Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2020 – 09:24 AM BST

PDB ID	:	5JQL
Title	:	Crystal Structure of Phosphatidic acid Transporter Ups1/Mdm35 Void of Bound Phospholipid from Saccharomyces Cerevisiae at 2.9 Angstroms Resolution
Authors	:	Lu, J.; Chan, K.C.; Zhai, Y.; Fan, J.; Sun, F.
Deposited on	:	2016-05-05
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.14.6
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)	:	2.14.6

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
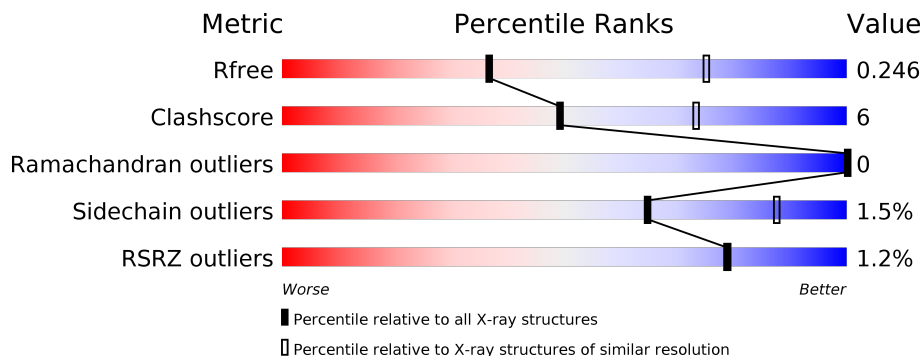
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	189	78% 12% · 10%
1	E	189	68% 19% · 12%
1	I	189	75% 9% · 15%
1	K	189	71% 15% · 13%
2	B	86	78% 5% · 16%
2	D	86	80% 6% 14%

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Mol	Chain	Length	Quality of chain
2	F	86	77% 7% 16%
2	J	86	3% 71% 12% 17%
2	L	86	71% 12% 17%
3	C	189	79% 12% 10%
4	G	189	77% 12% 11%
5	H	86	76% 7% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11018 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 Protein UPS1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	Se	0	0	0
			1278	814	218	241	1	4			
1	E	166	Total	C	N	O	S	Se	0	0	0
			1272	807	222	238	1	4			
1	I	160	Total	C	N	O	S	Se	0	0	0
			1229	779	218	227	1	4			
1	K	164	Total	C	N	O	S	Se	0	0	0
			1262	807	215	235	1	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q05776
A	-12	GLY	-	expression tag	UNP Q05776
A	-11	SER	-	expression tag	UNP Q05776
A	-10	SER	-	expression tag	UNP Q05776
A	-9	HIS	-	expression tag	UNP Q05776
A	-8	HIS	-	expression tag	UNP Q05776
A	-7	HIS	-	expression tag	UNP Q05776
A	-6	HIS	-	expression tag	UNP Q05776
A	-5	HIS	-	expression tag	UNP Q05776
A	-4	HIS	-	expression tag	UNP Q05776
A	-3	SER	-	expression tag	UNP Q05776
A	-2	GLN	-	expression tag	UNP Q05776
A	-1	ASP	-	expression tag	UNP Q05776
A	0	PRO	-	expression tag	UNP Q05776
E	-13	MET	-	expression tag	UNP Q05776
E	-12	GLY	-	expression tag	UNP Q05776
E	-11	SER	-	expression tag	UNP Q05776
E	-10	SER	-	expression tag	UNP Q05776
E	-9	HIS	-	expression tag	UNP Q05776
E	-8	HIS	-	expression tag	UNP Q05776
E	-7	HIS	-	expression tag	UNP Q05776

