Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:01 am GMT

PDB ID	:	4B7C
Title	:	Crystal structure of hypothetical protein PA1648 from Pseudomonas aeruginosa.
Authors	:	Alphey, M.S.; McMahon, S.A.; Duthie, F.G.; Naismith, J.H.
Deposited on	:	2012-08-17
Resolution	:	2.10 Å(reported)

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

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

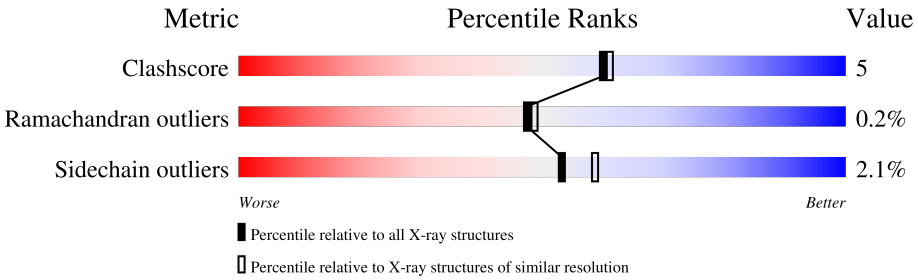
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	336	88% 7% • •
1	B	336	88% 10% ••
1	C	336	83% 11% • •
1	D	336	88% 9% •
1	E	336	87% 7% • 5%
1	F	336	88% 8% • •
1	G	336	85% 10% • •
1	H	336	86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	I	336	
1	J	336	
1	K	336	
1	L	336	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30125 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 PROBABLE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2473	1579	423	458	13			
1	B	331	Total	C	N	O	S	0	1	0
			2529	1613	437	466	13			
1	C	323	Total	C	N	O	S	0	0	0
			2450	1567	421	449	13			
1	D	325	Total	C	N	O	S	0	0	0
			2472	1579	423	457	13			
1	E	320	Total	C	N	O	S	0	0	0
			2424	1548	416	447	13			
1	F	325	Total	C	N	O	S	0	0	0
			2475	1581	425	456	13			
1	G	323	Total	C	N	O	S	0	0	0
			2452	1566	420	453	13			
1	H	320	Total	C	N	O	S	0	0	0
			2424	1548	415	448	13			
1	I	323	Total	C	N	O	S	0	0	0
			2454	1567	422	452	13			
1	J	302	Total	C	N	O	S	0	0	0
			2289	1463	392	422	12			
1	K	286	Total	C	N	O	S	0	0	0
			2172	1394	367	399	12			
1	L	325	Total	C	N	O	S	0	0	0
			2475	1581	425	456	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B7UV73
A	0	ALA	-	expression tag	UNP B7UV73
B	-1	GLY	-	expression tag	UNP B7UV73
B	0	ALA	-	expression tag	UNP B7UV73
C	-1	GLY	-	expression tag	UNP B7UV73

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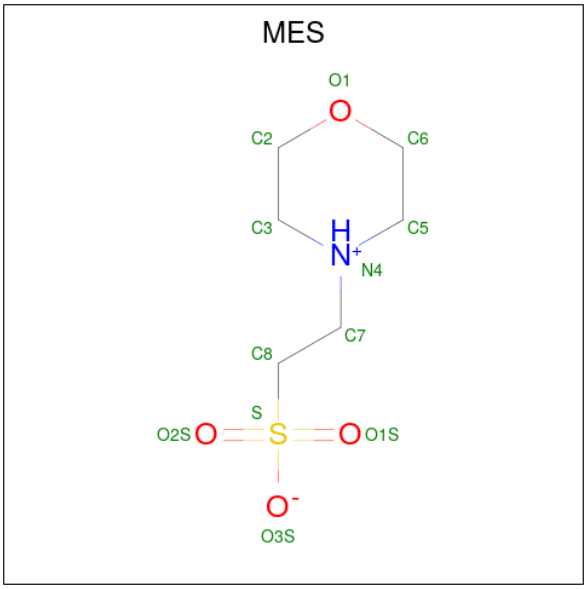
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP B7UV73
D	-1	GLY	-	expression tag	UNP B7UV73
D	0	ALA	-	expression tag	UNP B7UV73
E	-1	GLY	-	expression tag	UNP B7UV73
E	0	ALA	-	expression tag	UNP B7UV73
F	-1	GLY	-	expression tag	UNP B7UV73
F	0	ALA	-	expression tag	UNP B7UV73
G	-1	GLY	-	expression tag	UNP B7UV73
G	0	ALA	-	expression tag	UNP B7UV73
H	-1	GLY	-	expression tag	UNP B7UV73
H	0	ALA	-	expression tag	UNP B7UV73
I	-1	GLY	-	expression tag	UNP B7UV73
I	0	ALA	-	expression tag	UNP B7UV73
J	-1	GLY	-	expression tag	UNP B7UV73
J	0	ALA	-	expression tag	UNP B7UV73
K	-1	GLY	-	expression tag	UNP B7UV73
K	0	ALA	-	expression tag	UNP B7UV73
L	-1	GLY	-	expression tag	UNP B7UV73
L	0	ALA	-	expression tag	UNP B7UV73

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	88	Total	O	0	0
			88	88		
3	C	77	Total	O	0	0
			77	77		
3	D	141	Total	O	0	0
			141	141		
3	E	132	Total	O	0	0
			132	132		
3	F	55	Total	O	0	0
			55	55		
3	G	87	Total	O	0	0
			87	87		
3	H	36	Total	O	0	0
			36	36		
3	I	48	Total	O	0	0
			48	48		
3	J	72	Total	O	0	0
			72	72		
3	K	24	Total	O	0	0
			24	24		
3	L	70	Total	O	0	0
			70	70		

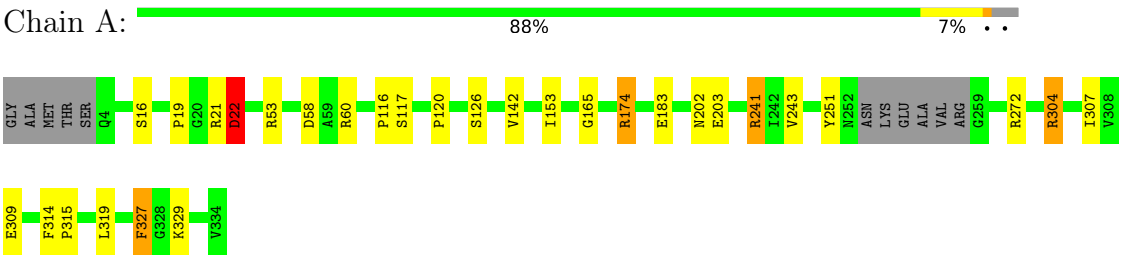
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

