	L	142	GLN
1	L	236	GLU
1	L	249	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	B	9	ASN
1	C	253	HIS
1	D	45	ASN
1	E	30	GLN
1	E	40	ASN

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Mol	Chain	Res	Type
1	E	45	ASN
1	F	25	ASN
1	F	40	ASN
1	H	96	GLN
1	I	196	HIS
1	I	249	GLN
1	J	253	HIS
1	J	297	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](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	$\# Z > 2$
2	BME	G	500	-	3,3,3	0.41	0	1,2,2	0.61	0
2	BME	E	500	-	3,3,3	0.16	0	1,2,2	0.64	0
2	BME	H	402	-	3,3,3	0.23	0	1,2,2	0.27	0
2	BME	I	500	-	3,3,3	0.28	0	1,2,2	0.70	0
2	BME	C	500	-	3,3,3	0.34	0	1,2,2	0.03	0
2	BME	D	402	-	3,3,3	0.31	0	1,2,2	0.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BME	F	402	-	3,3,3	0.21	0	1,2,2	0.64	0
2	BME	B	401	-	3,3,3	0.22	0	1,2,2	0.13	0
2	BME	J	402	-	3,3,3	0.32	0	1,2,2	0.08	0
2	BME	L	402	-	3,3,3	0.16	0	1,2,2	0.69	0
2	BME	A	401	-	3,3,3	0.23	0	1,2,2	0.39	0
2	BME	K	500	-	3,3,3	0.23	0	1,2,2	0.15	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	BME	G	500	-	-	1/1/1/1	-
2	BME	E	500	-	-	1/1/1/1	-
2	BME	H	402	-	-	1/1/1/1	-
2	BME	I	500	-	-	0/1/1/1	-
2	BME	C	500	-	-	0/1/1/1	-
2	BME	D	402	-	-	1/1/1/1	-
2	BME	F	402	-	-	0/1/1/1	-
2	BME	B	401	-	-	0/1/1/1	-
2	BME	J	402	-	-	1/1/1/1	-
2	BME	L	402	-	-	0/1/1/1	-
2	BME	A	401	-	-	1/1/1/1	-
2	BME	K	500	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	402	BME	O1-C1-C2-S2
2	G	500	BME	O1-C1-C2-S2
2	J	402	BME	O1-C1-C2-S2
2	D	402	BME	O1-C1-C2-S2
2	A	401	BME	O1-C1-C2-S2
2	E	500	BME	O1-C1-C2-S2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	402	BME	1	0
2	K	500	BME	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	327/333 (98%)	0.53	38 (11%) 4 4	39, 89, 151, 193	0
1	B	326/333 (97%)	0.49	45 (13%) 2 2	36, 87, 150, 193	0
1	C	327/333 (98%)	-0.14	13 (3%) 38 42	37, 55, 108, 147	0
1	D	326/333 (97%)	0.06	19 (5%) 23 24	35, 68, 135, 162	0
1	E	326/333 (97%)	0.31	40 (12%) 4 4	38, 79, 140, 164	0
1	F	326/333 (97%)	-0.19	8 (2%) 57 61	34, 59, 111, 153	0
1	G	328/333 (98%)	0.11	20 (6%) 21 22	35, 63, 119, 158	0
1	H	326/333 (97%)	-0.04	10 (3%) 49 53	35, 59, 113, 147	0
1	I	326/333 (97%)	-0.12	14 (4%) 35 39	35, 62, 117, 155	0
1	J	329/333 (98%)	-0.20	5 (1%) 73 76	35, 53, 94, 138	0
1	K	328/333 (98%)	-0.14	12 (3%) 41 45	35, 56, 94, 132	0
1	L	329/333 (98%)	0.04	18 (5%) 25 27	34, 68, 119, 150	0
All	All	3924/3996 (98%)	0.06	242 (6%) 20 22	34, 63, 128, 193	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	TYR	7.7
1	A	133	GLY	6.3
1	A	47	LYS	5.9
1	E	137	MET	5.8
1	D	142	GLN	5.7
1	A	50	TYR	5.5
1	A	44	GLY	5.3
1	B	23	TYR	5.2
1	A	52	GLU	5.1
1	B	142	GLN	5.0
1	E	75	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	L	49	LYS	4.9
1	J	330	VAL	4.9
1	A	51	TYR	4.8
1	D	144	LYS	4.8