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	HIS	-	expression tag	UNP Q05776
E	-5	HIS	-	expression tag	UNP Q05776
E	-4	HIS	-	expression tag	UNP Q05776
E	-3	SER	-	expression tag	UNP Q05776
E	-2	GLN	-	expression tag	UNP Q05776
E	-1	ASP	-	expression tag	UNP Q05776
E	0	PRO	-	expression tag	UNP Q05776
I	-13	MET	-	expression tag	UNP Q05776
I	-12	GLY	-	expression tag	UNP Q05776
I	-11	SER	-	expression tag	UNP Q05776
I	-10	SER	-	expression tag	UNP Q05776
I	-9	HIS	-	expression tag	UNP Q05776
I	-8	HIS	-	expression tag	UNP Q05776
I	-7	HIS	-	expression tag	UNP Q05776
I	-6	HIS	-	expression tag	UNP Q05776
I	-5	HIS	-	expression tag	UNP Q05776
I	-4	HIS	-	expression tag	UNP Q05776
I	-3	SER	-	expression tag	UNP Q05776
I	-2	GLN	-	expression tag	UNP Q05776
I	-1	ASP	-	expression tag	UNP Q05776
I	0	PRO	-	expression tag	UNP Q05776
K	-13	MET	-	expression tag	UNP Q05776
K	-12	GLY	-	expression tag	UNP Q05776
K	-11	SER	-	expression tag	UNP Q05776
K	-10	SER	-	expression tag	UNP Q05776
K	-9	HIS	-	expression tag	UNP Q05776
K	-8	HIS	-	expression tag	UNP Q05776
K	-7	HIS	-	expression tag	UNP Q05776
K	-6	HIS	-	expression tag	UNP Q05776
K	-5	HIS	-	expression tag	UNP Q05776
K	-4	HIS	-	expression tag	UNP Q05776
K	-3	SER	-	expression tag	UNP Q05776
K	-2	GLN	-	expression tag	UNP Q05776
K	-1	ASP	-	expression tag	UNP Q05776
K	0	PRO	-	expression tag	UNP Q05776

- Molecule 2 is a protein called Mitochondrial distribution and morphology protein 35.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	72	Total 529	C 343	N 85	O 96	S 5	0	0	0
2	D	74	Total 577	C 367	N 93	O 112	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	72	Total	C	N	O	S	0	0	0
			568	360	90	113	5			
2	J	71	Total	C	N	O	S	0	0	0
			535	342	86	103	4			
2	L	71	Total	C	N	O	S	0	0	0
			553	354	88	106	5			

- Molecule 3 is a protein called Protein UPS1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	171	Total	C	N	O	Se	0	0	0
			1328	842	232	249	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	expression tag	UNP Q05776
C	-12	GLY	-	expression tag	UNP Q05776
C	-11	SER	-	expression tag	UNP Q05776
C	-10	SER	-	expression tag	UNP Q05776
C	-9	HIS	-	expression tag	UNP Q05776
C	-8	HIS	-	expression tag	UNP Q05776
C	-7	HIS	-	expression tag	UNP Q05776
C	-6	HIS	-	expression tag	UNP Q05776
C	-5	HIS	-	expression tag	UNP Q05776
C	-4	HIS	-	expression tag	UNP Q05776
C	-3	SER	-	expression tag	UNP Q05776
C	-2	GLN	-	expression tag	UNP Q05776
C	-1	ASP	-	expression tag	UNP Q05776
C	0	PRO	-	expression tag	UNP Q05776
C	1	MSE	-	expression tag	UNP Q05776

- Molecule 4 is a protein called Protein UPS1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	169	Total	C	N	O	Se	0	0	0
			1327	842	229	251	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	expression tag	UNP Q05776

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	GLY	-	expression tag	UNP Q05776
G	-11	SER	-	expression tag	UNP Q05776
G	-10	SER	-	expression tag	UNP Q05776
G	-9	HIS	-	expression tag	UNP Q05776
G	-8	HIS	-	expression tag	UNP Q05776
G	-7	HIS	-	expression tag	UNP Q05776
G	-6	HIS	-	expression tag	UNP Q05776
G	-5	HIS	-	expression tag	UNP Q05776
G	-4	HIS	-	expression tag	UNP Q05776
G	-3	SER	-	expression tag	UNP Q05776
G	-2	GLN	-	expression tag	UNP Q05776
G	-1	ASP	-	expression tag	UNP Q05776
G	0	PRO	-	expression tag	UNP Q05776
G	1	MSE	-	expression tag	UNP Q05776