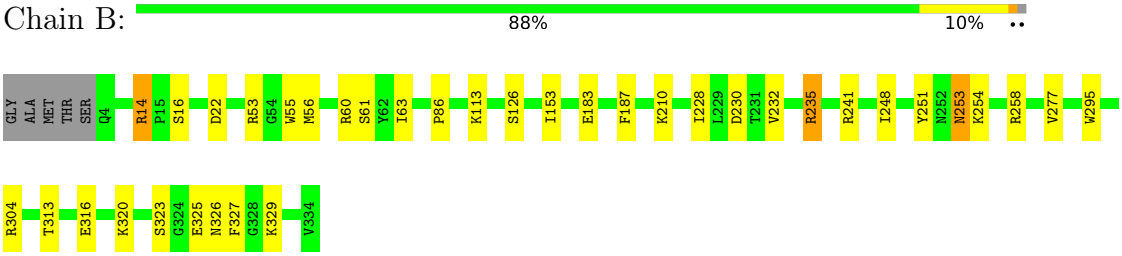
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain A:



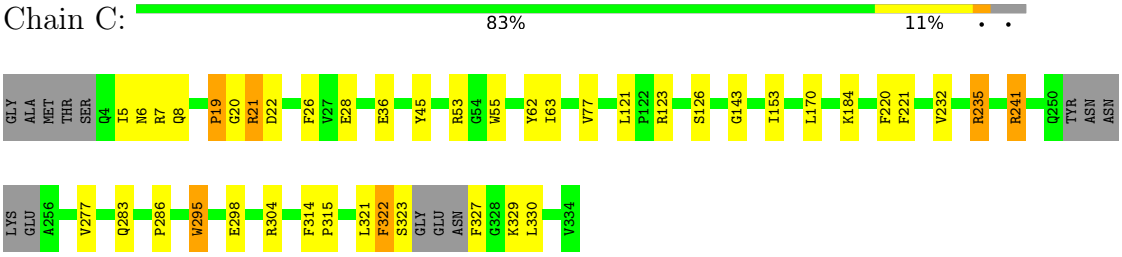
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain B:



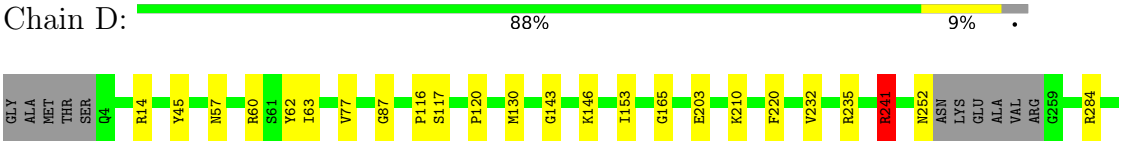
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain C:



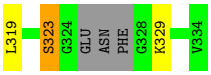
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain D:



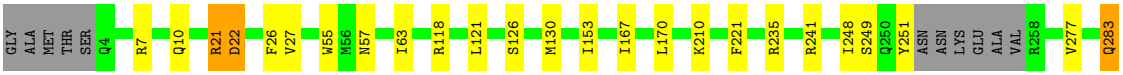
• Molecule 1: PROBABLE OXIDOREDUCTASE

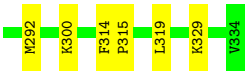
Chain E:



• Molecule 1: PROBABLE OXIDOREDUCTASE

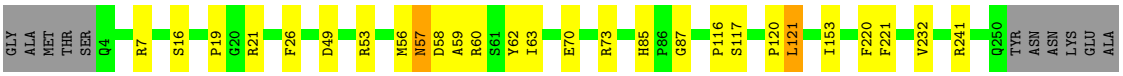
Chain F:

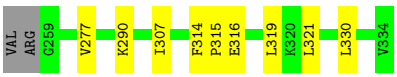




• Molecule 1: PROBABLE OXIDOREDUCTASE

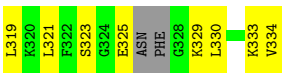
Chain G:





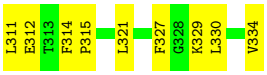
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain H:



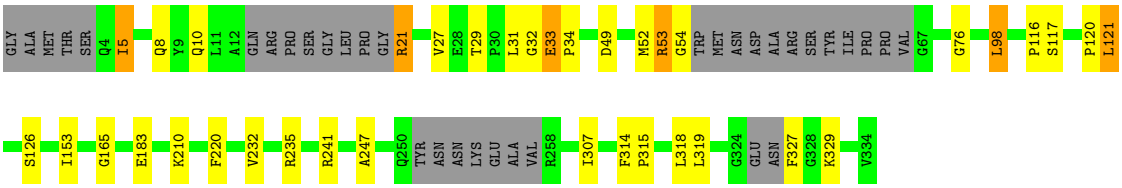
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain I:



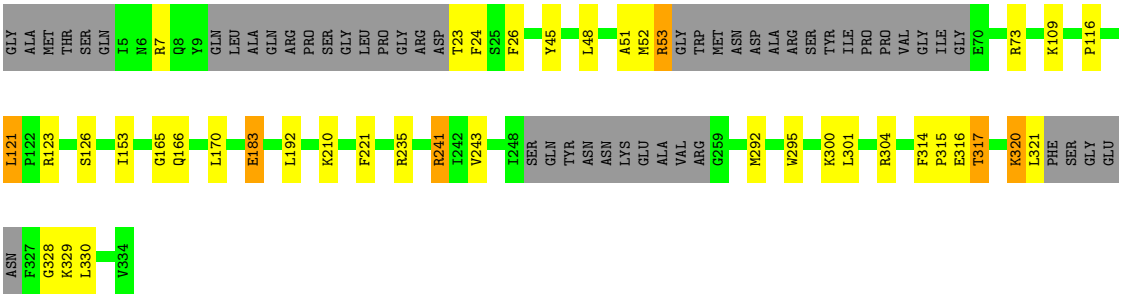
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain J:



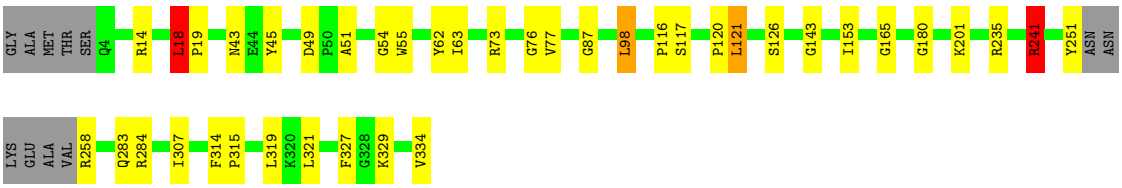
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain K:



• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain L:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	170.93Å 177.09Å 181.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.06 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (73.06-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.243	Depositor
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.180	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
Total number of atoms	30125	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.57	1/2520 (0.0%)	0.92	11/3401 (0.3%)
1	B	0.51	1/2580 (0.0%)	0.77	6/3483 (0.2%)
1	C	0.55	3/2495 (0.1%)	0.94	8/3367 (0.2%)
1	D	0.54	1/2519 (0.0%)	0.88	11/3401 (0.3%)
1	E	0.54	0/2468	0.74	2/3330 (0.1%)
1	F	0.52	1/2522 (0.0%)	0.69	2/3404 (0.1%)
1	G	0.49	0/2498	0.76	2/3372 (0.1%)
1	H	0.52	1/2468 (0.0%)	0.80	5/3330 (0.2%)
1	I	0.50	1/2500 (0.0%)	0.79	3/3374 (0.1%)
1	J	0.48	0/2325	0.73	3/3128 (0.1%)
1	K	0.52	3/2207 (0.1%)	0.78	7/2972 (0.2%)
1	L	0.49	0/2522	0.87	10/3404 (0.3%)
All	All	0.52	12/29624 (0.0%)	0.81	70/39966 (0.2%)

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	C	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	309	GLU	CD-OE1	-5.75	1.19	1.25
1	K	295	TRP	CD2-CE2	5.70	1.48	1.41
1	A	309	GLU	CD-OE1	-5.65	1.19	1.25
1	K	316	GLU	CD-OE2	-5.54	1.19	1.25
1	I	295	TRP	CD2-CE2	5.48	1.48	1.41
1	B	295	TRP	CD2-CE2	5.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	TRP	CD2-CE2	5.32	1.47	1.41
1	K	328	GLY	N-CA	5.32	1.54	1.46
1	C	298	GLU	CD-OE2	5.29	1.31	1.25
1	H	295	TRP	CD2-CE2	5.26	1.47	1.41
1	C	55	TRP	CD2-CE2	5.11	1.47	1.41
1	F	55	TRP	CD2-CE2	5.01	1.47	1.41

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	ARG	NE-CZ-NH1	23.92	132.26	120.30
1	C	241	ARG	NE-CZ-NH2	-22.66	108.97	120.30
1	A	241	ARG	NE-CZ-NH2	-17.07	111.77	120.30
1	H	241	ARG	NE-CZ-NH2	-16.97	111.82	120.30
1	L	241	ARG	NE-CZ-NH1	16.87	128.73	120.30
1	G	241	ARG	NE-CZ-NH2	-16.70	111.95	120.30
1	A	241	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	I	241	ARG	NE-CZ-NH1	16.46	128.53	120.30
1	D	241	ARG	NE-CZ-NH1	16.31	128.46	120.30
1	H	241	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	G	241	ARG	NE-CZ-NH1	16.21	128.40	120.30
1	I	241	ARG	NE-CZ-NH2	-14.79	112.91	120.30
1	L	241	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	D	241	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	L	284	ARG	NE-CZ-NH2	12.96	126.78	120.30
1	D	284	ARG	NE-CZ-NH2	12.86	126.73	120.30
1	D	284	ARG	NE-CZ-NH1	-11.42	114.59	120.30
1	L	284	ARG	NE-CZ-NH1	-10.91	114.84	120.30
1	K	123	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	K	123	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	E	241	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	241	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	K	241	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	F	241	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	22	ASP	CB-CG-OD2	8.46	125.91	118.30
1	J	241	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	B	14	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	241	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	304	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	F	241	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	K	241	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	J	241	ARG	NE-CZ-NH1	8.20	124.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	241	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	22	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	22	ASP	CB-CG-OD1	-7.36	111.68	118.30
1	B	14	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	L	284	ARG	CD-NE-CZ	-7.15	113.59	123.60
1	A	304	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	C	235	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	H	14	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	284	ARG	CD-NE-CZ	-6.85	114.01	123.60
1	C	298	GLU	CG-CD-OE2	6.84	131.98	118.30
1	C	235	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	D	304	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	D	309	GLU	CG-CD-OE2	6.45	131.20	118.30
1	H	28	GLU	OE1-CD-OE2	-6.43	115.59	123.30
1	A	309	GLU	CG-CD-OE2	6.38	131.05	118.30
1	L	14	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	14	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	309	GLU	CG-CD-OE1	-6.15	106.01	118.30
1	D	309	GLU	CG-CD-OE1	-6.10	106.09	118.30
1	L	18	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	235	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	H	14	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	L	235	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	304	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	K	183	GLU	N-CA-CB	-5.88	100.02	110.60
1	L	14	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	304	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	304	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	I	53	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	14	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	272	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	J	31	LEU	N-CA-C	5.43	125.67	111.00
1	C	298	GLU	CG-CD-OE1	-5.43	107.44	118.30
1	A	174	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	K	317	THR	CB-CA-C	-5.31	97.27	111.60
1	L	235	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	K	183	GLU	CA-CB-CG	5.14	124.71	113.40
1	A	174	ARG	CG-CD-NE	-5.04	101.21	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2473	0	2491	18	1
1	B	2529	0	2557	23	0
1	C	2450	0	2481	26	1
1	D	2472	0	2491	22	0
1	E	2424	0	2454	16	1
1	F	2475	0	2498	22	0
1	G	2452	0	2476	27	0
1	H	2424	0	2452	21	0
1	I	2454	0	2481	21	0
1	J	2289	0	2322	39	0
1	K	2172	0	2210	30	1
1	L	2475	0	2498	34	0
2	D	12	0	13	0	0
2	F	12	0	13	0	0
2	G	12	0	13	0	0
2	H	12	0	13	2	0
2	I	12	0	13	2	0
3	A	146	0	0	0	0
3	B	88	0	0	1	0
3	C	77	0	0	1	0
3	D	141	0	0	2	0
3	E	132	0	0	1	0
3	F	55	0	0	2	0
3	G	87	0	0	2	0
3	H	36	0	0	0	0
3	I	48	0	0	0	0
3	J	72	0	0	0	0
3	K	24	0	0	0	0
3	L	70	0	0	0	0
All	All	30125	0	29476	267	2

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 5.

