



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:30 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

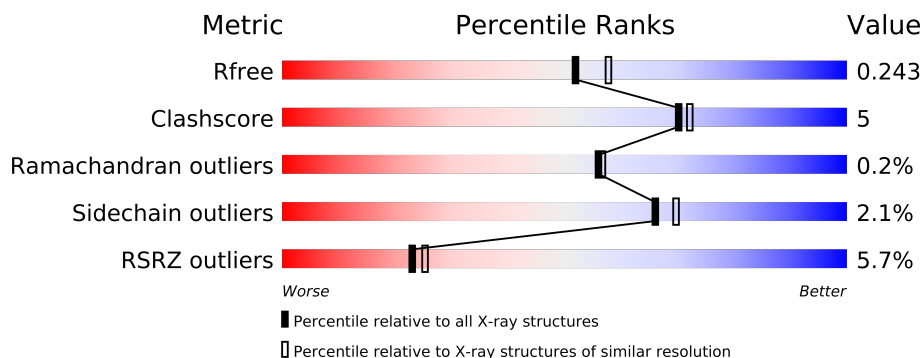
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
1	C	336	
1	D	336	
1	E	336	
1	F	336	
1	G	336	
1	H	336	
1	I	336	
1	J	336	
1	K	336	
1	L	336	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MES	H	1335	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30125 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

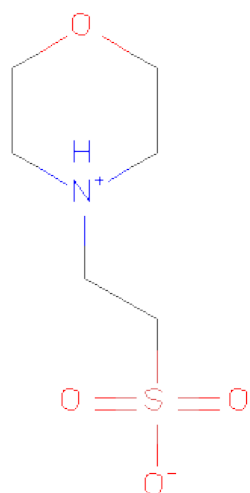
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP B7UV73
A	0	ALA	-	EXPRESSION TAG	UNP B7UV73
B	-1	GLY	-	EXPRESSION TAG	UNP B7UV73
B	0	ALA	-	EXPRESSION TAG	UNP B7UV73
C	-1	GLY	-	EXPRESSION TAG	UNP B7UV73

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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)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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.

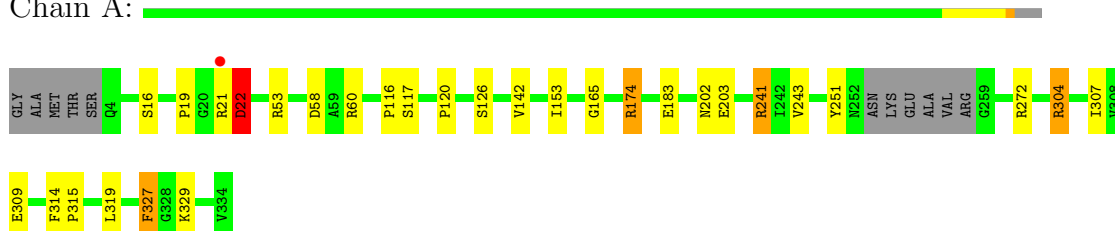
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	88	Total	O	0	0
			88	88		
3	C	77	Total	O	0	0
			77	77		
3	D	141	Total	O	0	0
			141	141		
3	E	132	Total	O	0	0
			132	132		
3	F	55	Total	O	0	0
			55	55		
3	G	87	Total	O	0	0
			87	87		
3	H	36	Total	O	0	0
			36	36		
3	I	48	Total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

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

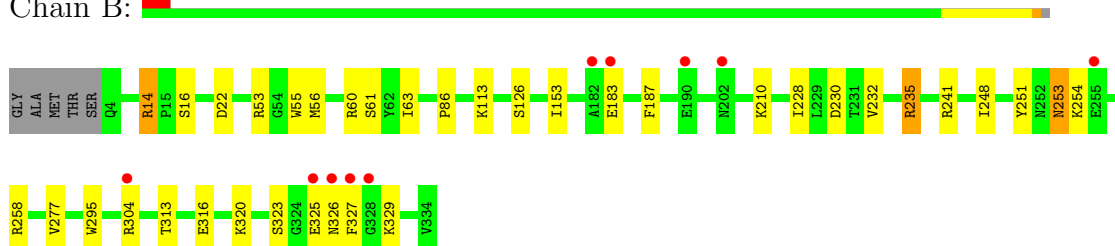
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain A:



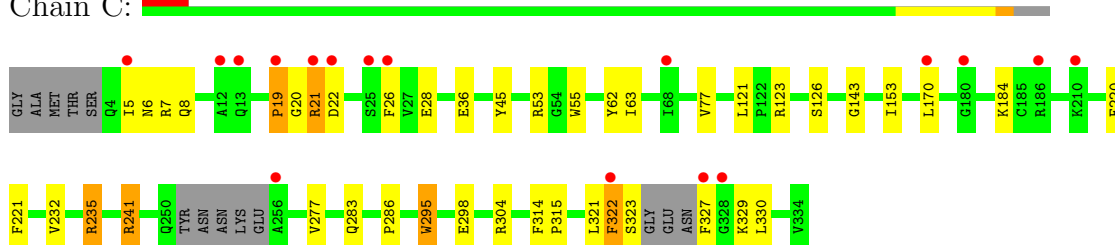
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain B:



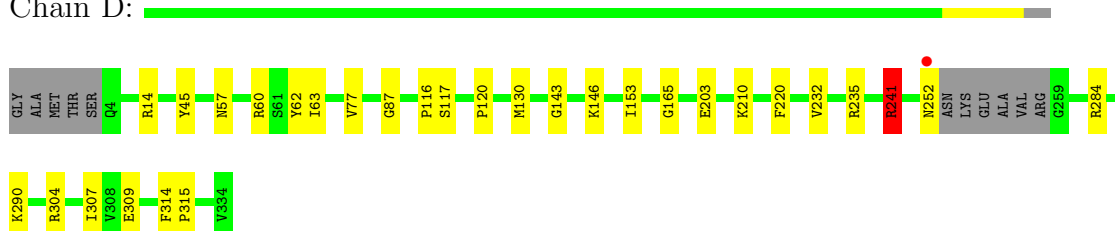
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain C:



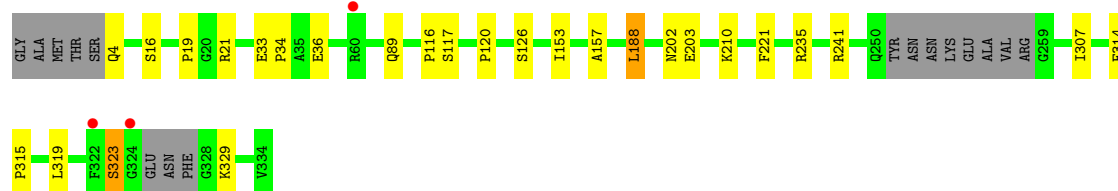
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain D:



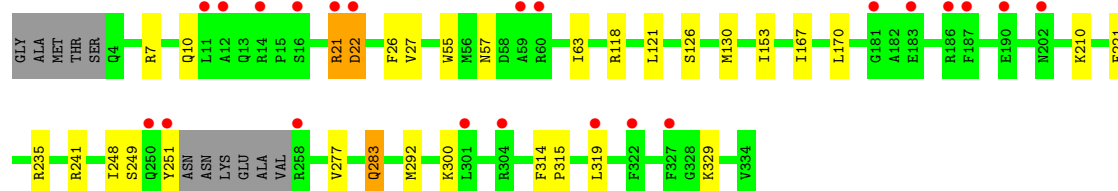
- Molecule 1: PROBABLE OXIDOREDUCTASE

Chain E:



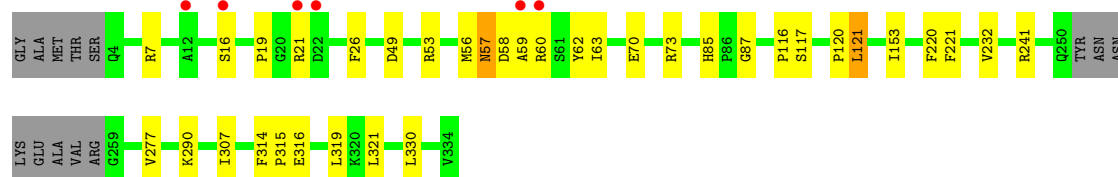
- Molecule 1: PROBABLE OXIDOREDUCTASE

Chain F:



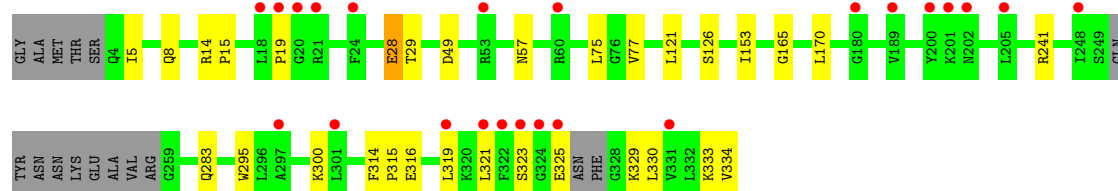
- Molecule 1: PROBABLE OXIDOREDUCTASE

Chain G:



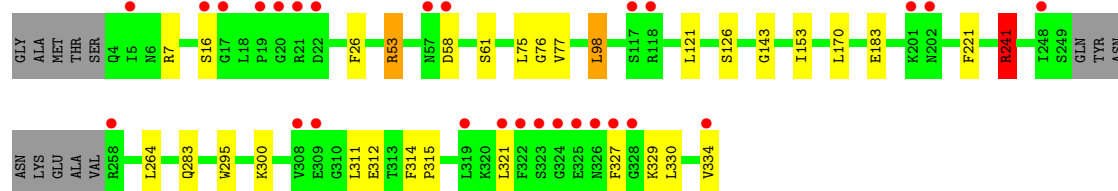
- Molecule 1: PROBABLE OXIDOREDUCTASE

Chain H:

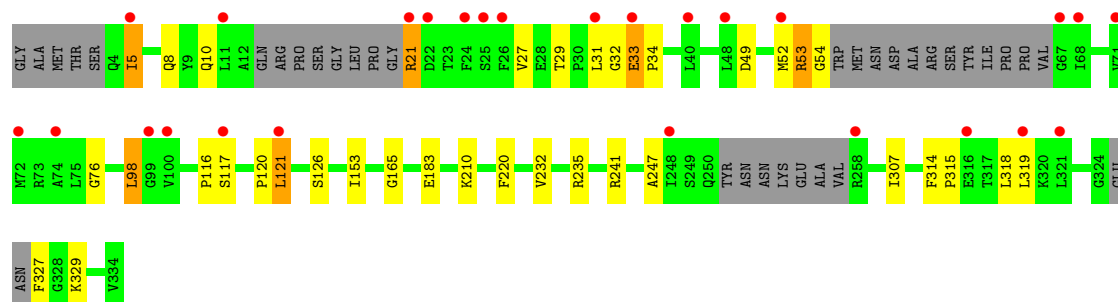


- Molecule 1: PROBABLE OXIDOREDUCTASE

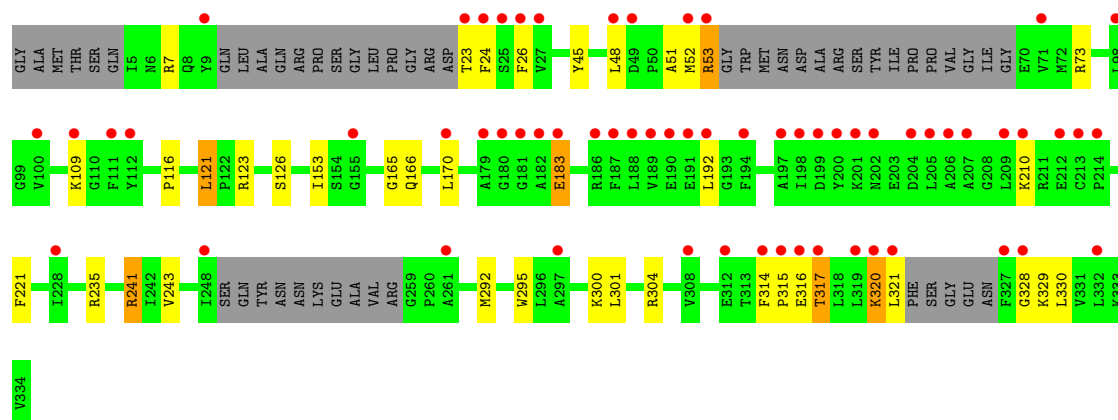
Chain I:



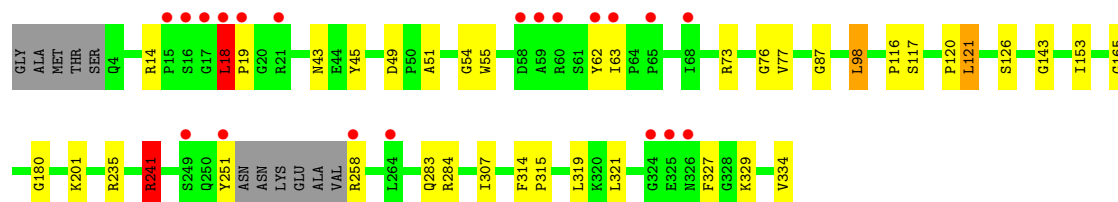
- Molecule 1: PROBABLE OXIDOREDUCTASE

Chain J: 

• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain K: 

• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain L: 