- Molecule 5 is a protein called Mitochondrial distribution and morphology protein 35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
5	H	71	560	357	89	109	4	1	0	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Protein UPS1, mitochondrial
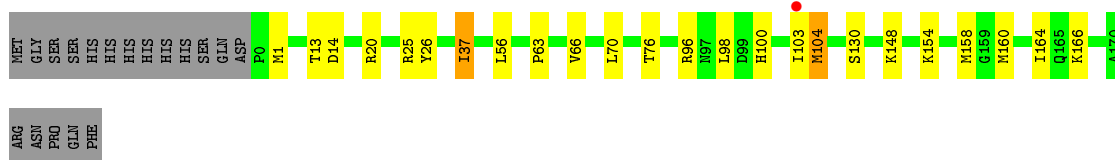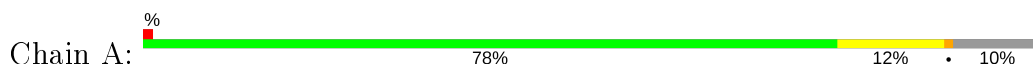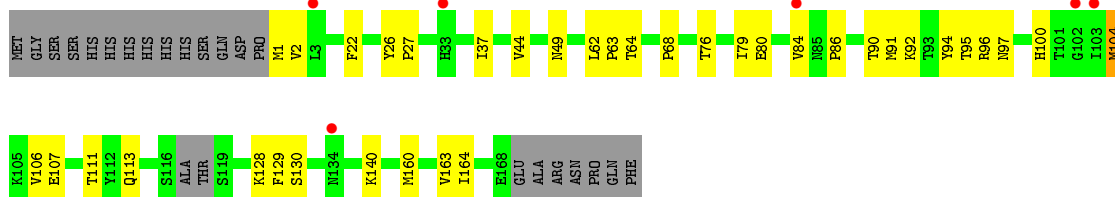
• Molecule 1: Protein UPS1, mitochondrial

• Molecule 1: Protein UPS1, mitochondrial

• Molecule 1: Protein UPS1, mitochondrial

Q113 S130 SER GLY PHE ASN MET G136 K140 R146 M158 V163 E168 GLU ALA ARG ASN PRO GLN PHE

• Molecule 2: Mitochondrial distribution and morphology protein 35

Chain B: 78%   5%   ·   16%

MET GLY ASN I4 S29 S43 A55 V58 A69 F75 GLU ASN GLY GLY LYS LEU LYS GLU VAL ASP LYS

• Molecule 2: Mitochondrial distribution and morphology protein 35

Chain D: %   80%   6%   14%

MET GLY ASN I4 K17 L33 V38 Y49 N54 V58 N77 GLY GLY LYS LEU LYS GLU VAL ASP LYS

• Molecule 2: Mitochondrial distribution and morphology protein 35

Chain F: 77%   7%   16%

MET GLY ASN I4 M5 S6 K17 K31 F32 L33 S37 Y49 F75 GLU ASN GLY GLY LYS LEU LYS GLU VAL ASP LYS

• Molecule 2: Mitochondrial distribution and morphology protein 35

Chain J: 3%   71%   12%   17%

MET GLY ASN ILE M5 S6 K17 L33 T50 N54 A55 A56 L57 V58 K59 Q60 G61 I62 F75 GLU ASN GLY GLY LYS LEU LYS GLU VAL ASP LYS

• Molecule 2: Mitochondrial distribution and morphology protein 35

Chain L: 71%   12%   17%

MET GLY ASN ILE M5 F9 W46 T50 N54 L57 V58 K59 Q60 G61 I62 F75 GLU ASN GLY GLY LYS LEU LYS GLU VAL ASP LYS
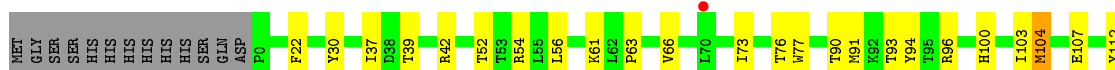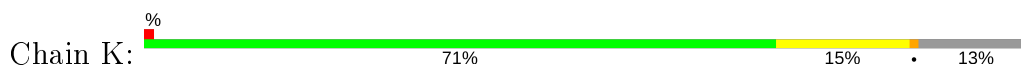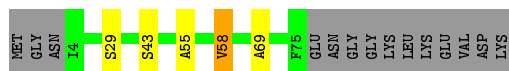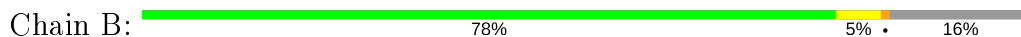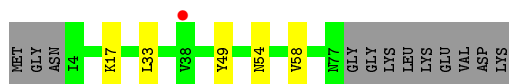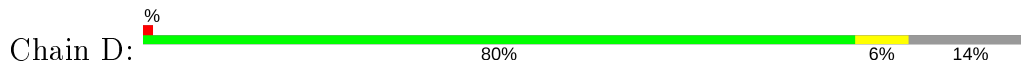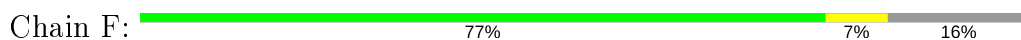
• Molecule 3: Protein UPS1, mitochondrial