All (267) 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:323:SER:OG	1:B:325:GLU:HB2	1.58	1.01
1:J:52:MET:C	1:J:54:GLY:H	1.76	0.85
1:J:52:MET:HE3	1:J:318:LEU:HD11	1.62	0.82
1:K:321:LEU:HD13	1:K:330:LEU:HD23	1.62	0.82
1:C:36:GLU:CG	1:J:5:ILE:HD12	2.16	0.76
1:G:120:PRO:HB3	1:J:116:PRO:O	1.86	0.76
1:H:15:PRO:O	1:H:57:ASN:ND2	2.20	0.75
1:D:120:PRO:HB3	1:E:116:PRO:O	1.87	0.74
1:A:304:ARG:NH2	1:A:327:PHE:CE1	2.56	0.74
1:F:283:GLN:HA	1:F:283:GLN:NE2	2.00	0.74
1:J:33:GLU:HG3	1:J:34:PRO:HD2	1.72	0.72
1:L:18:LEU:CD2	1:L:319:LEU:HD22	2.20	0.72
1:E:210:LYS:HA	1:E:235:ARG:HH12	1.55	0.71
1:K:48:LEU:HD12	1:K:330:LEU:HG	1.72	0.69
1:C:170:LEU:HD11	1:C:295:TRP:CD1	2.28	0.69
1:I:312:GLU:H	1:I:312:GLU:CD	1.96	0.69
1:I:75:LEU:HD22	2:I:1335:MES:S	2.33	0.68
1:A:116:PRO:O	1:L:120:PRO:HB3	1.93	0.68
1:I:76:GLY:C	1:I:98:LEU:HD22	2.15	0.68
1:J:52:MET:C	1:J:54:GLY:N	2.48	0.67
1:A:22:ASP:OD1	1:A:22:ASP:N	2.24	0.67
1:J:52:MET:O	1:J:54:GLY:N	2.28	0.66
1:A:53:ARG:NH1	1:A:251:TYR:O	2.29	0.65
1:B:210:LYS:HA	1:B:235:ARG:HH12	1.61	0.65
1:B:323:SER:OG	1:B:325:GLU:CB	2.41	0.65
1:L:18:LEU:HD21	1:L:319:LEU:HD22	1.77	0.65
1:K:166:GLN:CB	1:K:301:LEU:CD1	2.74	0.64
1:J:76:GLY:C	1:J:98:LEU:HD22	2.18	0.64
1:F:21:ARG:NH2	1:F:319:LEU:HD11	2.11	0.64
1:I:321:LEU:HD13	1:I:330:LEU:HD23	1.80	0.64
1:F:153:ILE:HD13	1:F:221:PHE:HB3	1.79	0.63
1:C:36:GLU:HG2	1:J:5:ILE:HD12	1.81	0.62
1:E:210:LYS:HA	1:E:235:ARG:NH1	2.14	0.62
1:G:153:ILE:HD13	1:G:221:PHE:HB3	1.79	0.62
1:K:166:GLN:HB2	1:K:301:LEU:CD1	2.29	0.62
1:I:283:GLN:HA	1:L:87:GLY:HA3	1.82	0.62
1:F:63:ILE:HD12	3:F:2012:HOH:O	1.98	0.62
1:B:210:LYS:HB2	1:B:235:ARG:HH22	1.64	0.62
1:J:52:MET:CE	1:J:318:LEU:HD11	2.29	0.62
1:K:317:THR:HG22	1:K:317:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ARG:NH1	1:G:316:GLU:OE2	2.33	0.61
1:L:76:GLY:C	1:L:98:LEU:HD22	2.20	0.61
1:J:49:ASP:O	1:J:52:MET:HE2	2.01	0.60
1:B:187:PHE:CZ	1:B:304:ARG:HD2	2.36	0.60
1:G:57:ASN:HD21	1:G:59:ALA:HB2	1.66	0.60
1:C:143:GLY:O	1:C:241:ARG:HD2	2.02	0.59
1:J:10:GLN:NE2	1:J:27:VAL:HG21	2.18	0.59
1:A:142:VAL:HG12	1:A:243:VAL:HG22	1.84	0.59
1:K:153:ILE:HD11	1:K:165:GLY:HA2	1.84	0.59
1:L:153:ILE:HD11	1:L:165:GLY:HA2	1.84	0.59
1:C:153:ILE:HD13	1:C:221:PHE:HB3	1.85	0.59
1:J:52:MET:CE	1:J:318:LEU:CD1	2.80	0.58
1:G:57:ASN:HD21	1:G:59:ALA:CB	2.17	0.58
1:F:283:GLN:HA	1:F:283:GLN:HE21	1.66	0.58
1:K:170:LEU:HD21	1:K:300:LYS:HB3	1.85	0.58
1:L:143:GLY:O	1:L:241:ARG:HD2	2.04	0.58
1:G:117:SER:HB2	1:J:307:ILE:CD1	2.35	0.57
1:I:143:GLY:O	1:I:241:ARG:HD2	2.05	0.57
1:B:86:PRO:HG2	3:E:2035:HOH:O	2.03	0.57
1:G:117:SER:CB	1:J:307:ILE:CD1	2.82	0.57
1:D:143:GLY:O	1:D:241:ARG:HD2	2.04	0.57
3:D:2067:HOH:O	1:G:290:LYS:HE2	2.03	0.57
1:J:153:ILE:HD11	1:J:165:GLY:HA2	1.87	0.57
1:H:153:ILE:HD11	1:H:165:GLY:HA2	1.87	0.57
1:J:33:GLU:HG3	1:J:34:PRO:CD	2.34	0.56
1:J:210:LYS:HA	1:J:235:ARG:HH21	1.70	0.56
1:D:57:ASN:HD21	1:D:252:ASN:HA	1.70	0.56
1:F:57:ASN:HD21	1:F:251:TYR:C	2.09	0.56
1:A:120:PRO:HB3	1:L:116:PRO:O	2.06	0.56
1:L:18:LEU:CD2	1:L:319:LEU:CD2	2.83	0.56
1:J:21:ARG:HH12	1:J:319:LEU:HD11	1.71	0.55
1:H:321:LEU:HD13	1:H:330:LEU:HD23	1.88	0.55
1:D:57:ASN:HD21	1:D:252:ASN:CA	2.20	0.55
1:J:153:ILE:CD1	1:J:165:GLY:HA2	2.36	0.55
1:F:22:ASP:OD1	1:F:22:ASP:N	2.39	0.55
1:F:210:LYS:HA	1:F:235:ARG:HH21	1.70	0.55
1:H:153:ILE:CD1	1:H:165:GLY:HA2	2.37	0.54
1:K:321:LEU:HD13	1:K:330:LEU:CD2	2.35	0.54
1:B:55:TRP:NE1	1:B:63:ILE:HD11	2.22	0.54
1:D:87:GLY:HA3	1:H:283:GLN:HA	1.89	0.54
1:D:210:LYS:HA	1:D:235:ARG:HH21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ILE:HD13	1:G:221:PHE:CB	2.38	0.54
1:E:19:PRO:O	1:E:319:LEU:HD21	2.06	0.54
1:A:153:ILE:HD11	1:A:165:GLY:HA2	1.89	0.54
1:K:166:GLN:NE2	1:K:192:LEU:HD22	2.23	0.54
1:L:55:TRP:HE1	1:L:63:ILE:HD12	1.72	0.54
1:C:283:GLN:HA	1:G:87:GLY:HA3	1.89	0.54
1:E:33:GLU:HB3	1:E:34:PRO:HD2	1.89	0.54
1:K:166:GLN:HB3	1:K:301:LEU:CD1	2.38	0.54
1:G:277:VAL:HG13	3:G:2071:HOH:O	2.08	0.53