4 Data and refinement statistics

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 73.06 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (73.06-2.10) 99.1 (73.06-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.243 0.225 , 0.243	Depositor DCC
R_{free} test set	16092 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 318881 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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(°)	Ideal(°)
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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (267) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:NE2	1:F:283:GLN:HA	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:B:323:SER:OG	1:B:325:GLU:CB	2.41	0.65
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: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:K:166:GLN:HB2	1:K:301:LEU:CD1	2.29	0.62
1:G:153:ILE:HD13	1:G:221:PHE:HB3	1.79	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:J:52:MET:CE	1:J:318:LEU:HD11	2.29	0.62
1:B:210:LYS:HB2	1:B:235:ARG:HH22	1.64	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:317:THR:O	1:K:317:THR:HG22	2.00	0.61
1:L:76:GLY:C	1:L:98:LEU:HD22	2.20	0.61
1:G:21:ARG:NH1	1:G:316:GLU:OE2	2.33	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:HE21	1:F:283:GLN:HA	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:I:143:GLY:O	1:I:241:ARG:HD2	2.05	0.57
1:G:117:SER:HB2	1:J:307:ILE:CD1	2.35	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:F:57:ASN:HD21	1:F:251:TYR:C	2.09	0.56
1:D:57:ASN:HD21	1:D:252:ASN:HA	1.70	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:N	1:F:22:ASP:OD1	2.39	0.55
1:F:210:LYS:HA	1:F:235:ARG:HH21	1.70	0.55
1:K:321:LEU:HD13	1:K:330:LEU:CD2	2.35	0.54
1:H:153:ILE:CD1	1:H:165:GLY:HA2	2.37	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:G:153:ILE:HD13	1:G:221:PHE:CB	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:210:LYS:HA	1:D:235:ARG:HH21	1.71	0.54
1:E:19:PRO:O	1:E:319:LEU:HD21	2.06	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:A:153:ILE:HD11	1:A:165:GLY:HA2	1.89	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:J:52:MET:HE3	1:J:318:LEU:CD1	2.34	0.53
1:G:277:VAL:HG13	3:G:2071:HOH:O	2.08	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:F:170:LEU:HD21	1:F:300:LYS:HB3	1.92	0.51
1:D:116:PRO:O	1:E:120:PRO:HB3	2.11	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:K:153:ILE:CD1	1:K:165:GLY:HA2	2.41	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:B:53:ARG:HA	1:B:56:MET:HE3	1.93	0.50
1:J:33:GLU:CG	1:J:34:PRO:HD2	2.40	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: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:J:52:MET:HE1	1:J:318:LEU:CD1	2.43	0.49
1:B:304:ARG:HH12	1:B:327:PHE:HD2	1.61	0.49
1:C:153:ILE:HD13	1:C:221:PHE:CB	2.43	0.49
1:A:153:ILE:CD1	1:A:165:GLY:HA2	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:K:170:LEU:CD2	1:K:300:LYS:HB3	2.44	0.47
1:F:277:VAL:HG13	3:F:2047:HOH:O	2.14	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:K:210:LYS:HA	1:K:235:ARG:HH21	1.78	0.47
1:I:58:ASP:HB3	1:I:61:SER:OG	2.15	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:H:153:ILE:CD1	1:H:165:GLY:CA	2.93	0.46
1:B:228:ILE:O	1:B:232:VAL:HG23	2.15	0.46
1:H:75:LEU:HD12	2:H:1335:MES:O2S	2.16	0.46
1:B:183:GLU:OE1	1:B:183:GLU:HA	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: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:D:130:MET:HA	1:D:130:MET:CE	2.47	0.45
1:L:43:ASN:O	1:L:334:VAL:HG23	2.17	0.45
1:K:166:GLN:CB	1:K:301:LEU:HD13	2.47	0.45
1:I:153:ILE:HD13	1:I:221:PHE:CB	2.46	0.45
1:C:77:VAL:HG11	1:C:121:LEU:HD22	1.99	0.45