Chain C: 79%   12%   10%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER GLN ASP P0 F22 R25 R42 T52 L55 P63 T64 W65 V66 K67 P68 F69 L70 R71 T74 E75 V84 M91 K92 T93 Y94 T95 R96 I137 W144 R157 M158 A170 ARG ASN PRO GLN PHE
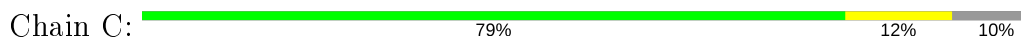
• Molecule 4: Protein UPS1, mitochondrial

Chain G: 77%   12%   ·   11%

MET GLY SER HIS HIS HIS HIS HIS SER GLN ASP P0 F22 F23 Y30 I37 R54 L55 L56 L62 P63 T64 P68 F69 L70 R71 T74 E75 M91 I103 M104 T110 D124 I137 K148 M158 V163 K166 L167 E168 GLU ALA

ARG ASN PRO GLN PHE
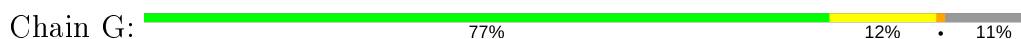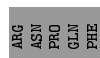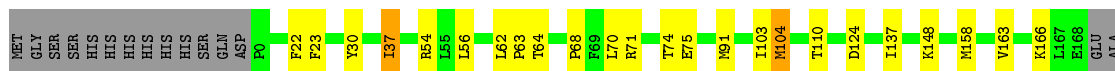
• Molecule 5: Mitochondrial distribution and morphology protein 35

Chain H:

76%   7%   17%

MET GLY ASN ILE M5 S6 S37 VAL GLU N40 W46 T50 A55 V58 N77 GLY GLY LYS LEU LYS GLU VAL ASP LYS
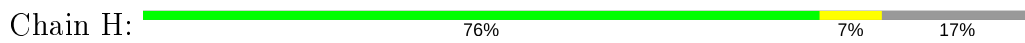
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.31Å 130.74Å 84.27Å 90.00° 103.09° 90.00°	Depositor
Resolution (Å)	48.40 – 2.90 48.40 – 2.87	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.40-2.90) 94.2 (48.40-2.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.98 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.200 , 0.248 0.200 , 0.246	Depositor DCC
R_{free} test set	1950 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.0	EDS
L-test for twinning[2]	$<|L|>$ = 0.48, $<L^2>$ = 0.31	Xtriage
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11018	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

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	0.49	0/1303	0.63	0/1770
1	E	0.47	0/1295	0.66	0/1753
1	I	0.48	0/1253	0.66	0/1694
1	K	0.45	0/1288	0.61	0/1744
2	B	0.57	0/543	0.66	0/738
2	D	0.63	0/591	0.64	0/799
2	F	0.43	0/582	0.55	0/785
2	J	0.56	0/549	0.65	0/746
2	L	0.48	0/567	0.63	0/768
3	C	0.55	0/1353	0.68	0/1828
4	G	0.55	0/1351	0.68	0/1822
5	H	0.58	0/573	0.65	0/772
All	All	0.51	0/11248	0.65	0/15219

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1278	0	1201	19	0
1	E	1272	0	1218	23	0
1	I	1229	0	1155	14	0
1	K	1262	0	1209	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	529	0	482	3	0
2	D	577	0	536	3	0
2	F	568	0	522	5	0
2	J	535	0	478	8	0
2	L	553	0	509	10	0
3	C	1328	0	1289	18	0
4	G	1327	0	1308	21	0
5	H	560	0	519	2	0
All	All	11018	0	10426	127	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 6.