1	A	136	ILE	4.7
1	G	51	TYR	4.7
1	B	53	LEU	4.6
1	G	132	VAL	4.6
1	B	47	LYS	4.6
1	B	56	LYS	4.6
1	L	142	GLN	4.5
1	B	59	PHE	4.5
1	L	141	LYS	4.4
1	G	134	GLU	4.4
1	E	8	ALA	4.3
1	A	59	PHE	4.3
1	A	31	ALA	4.3
1	F	239	ARG	4.3
1	L	50	TYR	4.2
1	A	37	ASN	4.1
1	E	132	VAL	4.1
1	B	144	LYS	4.0
1	L	236	GLU	4.0
1	B	60	GLU	4.0
1	E	9	ASN	4.0
1	B	252	HIS	4.0
1	A	96	GLN	3.9
1	D	137	MET	3.9
1	E	50	TYR	3.9
1	B	51	TYR	3.8
1	K	329	LYS	3.8
1	A	137	MET	3.8
1	B	240	LEU	3.7
1	E	70	ARG	3.6
1	A	9	ASN	3.6
1	D	139	LEU	3.6
1	I	49	LYS	3.6
1	E	141	LYS	3.5
1	E	62	TYR	3.5
1	I	144	LYS	3.5
1	G	329	LYS	3.5
1	I	142	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	57	GLU	3.4
1	F	134	GLU	3.4
1	H	75	LEU	3.4
1	B	137	MET	3.4
1	G	9	ASN	3.4
1	A	97	GLY	3.3
1	I	138	ASP	3.3
1	B	61	VAL	3.3
1	B	96	GLN	3.3
1	C	327	GLY	3.3
1	E	53	LEU	3.3
1	B	141	LYS	3.3
1	G	50	TYR	3.3
1	D	50	TYR	3.2
1	E	243	GLU	3.2
1	C	132	VAL	3.2
1	A	58	GLY	3.2
1	A	252	HIS	3.2
1	B	58	GLY	3.2
1	B	55	LYS	3.2
1	J	329	LYS	3.2
1	F	234	LEU	3.1
1	H	252	HIS	3.1
1	E	156	ALA	3.1
1	L	140	HIS	3.1
1	F	236	GLU	3.1
1	D	23	TYR	3.1
1	B	54	ALA	3.1
1	E	76	LEU	3.1
1	B	236	GLU	3.0
1	I	143	GLY	3.0
1	E	138	ASP	3.0
1	D	131	MET	3.0
1	A	141	LYS	3.0
1	B	133	GLY	3.0
1	G	49	LYS	3.0
1	H	240	LEU	3.0
1	E	7	ASP	2.9
1	B	70	ARG	2.9
1	H	239	ARG	2.9
1	L	59	PHE	2.9
1	A	135	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	2.9
1	B	139	LEU	2.9
1	B	239	ARG	2.9
1	C	142	GLN	2.9
1	G	53	LEU	2.9
1	I	50	TYR	2.9
1	B	62	TYR	2.9
1	A	140	HIS	2.9
1	A	329	LYS	2.9
1	C	138	ASP	2.8
1	D	11	ASP	2.8
1	B	233	GLU	2.8
1	B	40	ASN	2.8
1	I	141	LYS	2.8
1	E	28	ARG	2.8
1	E	142	GLN	2.8
1	K	132	VAL	2.8
1	E	106	ALA	2.8
1	B	9	ASN	2.7
1	D	9	ASN	2.7
1	B	128	ALA	2.7
1	A	139	LEU	2.7
1	D	233	GLU	2.7
1	E	51	TYR	2.7
1	B	138	ASP	2.7
1	E	77	LEU	2.7
1	A	134	GLU	2.7
1	K	141	LYS	2.7
1	B	43	VAL	2.7
1	D	174	ILE	2.7
1	D	252	HIS	2.7
1	E	74	ALA	2.7
1	H	49	LYS	2.7
1	G	75	LEU	2.6
1	E	19	GLY	2.6
1	C	2	ASP	2.6
1	E	252	HIS	2.6
1	A	236	GLU	2.6
1	B	38	GLY	2.6
1	C	134	GLU	2.6
1	E	55	LYS	2.6
1	B	143	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	14	LYS	2.6
1	K	233	GLU	2.6
1	B	145	GLY	2.6
1	B	251	VAL	2.6
1	E	23	TYR	2.6
1	L	138	ASP	2.6
1	B	127	VAL	2.6
1	J	236	GLU	2.6
1	B	50	TYR	2.6
1	G	139	LEU	2.5
1	L	23	TYR	2.5
1	E	240	LEU	2.5
1	A	239	ARG	2.5
1	B	140	HIS	2.5
1	A	39	LEU	2.5
1	C	53	LEU	2.5
1	A	327	GLY	2.5
1	G	97	GLY	2.5
1	K	330	VAL	2.5
1	H	243	GLU	2.5
1	E	104	ASP	2.5
1	A	243	GLU	2.5
1	B	132	VAL	2.4
1	D	143	GLY	2.4
1	F	3	LYS	2.4
1	A	8	ALA	2.4
1	K	142	GLN	2.4
1	I	51	TYR	2.4
1	A	138	ASP	2.4
1	D	327	GLY	2.3
1	D	36	GLU	2.3
1	G	52	GLU	2.3
1	C	50	TYR	2.3
1	D	141	LYS	2.3
1	A	27	GLY	2.3
1	E	143	GLY	2.3
1	E	56	LYS	2.3
1	L	137	MET	2.3
1	C	233	GLU	2.3
1	L	330	VAL	2.3
1	A	89	LYS	2.3