1:K:7:ARG:HD2	1:K:26:PHE:HZ	1.82	0.45
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:75:LEU:HD22	2:I:1335:MES:O2S	2.17	0.44
1:G:63:ILE:HG22	1:G:73:ARG:NH1	2.32	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: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:48:LEU:HD11	1:K:317:THR:O	2.18	0.44
1:G:7:ARG:HD2	1:G:26:PHE:HZ	1.83	0.44
1:K:292:MET:SD	1:K:301:LEU:CD2	3.05	0.44
1:B:277:VAL:HG13	3:B:2073:HOH:O	2.17	0.44
1:K:320:LYS:HE3	1:K:320:LYS:HB2	1.72	0.44
1:D:117:SER:HB2	1:E:307:ILE:CD1	2.48	0.43
1:I:7:ARG:HD2	1:I:26:PHE:HZ	1.82	0.43
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.17	0.43
1:G:220:PHE:CG	1:G:232:VAL:HG11	2.52	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:A:126:SER:HB3	1:A:329:LYS:HG2	2.00	0.43
1:H:8:GLN:OE1	1:H:29:THR:HG21	2.19	0.43
1:E:157:ALA:HA	1:E:188:LEU:HD11	2.00	0.43
1:G:19:PRO:O	1:G:319:LEU:HD21	2.19	0.43
1:C:7:ARG:HD2	1:C:26:PHE:HZ	1.82	0.43
1:L:51:ALA:HA	1:L:251:TYR:CZ	2.53	0.43
1:F:130:MET:HA	1:F:130:MET:HE2	2.00	0.43
1:D:290:LYS:HE2	3:G:2030:HOH:O	2.18	0.43
1:E:153:ILE:HD13	1:E:221:PHE:CB	2.49	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: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:J:116:PRO:HB3	1:J:121:LEU:CD1	2.48	0.43
1:H:153:ILE:HD13	1:H:165:GLY:CA	2.49	0.43
1:J:183:GLU:OE1	1:J:183:GLU:HA	2.18	0.42
1:H:314:PHE:HB3	1:H:315:PRO:HD3	2.01	0.42
1:H:126:SER:HB3	1:H:329:LYS:HG2	2.01	0.42
1:J:126:SER:HB3	1:J:329:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:314:PHE:HB3	1:C:315:PRO:HD3	2.01	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:K:126:SER:HB3	1:K:329:LYS:HG2	2.01	0.42
1:E:314:PHE:HB3	1:E:315:PRO:HD3	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:H:49:ASP:C	1:H:321:LEU:HD21	2.41	0.42
1:G:116:PRO:HB3	1:G:121:LEU:HD11	2.02	0.42
1:D:87:GLY:CA	1:H:283:GLN:HA	2.50	0.42
1:K:116:PRO:HB3	1:K:121:LEU:HD13	2.01	0.42
1:F:126:SER:HB3	1:F:329:LYS:HG2	2.01	0.42
1:C:277:VAL:HG13	3:C:2066:HOH:O	2.18	0.42
1:A:314:PHE:HB3	1:A:315:PRO:HD3	2.01	0.41
1:I:283:GLN:HA	1:L:87:GLY:CA	2.48	0.41
1:B:53:ARG:HD2	1:B:53:ARG:HA	1.87	0.41
1:I:264:LEU:HD11	1:J:247:ALA:CB	2.50	0.41
1:K:116:PRO:HB3	1:K:121:LEU:CD1	2.49	0.41
1:K:314:PHE:HB3	1:K:315:PRO:HD3	2.02	0.41
1:K:221:PHE:HA	1:K:243:VAL:HG13	2.02	0.41
1:L:126:SER:HB3	1:L:329:LYS:HG2	2.02	0.41
1:D:45:TYR:HB2	1:D:77:VAL:CG2	2.50	0.41
1:L:55:TRP:NE1	1:L:63:ILE:HD12	2.34	0.41
1:E:126:SER:HB3	1:E:329:LYS:HG2	2.01	0.41
1:K:292:MET:SD	1:K:301:LEU:HD23	2.60	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:L:62:TYR:CD2	1:L:63:ILE:HG13	2.56	0.41
1:J:8:GLN:OE1	1:J:29:THR:HG21	2.21	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:L:49:ASP:C	1:L:321:LEU:HD21	2.41	0.41
1:I:311:LEU:HB2	1:I:334:VAL:HG13	2.03	0.41
1:L:54:GLY:HA3	1:L:251:TYR:CE1	2.55	0.41
1:F:10:GLN:NE2	1:F:27:VAL:HG21	2.36	0.41
1:D:62:TYR:CD2	1:D:63:ILE:HG13	2.56	0.41
1:K:166:GLN:CB	1:K:301:LEU:HD12	2.49	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:J:116:PRO:HB3	1:J:121:LEU:HD11	2.03	0.41
1:L:19:PRO:O	1:L:319:LEU:HD21	2.21	0.41
1:K:51:ALA:O	1:K:53:ARG:N	2.54	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: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: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:A:307:ILE:CD1	1:L:117:SER:CB	2.99	0.40
1:C:220:PHE:CG	1:C:232:VAL:HG11	2.56	0.40
1:K:51:ALA:HB1	1:K:73:ARG:HH22	1.86	0.40
1:D:307:ILE:CD1	1:E:117:SER:HB3	2.51	0.40
1:B:126:SER:HB3	1:B:329:LYS:HG2	2.02	0.40
1:J:32:GLY:O	1:J:33:GLU:HB2	2.22	0.40
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.93	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	Distance(Å)	Clash(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