1:J:52:MET:HE3	1:J:318:LEU:CD1	2.34	0.53
1:L:180:GLY:HA3	1:L:201:LYS:HE3	1.90	0.53
1:C:321:LEU:C	1:C:323:SER:H	2.11	0.53
1:I:153:ILE:HD13	1:I:221:PHE:HB3	1.89	0.53
1:F:21:ARG:HH22	1:F:319:LEU:HD11	1.73	0.52
1:F:153:ILE:HD13	1:F:221:PHE:CB	2.40	0.52
1:C:6:ASN:ND2	1:C:8:GLN:HE21	2.07	0.52
1:F:248:ILE:C	1:F:248:ILE:HD12	2.29	0.52
1:C:286:PRO:HG2	1:G:85:HIS:NE2	2.25	0.52
1:K:23:THR:HG23	1:K:24:PHE:H	1.76	0.51
1:F:21:ARG:HH22	1:F:319:LEU:CD1	2.23	0.51
1:D:116:PRO:O	1:E:120:PRO:HB3	2.11	0.51
1:F:170:LEU:HD21	1:F:300:LYS:HB3	1.92	0.51
1:B:113:LYS:NZ	1:E:36:GLU:OE2	2.39	0.51
1:L:153:ILE:CD1	1:L:165:GLY:HA2	2.41	0.51
1:C:184:LYS:HG2	1:C:327:PHE:CE1	2.45	0.51
1:B:53:ARG:HA	1:B:56:MET:HE3	1.93	0.50
1:D:146:LYS:NZ	3:D:2064:HOH:O	2.44	0.50
1:D:153:ILE:HD11	1:D:165:GLY:HA2	1.93	0.50
1:K:153:ILE:CD1	1:K:165:GLY:HA2	2.41	0.50
1:A:117:SER:HB3	1:L:307:ILE:CD1	2.41	0.50
1:C:62:TYR:CD2	1:C:63:ILE:HG13	2.46	0.50
1:J:33:GLU:CG	1:J:34:PRO:HD2	2.40	0.50
1:B:248:ILE:HA	1:B:251:TYR:CD2	2.47	0.50
1:C:5:ILE:HD11	1:C:28:GLU:HB3	1.93	0.50
1:H:170:LEU:HD21	1:H:300:LYS:HB3	1.94	0.50
1:L:63:ILE:HG22	1:L:73:ARG:NH1	2.27	0.49
1:C:36:GLU:HG3	1:J:5:ILE:HD12	1.91	0.49
1:J:153:ILE:CD1	1:J:165:GLY:CA	2.90	0.49
1:B:304:ARG:HH12	1:B:327:PHE:HD2	1.61	0.49
1:J:52:MET:HE1	1:J:318:LEU:CD1	2.43	0.49
1:C:153:ILE:HD13	1:C:221:PHE:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:CD1	1:A:165:GLY:HA2	2.43	0.49
1:E:153:ILE:HD13	1:E:221:PHE:HB3	1.93	0.49
1:B:230:ASP:HB2	1:B:258:ARG:HH12	1.78	0.49
1:D:117:SER:CB	1:E:307:ILE:CD1	2.91	0.49
1:F:57:ASN:ND2	1:F:251:TYR:C	2.67	0.48
1:H:323:SER:OG	1:H:325:GLU:HG3	2.14	0.48
1:L:116:PRO:HB3	1:L:121:LEU:HD11	1.96	0.48
1:F:277:VAL:HG13	3:F:2047:HOH:O	2.14	0.47
1:K:170:LEU:CD2	1:K:300:LYS:HB3	2.44	0.47
1:G:321:LEU:HD13	1:G:330:LEU:HD23	1.97	0.47
1:D:153:ILE:CD1	1:D:165:GLY:HA2	2.45	0.47
1:A:117:SER:CB	1:L:307:ILE:CD1	2.92	0.47
1:H:75:LEU:HD12	2:H:1335:MES:S	2.54	0.47
1:I:58:ASP:HB3	1:I:61:SER:OG	2.15	0.47
1:K:210:LYS:HA	1:K:235:ARG:HH21	1.78	0.47
1:I:321:LEU:HD13	1:I:330:LEU:CD2	2.43	0.47
1:H:77:VAL:HG11	1:H:121:LEU:HD22	1.97	0.47
1:G:53:ARG:HA	1:G:56:MET:HE2	1.96	0.46
1:C:170:LEU:HD11	1:C:295:TRP:CG	2.50	0.46
1:B:228:ILE:O	1:B:232:VAL:HG23	2.15	0.46
1:H:153:ILE:CD1	1:H:165:GLY:CA	2.93	0.46
1:H:75:LEU:HD12	2:H:1335:MES:O2S	2.16	0.46
1:B:183:GLU:HA	1:B:183:GLU:OE1	2.15	0.46
1:B:210:LYS:CA	1:B:235:ARG:HH12	2.29	0.46
1:A:116:PRO:HG2	1:L:45:TYR:OH	2.16	0.45
1:D:220:PHE:CG	1:D:232:VAL:HG11	2.51	0.45
1:L:45:TYR:HB2	1:L:77:VAL:CG2	2.47	0.45
1:I:170:LEU:HD21	1:I:300:LYS:HB3	1.98	0.45
1:G:117:SER:HB3	1:J:307:ILE:CD1	2.47	0.45
1:L:63:ILE:CG2	1:L:73:ARG:NH1	2.79	0.45
1:I:76:GLY:CA	1:I:98:LEU:HD22	2.47	0.45
1:K:153:ILE:CD1	1:K:165:GLY:CA	2.95	0.45
1:L:153:ILE:CD1	1:L:165:GLY:CA	2.95	0.45
1:D:130:MET:CE	1:D:130:MET:HA	2.47	0.45
1:F:167:ILE:HD11	1:F:292:MET:HE1	1.99	0.45
1:I:264:LEU:HD11	1:J:247:ALA:HB3	1.99	0.45
1:L:43:ASN:O	1:L:334:VAL:HG23	2.17	0.45
1:C:77:VAL:HG11	1:C:121:LEU:HD22	1.99	0.45
1:I:153:ILE:HD13	1:I:221:PHE:CB	2.46	0.45
1:K:166:GLN:CB	1:K:301:LEU:HD13	2.47	0.45
1:K:7:ARG:HD2	1:K:26:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:LEU:HD23	1:L:19:PRO:HD2	1.98	0.44
1:A:19:PRO:O	1:A:319:LEU:HD21	2.18	0.44
1:G:63:ILE:HG22	1:G:73:ARG:NH1	2.32	0.44
1:I:75:LEU:HD22	2:I:1335:MES:O2S	2.17	0.44
1:G:314:PHE:HB3	1:G:315:PRO:HD3	1.99	0.44
1:J:220:PHE:CG	1:J:232:VAL:HG11	2.52	0.44
1:K:166:GLN:CD	1:K:301:LEU:HD12	2.38	0.44
1:L:314:PHE:HB3	1:L:315:PRO:HD3	2.00	0.44
1:G:7:ARG:HD2	1:G:26:PHE:HZ	1.83	0.44
1:K:48:LEU:HD11	1:K:317:THR:O	2.18	0.44
1:B:277:VAL:HG13	3:B:2073:HOH:O	2.17	0.44
1:K:292:MET:SD	1:K:301:LEU:CD2	3.05	0.44
1:K:320:LYS:HE3	1:K:320:LYS:HB2	1.72	0.44
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.17	0.43
1:B:320:LYS:HE2	1:B:326:ASN:HA	1.99	0.43
1:C:19:PRO:HG3	1:C:322:PHE:HE2	1.84	0.43
1:D:117:SER:HB2	1:E:307:ILE:CD1	2.48	0.43