1	K	138	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	53	LEU	2.3
1	F	243	GLU	2.3
1	I	52	GLU	2.3
1	A	42	ILE	2.3
1	F	132	VAL	2.2
1	E	21	ILE	2.2
1	G	125	ILE	2.2
1	G	47	LYS	2.2
1	K	75	LEU	2.2
1	L	139	LEU	2.2
1	B	99	LYS	2.2
1	C	141	LYS	2.2
1	D	156	ALA	2.2
1	I	47	LYS	2.2
1	B	156	ALA	2.2
1	A	38	GLY	2.2
1	A	159	LYS	2.2
1	E	49	LYS	2.2
1	C	239	ARG	2.2
1	F	327	GLY	2.2
1	G	77	LEU	2.2
1	I	53	LEU	2.2
1	B	49	LYS	2.2
1	C	49	LYS	2.2
1	K	251	VAL	2.2
1	K	324	LYS	2.2
1	H	9	ASN	2.2
1	E	139	LEU	2.2
1	E	134	GLU	2.2
1	E	140	HIS	2.1
1	L	127	VAL	2.1
1	G	167	ILE	2.1
1	B	129	PRO	2.1
1	E	129	PRO	2.1
1	I	56	LYS	2.1
1	I	99	LYS	2.1
1	E	127	VAL	2.1
1	B	6	LEU	2.1
1	K	231	SER	2.1
1	G	76	LEU	2.1
1	E	11	ASP	2.1
1	G	233	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	244	GLU	2.1
1	J	97	GLY	2.1
1	D	134	GLU	2.1
1	E	239	ARG	2.1
1	H	236	GLU	2.1
1	A	143	GLY	2.1
1	A	43	VAL	2.1
1	G	74	ALA	2.1
1	H	74	ALA	2.1
1	E	144	LYS	2.1
1	K	252	HIS	2.1
1	E	48	ASP	2.0
1	J	242	ALA	2.0
1	L	120	LYS	2.0
1	L	237	ILE	2.0
1	L	329	LYS	2.0
1	B	97	GLY	2.0
1	G	48	ASP	2.0
1	C	99	LYS	2.0
1	L	331	LYS	2.0
1	I	139	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. 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(\AA^2)	Q<0.9
3	MG	C	501	1/1	0.63	0.25	84,84,84,84	0
3	MG	H	403	1/1	0.72	0.39	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	E	502	1/1	0.73	0.30	78,78,78,78	0
3	MG	D	403	1/1	0.81	0.40	74,74,74,74	0
3	MG	A	402	1/1	0.84	0.39	81,81,81,81	0
3	MG	B	402	1/1	0.86	0.42	76,76,76,76	0
3	MG	I	501	1/1	0.87	0.37	72,72,72,72	0
3	MG	J	401	1/1	0.88	0.53	72,72,72,72	0
3	MG	I	502	1/1	0.88	0.61	66,66,66,66	0
3	MG	F	401	1/1	0.89	0.49	70,70,70,70	0
3	MG	F	403	1/1	0.90	0.41	74,74,74,74	0
3	MG	A	403	1/1	0.91	0.63	78,78,78,78	0
2	BME	A	401	4/4	0.91	0.19	74,76,82,91	0
3	MG	L	403	1/1	0.91	0.66	78,78,78,78	0
2	BME	B	401	4/4	0.92	0.23	65,68,71,84	0
3	MG	K	501	1/1	0.92	0.59	76,76,76,76	0
3	MG	D	401	1/1	0.92	0.39	64,64,64,64	0
3	MG	E	501	1/1	0.92	0.25	78,78,78,78	0
3	MG	L	401	1/1	0.93	0.47	60,60,60,60	0
2	BME	L	402	4/4	0.93	0.17	62,64,65,67	0
2	BME	I	500	4/4	0.94	0.16	57,57,65,78	0
2	BME	J	402	4/4	0.94	0.22	51,54,68,69	0
2	BME	E	500	4/4	0.94	0.15	59,59,78,82	0
3	MG	J	403	1/1	0.95	0.43	73,73,73,73	0
2	BME	G	500	4/4	0.95	0.13	63,67,70,73	0
2	BME	H	402	4/4	0.95	0.12	65,65,74,75	0
3	MG	K	502	1/1	0.95	0.89	73,73,73,73	0
3	MG	C	502	1/1	0.95	0.70	74,74,74,74	0
3	MG	G	502	1/1	0.95	0.66	70,70,70,70	0
3	MG	H	401	1/1	0.96	0.49	64,64,64,64	0
2	BME	C	500	4/4	0.96	0.16	66,70,74,76	0
2	BME	K	500	4/4	0.96	0.14	60,62,70,75	0
3	MG	A	404	1/1	0.97	0.76	76,76,76,76	0
3	MG	G	501	1/1	0.97	0.44	74,74,74,74	0
2	BME	F	402	4/4	0.97	0.17	60,61,66,72	0
2	BME	D	402	4/4	0.97	0.15	53,55,60,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.