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	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%)	33	28
1	D	321/336 (96%)	317 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	314/336 (94%)	309 (98%)	4 (1%)	1 (0%)	50	49
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%)	50	49
1	J	292/336 (87%)	286 (98%)	5 (2%)	1 (0%)	50	49
1	K	276/336 (82%)	269 (98%)	6 (2%)	1 (0%)	43	39
1	L	321/336 (96%)	316 (98%)	5 (2%)	0	100	100
All	All	3765/4032 (93%)	3697 (98%)	62 (2%)	6 (0%)	56	57

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 ⓘ

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%)	48	48
1	B	261/263 (99%)	257 (98%)	4 (2%)	76	81
1	C	252/263 (96%)	248 (98%)	4 (2%)	75	79
1	D	255/263 (97%)	252 (99%)	3 (1%)	82	87
1	E	250/263 (95%)	243 (97%)	7 (3%)	56	59
1	F	255/263 (97%)	250 (98%)	5 (2%)	68	72
1	G	253/263 (96%)	247 (98%)	6 (2%)	61	65
1	H	250/263 (95%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	253/263 (96%)	248 (98%)	5 (2%)	68	72
1	J	235/263 (89%)	228 (97%)	7 (3%)	53	55
1	K	224/263 (85%)	217 (97%)	7 (3%)	52	54
1	L	255/263 (97%)	248 (97%)	7 (3%)	57	60
All	All	2998/3156 (95%)	2934 (98%)	64 (2%)	66	70

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
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

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Mol	Chain	Res	Type
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

Some 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

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Mol	Chain	Res	Type
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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	D	1335	-	12,12,12	1.39	1 (8%)	16,16,16	2.01	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	F	1335	-	12,12,12	1.84	2 (16%)	16,16,16	5.46	8 (50%)
2	MES	G	1335	-	12,12,12	1.83	1 (8%)	16,16,16	1.95	5 (31%)
2	MES	H	1335	-	12,12,12	1.96	1 (8%)	16,16,16	5.43	7 (43%)
2	MES	I	1335	-	12,12,12	1.90	2 (16%)	16,16,16	5.45	7 (43%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1335	MES	C8-S	-5.81	1.67	1.78
2	G	1335	MES	C8-S	-5.75	1.68	1.78
2	I	1335	MES	C8-S	-5.65	1.68	1.78
2	F	1335	MES	C8-S	-5.27	1.68	1.78
2	D	1335	MES	C8-S	-4.29	1.70	1.78
2	F	1335	MES	O1S-S	2.18	1.50	1.45
2	I	1335	MES	O3S-S	2.12	1.50	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1335	MES	O2S-S-O1S	-16.38	80.85	112.44
2	I	1335	MES	O2S-S-O1S	-16.04	81.50	112.44
2	H	1335	MES	O2S-S-O1S	-14.67	84.15	112.44
2	H	1335	MES	O3S-S-O1S	-12.39	80.62	112.48
2	I	1335	MES	O3S-S-O1S	-11.10	83.93	112.48
2	F	1335	MES	O3S-S-O1S	-9.43	88.23	112.48
2	H	1335	MES	O1S-S-C8	-6.11	87.54	106.36
2	I	1335	MES	O1S-S-C8	-6.07	87.65	106.36
2	H	1335	MES	O3S-S-C8	6.04	121.58	105.99
2	F	1335	MES	O1S-S-C8	-5.31	89.98	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1335	MES	O3S-S-C8	5.14	119.26	105.99
2	F	1335	MES	O3S-S-C8	4.62	117.92	105.99
2	F	1335	MES	O2S-S-C8	4.53	120.31	106.36
2	D	1335	MES	C6-C5-N4	4.19	115.34	109.96
2	G	1335	MES	C6-C5-N4	4.14	115.27	109.96
2	G	1335	MES	C2-C3-N4	4.11	115.24	109.96
2	F	1335	MES	C2-C3-N4	3.80	114.83	109.96
2	F	1335	MES	C6-C5-N4	3.70	114.70	109.96
2	I	1335	MES	O2S-S-C8	3.58	117.40	106.36
2	D	1335	MES	O1-C2-C3	-3.21	107.51	111.34
2	H	1335	MES	O3S-S-O2S	3.20	120.70	112.48
2	F	1335	MES	O3S-S-O2S	3.13	120.53	112.48
2	I	1335	MES	O3S-S-O2S	3.10	120.45	112.48
2	D	1335	MES	C2-C3-N4	3.01	113.82	109.96
2	D	1335	MES	C8-C7-N4	3.00	117.58	112.44
2	D	1335	MES	C5-N4-C3	2.74	115.19	109.75
2	H	1335	MES	C6-C5-N4	2.68	113.40	109.96
2	H	1335	MES	O2S-S-C8	2.64	114.50	106.36
2	G	1335	MES	C8-C7-N4	2.55	116.80	112.44
2	G	1335	MES	C5-N4-C3	2.35	114.41	109.75
2	D	1335	MES	O3S-S-O2S	-2.23	106.76	112.48
2	G	1335	MES	O1-C2-C3	-2.20	108.72	111.34
2	I	1335	MES	C6-C5-N4	2.05	112.60	109.96