1:G:220:PHE:CG	1:G:232:VAL:HG11	2.52	0.43
1:I:7:ARG:HD2	1:I:26:PHE:HZ	1.82	0.43
1:A:126:SER:HB3	1:A:329:LYS:HG2	2.00	0.43
1:E:157:ALA:HA	1:E:188:LEU:HD11	2.00	0.43
1:H:8:GLN:OE1	1:H:29:THR:HG21	2.19	0.43
1:C:7:ARG:HD2	1:C:26:PHE:HZ	1.82	0.43
1:G:19:PRO:O	1:G:319:LEU:HD21	2.19	0.43
1:L:51:ALA:HA	1:L:251:TYR:CZ	2.53	0.43
1:D:290:LYS:HE2	3:G:2030:HOH:O	2.18	0.43
1:F:130:MET:HE2	1:F:130:MET:HA	2.00	0.43
1:A:307:ILE:CD1	1:L:117:SER:HB2	2.48	0.43
1:B:60:ARG:HD2	1:B:61:SER:N	2.34	0.43
1:E:153:ILE:HD13	1:E:221:PHE:CB	2.49	0.43
1:G:116:PRO:O	1:J:120:PRO:HB3	2.18	0.43
1:C:170:LEU:HD11	1:C:295:TRP:CE2	2.54	0.43
1:C:170:LEU:HD11	1:C:295:TRP:NE1	2.33	0.43
1:J:314:PHE:HB3	1:J:315:PRO:HD3	2.01	0.43
1:H:19:PRO:O	1:H:319:LEU:HD21	2.18	0.43
1:I:314:PHE:HB3	1:I:315:PRO:HD3	2.01	0.43
1:G:63:ILE:CG2	1:G:73:ARG:NH1	2.81	0.43
1:H:316:GLU:OE1	1:H:316:GLU:HA	2.18	0.43
1:H:153:ILE:HD13	1:H:165:GLY:CA	2.49	0.43
1:J:116:PRO:HB3	1:J:121:LEU:CD1	2.48	0.43
1:J:183:GLU:HA	1:J:183:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:SER:HB3	1:H:329:LYS:HG2	2.01	0.42
1:H:314:PHE:HB3	1:H:315:PRO:HD3	2.01	0.42
1:J:126:SER:HB3	1:J:329:LYS:HG2	2.01	0.42
1:C:314:PHE:HB3	1:C:315:PRO:HD3	2.01	0.42
1:D:314:PHE:HB3	1:D:315:PRO:HD3	2.00	0.42
1:F:314:PHE:HB3	1:F:315:PRO:HD3	2.00	0.42
1:H:5:ILE:HD13	1:H:28:GLU:OE2	2.20	0.42
1:B:230:ASP:CB	1:B:258:ARG:HH12	2.31	0.42
1:I:126:SER:HB3	1:I:329:LYS:HG2	2.01	0.42
1:E:314:PHE:HB3	1:E:315:PRO:HD3	2.01	0.42
1:K:126:SER:HB3	1:K:329:LYS:HG2	2.01	0.42
1:F:7:ARG:HD2	1:F:26:PHE:HZ	1.85	0.42
1:H:333:LYS:O	1:H:334:VAL:HB	2.20	0.42
1:G:116:PRO:HB3	1:G:121:LEU:HD11	2.02	0.42
1:H:49:ASP:C	1:H:321:LEU:HD21	2.41	0.42
1:C:277:VAL:HG13	3:C:2066:HOH:O	2.18	0.42
1:D:87:GLY:CA	1:H:283:GLN:HA	2.50	0.42
1:F:126:SER:HB3	1:F:329:LYS:HG2	2.01	0.42
1:K:116:PRO:HB3	1:K:121:LEU:HD13	2.01	0.42
1:A:314:PHE:HB3	1:A:315:PRO:HD3	2.01	0.41
1:B:53:ARG:HA	1:B:53:ARG:HD2	1.87	0.41
1:I:264:LEU:HD11	1:J:247:ALA:CB	2.50	0.41
1:I:283:GLN:HA	1:L:87:GLY:CA	2.48	0.41
1:K:116:PRO:HB3	1:K:121:LEU:CD1	2.49	0.41
1:D:45:TYR:HB2	1:D:77:VAL:CG2	2.50	0.41
1:K:221:PHE:HA	1:K:243:VAL:HG13	2.02	0.41
1:K:314:PHE:HB3	1:K:315:PRO:HD3	2.02	0.41
1:L:126:SER:HB3	1:L:329:LYS:HG2	2.02	0.41
1:E:126:SER:HB3	1:E:329:LYS:HG2	2.01	0.41
1:L:55:TRP:NE1	1:L:63:ILE:HD12	2.34	0.41
1:A:153:ILE:CD1	1:A:165:GLY:CA	2.99	0.41
1:G:49:ASP:C	1:G:321:LEU:HD21	2.40	0.41
1:K:292:MET:SD	1:K:301:LEU:HD23	2.60	0.41
1:B:313:THR:O	1:B:316:GLU:HG2	2.21	0.41
1:I:77:VAL:HG11	1:I:121:LEU:HD22	2.02	0.41
1:I:311:LEU:HB2	1:I:334:VAL:HG13	2.03	0.41
1:J:8:GLN:OE1	1:J:29:THR:HG21	2.21	0.41
1:L:49:ASP:C	1:L:321:LEU:HD21	2.41	0.41
1:L:62:TYR:CD2	1:L:63:ILE:HG13	2.56	0.41
1:D:62:TYR:CD2	1:D:63:ILE:HG13	2.56	0.41
1:F:10:GLN:NE2	1:F:27:VAL:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:GLY:HA3	1:L:251:TYR:CE1	2.55	0.41
1:C:20:GLY:O	1:C:22:ASP:N	2.53	0.41
1:C:126:SER:HB3	1:C:329:LYS:HG2	2.03	0.41
1:D:117:SER:HB3	1:E:307:ILE:CD1	2.51	0.41
1:G:62:TYR:CD2	1:G:63:ILE:HG13	2.56	0.41
1:K:166:GLN:CB	1:K:301:LEU:HD12	2.49	0.41
1:B:253:ASN:HD22	1:B:254:LYS:N	2.18	0.41
1:G:307:ILE:CD1	1:J:117:SER:CB	2.99	0.41
1:J:116:PRO:HB3	1:J:121:LEU:HD11	2.03	0.41
1:K:51:ALA:O	1:K:53:ARG:N	2.54	0.41
1:L:19:PRO:O	1:L:319:LEU:HD21	2.21	0.41
1:G:117:SER:HB2	1:J:307:ILE:HD11	2.03	0.41
1:L:180:GLY:CA	1:L:201:LYS:HE3	2.51	0.41
1:A:307:ILE:CD1	1:L:117:SER:CB	2.99	0.40
1:C:321:LEU:HD13	1:C:330:LEU:HD23	2.03	0.40
1:D:153:ILE:CD1	1:D:165:GLY:CA	2.99	0.40
1:C:220:PHE:CG	1:C:232:VAL:HG11	2.56	0.40
1:B:126:SER:HB3	1:B:329:LYS:HG2	2.02	0.40
1:D:307:ILE:CD1	1:E:117:SER:HB3	2.51	0.40
1:K:51:ALA:HB1	1:K:73:ARG:HH22	1.86	0.40
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.93	0.40
1:J:32:GLY:O	1:J:33:GLU:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:OD1	1:K:45:TYR:OH[2_554]	1.54	0.66
1:C:45:TYR:OH	1:E:202:ASN:OD1[3_655]	1.58	0.62