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1335	MES	C2-C3-C5-C6-N4-O1
2	H	1335	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	325/336 (96%)	0.22	1 (0%) 91 94	20, 31, 66, 88	0
1	B	331/336 (98%)	0.15	10 (3%) 48 53	27, 42, 70, 102	0
1	C	323/336 (96%)	0.24	17 (5%) 25 28	26, 46, 77, 98	0
1	D	325/336 (96%)	0.06	1 (0%) 91 94	21, 32, 53, 73	0
1	E	320/336 (95%)	0.25	3 (0%) 81 85	20, 30, 61, 93	0
1	F	325/336 (96%)	0.38	22 (6%) 17 19	30, 49, 80, 101	0
1	G	323/336 (96%)	0.20	6 (1%) 64 68	23, 42, 77, 100	0
1	H	320/336 (95%)	0.37	23 (7%) 15 17	31, 54, 82, 102	0
1	I	323/336 (96%)	0.48	27 (8%) 11 12	33, 53, 83, 117	0
1	J	302/336 (89%)	0.49	26 (8%) 11 11	27, 45, 83, 109	0
1	K	286/336 (85%)	1.14	62 (21%) 1 1	39, 66, 99, 115	0
1	L	325/336 (96%)	0.21	20 (6%) 20 22	25, 39, 80, 118	0
All	All	3828/4032 (94%)	0.34	218 (5%) 23 25	20, 44, 81, 118	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	PHE	7.1
1	K	319	LEU	6.3
1	I	327	PHE	6.1
1	J	67	GLY	5.8
1	I	21	ARG	5.7
1	J	68	ILE	5.6
1	K	24	PHE	5.4
1	J	11	LEU	5.3
1	I	324	GLY	5.1
1	K	191	GLU	4.9
1	J	24	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	205	LEU	4.8
1	F	327	PHE	4.7
1	K	198	ILE	4.7
1	I	323	SER	4.6
1	L	258	ARG	4.5
1	H	248	ILE	4.4
1	H	323	SER	4.4
1	K	25	SER	4.4
1	I	326	ASN	4.4
1	I	248	ILE	4.3
1	K	200	TYR	4.2
1	L	21	ARG	4.2
1	K	52	MET	4.2
1	C	21	ARG	4.2
1	H	21	ARG	4.1
1	K	26	PHE	4.1
1	K	209	LEU	4.0
1	J	319	LEU	3.9
1	K	155	GLY	3.9
1	K	228	ILE	3.9
1	L	324	GLY	3.9
1	F	21	ARG	3.8
1	J	21	ARG	3.7
1	L	59	ALA	3.7
1	H	18	LEU	3.7
1	K	202	ASN	3.7
1	K	214	PRO	3.6
1	K	327	PHE	3.6
1	F	251	TYR	3.6
1	K	201	LYS	3.6
1	K	112	TYR	3.6
1	K	49	ASP	3.6
1	J	71	VAL	3.5
1	I	325	GLU	3.5
1	J	26	PHE	3.5
1	J	52	MET	3.5
1	K	248	ILE	3.5
1	B	255	GLU	3.5
1	K	213	CYS	3.5
1	K	27	VAL	3.5
1	I	319	LEU	3.4
1	C	327	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	207	ALA	3.4
1	K	206	ALA	3.4
1	G	21	ARG	3.4
1	A	21	ARG	3.3
1	J	25	SER	3.3
1	I	19	PRO	3.3
1	E	60	ARG	3.3
1	K	199	ASP	3.3
1	C	328	GLY	3.3
1	K	321	LEU	3.3
1	H	319	LEU	3.2
1	C	186	ARG	3.2
1	H	60	ARG	3.2
1	F	319	LEU	3.2
1	F	12	ALA	3.2
1	K	312	GLU	3.1
1	K	170	LEU	3.1
1	L	58	ASP	3.1
1	K	182	ALA	3.1
1	K	23	THR	3.1
1	C	26	PHE	3.1
1	L	18	LEU	3.1
1	L	60	ARG	3.1
1	C	210	LYS	3.1
1	I	322	PHE	3.0
1	K	71	VAL	3.0
1	K	194	PHE	3.0
1	K	186	ARG	3.0
1	L	325	GLU	3.0
1	C	25	SER	3.0
1	I	308	VAL	3.0
1	K	317	THR	3.0
1	K	180	GLY	3.0
1	G	12	ALA	3.0
1	K	204	ASP	2.9
1	L	17	GLY	2.9
1	K	197	ALA	2.9
1	K	261	ALA	2.9
1	L	63	ILE	2.9
1	I	20	GLY	2.9
1	K	181	GLY	2.9
1	K	188	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	16	SER	2.9
1	C	19	PRO	2.9
1	I	201	LYS	2.8
1	J	248	ILE	2.8
1	I	22	ASP	2.8
1	H	189	VAL	2.8
1	K	189	VAL	2.8
1	K	332	LEU	2.8
1	K	183	GLU	2.8
1	F	202	ASN	2.8
1	K	53	ARG	2.8
1	H	202	ASN	2.7
1	K	192	LEU	2.7
1	K	210	LYS	2.7
1	J	258	ARG	2.7
1	K	187	PHE	2.7
1	B	182	ALA	2.7
1	G	60	ARG	2.7
1	K	315	PRO	2.7
1	C	5	ILE	2.7
1	B	190	GLU	2.6
1	I	16	SER	2.6
1	K	314	PHE	2.6
1	H	201	LYS	2.6
1	G	59	ALA	2.6
1	B	183	GLU	2.6
1	J	99	GLY	2.6
1	L	326	ASN	2.6
1	I	258	ARG	2.6
1	H	53	ARG	2.6
1	H	324	GLY	2.5
1	I	328	GLY	2.5
1	L	19	PRO	2.5
1	B	304	ARG	2.5
1	C	22	ASP	2.5
1	H	205	LEU	2.5
1	H	321	LEU	2.5
1	H	20	GLY	2.5
1	F	258	ARG	2.5
1	K	212	GLU	2.5
1	L	15	PRO	2.5
1	J	74	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	297	ALA	2.5
1	F	301	LEU	2.5
1	K	316	GLU	2.5
1	I	117	SER	2.4
1	J	40	LEU	2.4
1	J	100	VAL	2.4
1	F	60	ARG	2.4
1	J	31	LEU	2.4
1	J	121	LEU	2.4
1	H	331	VAL	2.4
1	J	72	MET	2.4
1	L	264	LEU	2.4
1	K	98	LEU	2.4
1	K	9	TYR	2.4
1	B	325	GLU	2.4
1	L	251	TYR	2.3
1	J	316	GLU	2.3
1	C	180	GLY	2.3
1	F	187	PHE	2.3
1	J	5	ILE	2.3
1	H	322	PHE	2.3
1	F	190	GLU	2.3
1	I	321	LEU	2.3
1	I	309	GLU	2.3
1	C	68	ILE	2.3
1	F	186	ARG	2.3
1	K	179	ALA	2.3
1	J	117	SER	2.3
1	I	118	ARG	2.3
1	F	181	GLY	2.3
1	J	48	LEU	2.3
1	K	328	GLY	2.3
1	F	59	ALA	2.3
1	F	304	ARG	2.3
1	B	328	GLY	2.2
1	H	297	ALA	2.2
1	H	24	PHE	2.2
1	J	321	LEU	2.2
1	C	256	ALA	2.2
1	E	324	GLY	2.2
1	L	62	TYR	2.2
1	C	322	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	111	PHE	2.2
1	J	33	GLU	2.2
1	H	301	LEU	2.2
1	F	14	ARG	2.2
1	K	308	VAL	2.2
1	F	16	SER	2.2
1	F	22	ASP	2.2
1	J	22	ASP	2.2
1	H	19	PRO	2.2
1	H	180	GLY	2.1
1	L	68	ILE	2.1
1	K	320	LYS	2.1
1	C	170	LEU	2.1
1	F	250	GLN	2.1
1	L	16	SER	2.1
1	E	322	PHE	2.1
1	K	48	LEU	2.1
1	D	252	ASN	2.1
1	F	183	GLU	2.1
1	K	190	GLU	2.1
1	I	58	ASP	2.1
1	F	322	PHE	2.1
1	H	325	GLU	2.1
1	B	202	ASN	2.1
1	I	202	ASN	2.1
1	I	334	VAL	2.1
1	K	100	VAL	2.1
1	L	249	SER	2.1
1	C	12	ALA	2.0
1	H	200	TYR	2.0
1	I	5	ILE	2.0
1	K	109	LYS	2.0
1	L	65	PRO	2.0
1	G	22	ASP	2.0
1	B	326	ASN	2.0
1	I	57	ASN	2.0
1	F	11	LEU	2.0
1	C	13	GLN	2.0
1	I	17	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MES	H	1335	12/12	0.19	2.47	73,75,77,78	0
2	MES	F	1335	12/12	0.13	0.34	41,51,52,53	0
2	MES	I	1335	12/12	0.14	0.12	61,65,73,73	0
2	MES	D	1335	12/12	0.11	-0.60	28,32,33,34	0
2	MES	G	1335	12/12	0.10	-0.78	40,41,41,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.