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	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	B	330/336 (98%)	324 (98%)	6 (2%)	0	100	100
1	C	317/336 (94%)	311 (98%)	4 (1%)	2 (1%)	25	21
1	D	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	E	314/336 (94%)	309 (98%)	4 (1%)	1 (0%)	41	41
1	F	321/336 (96%)	317 (99%)	4 (1%)	0	100	100
1	G	319/336 (95%)	315 (99%)	4 (1%)	0	100	100
1	H	314/336 (94%)	307 (98%)	7 (2%)	0	100	100
1	I	319/336 (95%)	309 (97%)	9 (3%)	1 (0%)	41	41
1	J	292/336 (87%)	286 (98%)	5 (2%)	1 (0%)	41	41
1	K	276/336 (82%)	269 (98%)	6 (2%)	1 (0%)	34	32
1	L	321/336 (96%)	316 (98%)	5 (2%)	0	100	100
All	All	3765/4032 (93%)	3697 (98%)	62 (2%)	6 (0%)	47	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	53	ARG
1	C	21	ARG
1	C	322	PHE
1	E	323	SER
1	I	327	PHE
1	K	52	MET

5.3.2 Protein sidechains (i)

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	255/263 (97%)	246 (96%)	9 (4%)	36	38
1	B	261/263 (99%)	257 (98%)	4 (2%)	65	71
1	C	252/263 (96%)	248 (98%)	4 (2%)	62	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	255/263 (97%)	252 (99%)	3 (1%)	71	77
1	E	250/263 (95%)	243 (97%)	7 (3%)	43	47
1	F	255/263 (97%)	250 (98%)	5 (2%)	55	60
1	G	253/263 (96%)	247 (98%)	6 (2%)	49	53
1	H	250/263 (95%)	250 (100%)	0	100	100
1	I	253/263 (96%)	248 (98%)	5 (2%)	55	60
1	J	235/263 (89%)	228 (97%)	7 (3%)	41	44
1	K	224/263 (85%)	217 (97%)	7 (3%)	40	43
1	L	255/263 (97%)	248 (97%)	7 (3%)	44	48
All	All	2998/3156 (95%)	2934 (98%)	64 (2%)	53	59

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	21	ARG
1	A	22	ASP
1	A	58	ASP
1	A	60	ARG
1	A	174	ARG
1	A	203	GLU
1	A	241	ARG
1	A	327	PHE
1	B	14	ARG
1	B	16	SER
1	B	153	ILE
1	B	253	ASN
1	C	21	ARG
1	C	53	ARG
1	C	123	ARG
1	C	235	ARG
1	D	60	ARG
1	D	203	GLU
1	D	241	ARG
1	E	4	GLN
1	E	16	SER
1	E	21	ARG
1	E	89	GLN
1	E	188	LEU

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Mol	Chain	Res	Type
1	E	203	GLU
1	E	323	SER
1	F	21	ARG
1	F	22	ASP
1	F	118	ARG
1	F	249	SER
1	F	283	GLN
1	G	16	SER
1	G	57	ASN
1	G	58	ASP
1	G	60	ARG
1	G	70	GLU
1	G	121	LEU
1	I	16	SER
1	I	53	ARG
1	I	98	LEU
1	I	183	GLU
1	I	241	ARG
1	J	5	ILE
1	J	21	ARG
1	J	33	GLU
1	J	53	ARG
1	J	98	LEU
1	J	121	LEU
1	J	327	PHE
1	K	53	ARG
1	K	109	LYS
1	K	121	LEU
1	K	183	GLU
1	K	241	ARG
1	K	304	ARG
1	K	320	LYS
1	L	18	LEU
1	L	98	LEU
1	L	121	LEU
1	L	241	ARG
1	L	258	ARG
1	L	283	GLN
1	L	327	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	B	253	ASN
1	B	326	ASN
1	C	8	GLN
1	D	57	ASN
1	E	283	GLN
1	F	57	ASN
1	F	283	GLN
1	F	326	ASN
1	G	4	GLN
1	G	8	GLN
1	G	57	ASN
1	G	89	GLN
1	I	4	GLN
1	I	89	GLN
1	I	326	ASN
1	J	302	GLN
1	L	89	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	MES	G	1335	-	12,12,12	2.08	1 (8%)	14,16,16	1.82	4 (28%)
2	MES	F	1335	-	12,12,12	1.96	1 (8%)	14,16,16	6.54	8 (57%)
2	MES	H	1335	-	12,12,12	2.10	1 (8%)	14,16,16	6.81	7 (50%)
2	MES	D	1335	-	12,12,12	1.61	1 (8%)	14,16,16	1.81	4 (28%)
2	MES	I	1335	-	12,12,12	2.03	1 (8%)	14,16,16	6.73	6 (42%)

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	MES	G	1335	-	-	1/6/14/14	0/1/1/1
2	MES	F	1335	-	-	2/6/14/14	0/1/1/1
2	MES	H	1335	-	-	3/6/14/14	0/1/1/1
2	MES	D	1335	-	-	1/6/14/14	0/1/1/1
2	MES	I	1335	-	-	3/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1335	MES	C8-S	-6.73	1.67	1.77
2	G	1335	MES	C8-S	-6.66	1.68	1.77
2	I	1335	MES	C8-S	-6.53	1.68	1.77
2	F	1335	MES	C8-S	-6.06	1.68	1.77
2	D	1335	MES	C8-S	-4.84	1.70	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1335	MES	O1S-S-C8	-16.09	87.54	106.92
2	I	1335	MES	O1S-S-C8	-16.00	87.65	106.92
2	F	1335	MES	O1S-S-C8	-14.07	89.98	106.92
2	H	1335	MES	O3S-S-O1S	-12.55	80.62	111.27
2	I	1335	MES	O3S-S-O1S	-11.19	83.93	111.27
2	F	1335	MES	O2S-S-C8	11.13	120.31	106.92
2	H	1335	MES	O3S-S-C8	9.78	121.58	105.77
2	F	1335	MES	O2S-S-O1S	-9.56	80.85	113.95
2	F	1335	MES	O3S-S-O1S	-9.43	88.23	111.27
2	I	1335	MES	O2S-S-O1S	-9.38	81.50	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1335	MES	O2S-S-C8	8.71	117.40	106.92
2	H	1335	MES	O2S-S-O1S	-8.61	84.15	113.95
2	I	1335	MES	O3S-S-C8	8.34	119.26	105.77
2	F	1335	MES	O3S-S-C8	7.52	117.92	105.77
2	H	1335	MES	O2S-S-C8	6.30	114.50	106.92
2	H	1335	MES	O3S-S-O2S	3.86	120.70	111.27
2	F	1335	MES	O3S-S-O2S	3.79	120.53	111.27
2	I	1335	MES	O3S-S-O2S	3.76	120.45	111.27
2	D	1335	MES	C6-C5-N4	3.45	115.34	110.10
2	G	1335	MES	C6-C5-N4	3.41	115.27	110.10
2	G	1335	MES	C2-C3-N4	3.39	115.24	110.10
2	F	1335	MES	C2-C3-N4	3.12	114.83	110.10
2	F	1335	MES	C6-C5-N4	3.03	114.70	110.10
2	D	1335	MES	C5-N4-C3	2.83	115.19	108.83
2	D	1335	MES	O3S-S-C8	2.57	109.92	105.77
2	G	1335	MES	C5-N4-C3	2.48	114.41	108.83
2	D	1335	MES	C2-C3-N4	2.45	113.82	110.10
2	G	1335	MES	O1S-S-C8	2.21	109.58	106.92
2	H	1335	MES	C6-C5-N4	2.17	113.40	110.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1335	MES	C8-C7-N4-C5
2	G	1335	MES	C8-C7-N4-C5
2	H	1335	MES	N4-C7-C8-S
2	H	1335	MES	C7-C8-S-O3S
2	I	1335	MES	C7-C8-S-O2S
2	F	1335	MES	C7-C8-S-O3S
2	I	1335	MES	N4-C7-C8-S
2	I	1335	MES	C7-C8-S-O3S
2	F	1335	MES	C7-C8-S-O2S
2	H	1335	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1335	MES	2	0
2	I	1335	MES	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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.