All (127) 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:K:76:THR:HG22	1:K:100:HIS:HD2	1.33	0.93
1:K:76:THR:HG22	1:K:100:HIS:CD2	2.12	0.84
3:C:68:PRO:HA	3:C:71:ARG:HG3	1.64	0.77
1:E:68:PRO:HG2	4:G:68:PRO:HG2	1.65	0.76
3:C:64:THR:O	3:C:71:ARG:NH1	2.19	0.75
1:E:96:ARG:NH1	1:E:97:ASN:O	2.21	0.72
1:K:77:TRP:NE1	2:L:62:ILE:HG12	2.06	0.70
3:C:158:MSE:HE3	4:G:30:TYR:CE1	2.29	0.68
3:C:157:ARG:NH2	2:L:5:MET:O	2.24	0.68
3:C:69:PHE:O	1:K:140:LYS:NZ	2.24	0.67
2:L:60:GLN:HB3	2:L:62:ILE:HD13	1.76	0.67
1:I:77:TRP:CD1	2:J:62:ILE:HG12	2.32	0.64
1:E:84:VAL:HG22	1:E:91:MSE:HG3	1.77	0.64
4:G:23:PHE:O	4:G:54:ARG:NH2	2.29	0.64
1:E:27:PRO:HG3	4:G:158:MSE:HE1	1.80	0.64
4:G:64:THR:O	4:G:71:ARG:NH1	2.31	0.64
2:J:60:GLN:HB3	2:J:62:ILE:HD13	1.78	0.64
1:K:91:MSE:HE2	1:K:112:TYR:CD1	2.33	0.64
3:C:22:PHE:CD2	3:C:91:MSE:HE1	2.33	0.63
3:C:137:ILE:HG21	4:G:137:ILE:HD11	1.81	0.63
1:A:103:ILE:HG22	1:A:104:MSE:HG2	1.81	0.61
1:E:94:TYR:OH	1:E:107:GLU:OE1	2.17	0.61
4:G:64:THR:HA	4:G:71:ARG:HD3	1.82	0.60
1:E:92:LYS:HG2	1:E:111:THR:HG22	1.83	0.60
1:K:63:PRO:O	1:K:66:VAL:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:TYR:HB2	1:E:37:ILE:HD11	1.85	0.59
1:A:26:TYR:HB2	1:A:37:ILE:HD11	1.86	0.58
1:I:42:ARG:HH21	1:I:52:THR:HG21	1.69	0.57
1:K:77:TRP:CE2	2:L:62:ILE:HG12	2.39	0.57
1:A:158:MSE:HE3	1:K:30:TYR:CZ	2.39	0.57
1:K:94:TYR:OH	1:K:107:GLU:OE1	2.14	0.55
4:G:103:ILE:HG22	4:G:104:MSE:HG2	1.88	0.55
1:A:63:PRO:O	1:A:66:VAL:HG22	2.07	0.54
1:A:37:ILE:HG23	1:A:56:LEU:HG	1.88	0.54
2:F:6:SER:HB2	2:F:17:LYS:NZ	2.23	0.53
4:G:68:PRO:HA	4:G:71:ARG:HB2	1.90	0.53
5:H:55:ALA:O	5:H:58:VAL:HG22	2.08	0.53
1:I:84:VAL:HG22	1:I:91:MSE:HG3	1.91	0.52
1:E:163:VAL:HG21	1:I:25:ARG:HA	1.92	0.52
3:C:84:VAL:HG22	3:C:91:MSE:HG3	1.91	0.52
1:E:106:VAL:HG22	1:E:129:PHE:HD1	1.75	0.52
1:I:42:ARG:NH2	1:I:52:THR:HG21	2.24	0.52
1:I:22:PHE:CD2	1:I:91:MSE:HE1	2.45	0.52
4:G:74:THR:OG1	4:G:75:GLU:N	2.41	0.51
2:F:31:LYS:HB3	2:F:37:SER:HB3	1.92	0.51
2:B:55:ALA:O	2:B:58:VAL:HG13	2.10	0.51
1:E:2:VAL:HG11	1:E:128:LYS:HE3	1.93	0.51
1:E:104:MSE:HB3	1:E:129:PHE:CE1	2.45	0.51
1:A:1:MET:O	1:A:130:SER:HA	2.10	0.51
2:F:6:SER:HB2	2:F:17:LYS:HZ1	1.76	0.50
1:E:79:ILE:O	1:E:95:THR:HA	2.12	0.50
1:I:103:ILE:HG22	1:I:104:MSE:HG2	1.94	0.50
1:I:29:PRO:HG2	1:I:30:TYR:CE2	2.47	0.50
2:J:6:SER:HB2	2:J:17:LYS:NZ	2.27	0.50
1:K:90:THR:HG22	1:K:113:GLN:HG3	1.94	0.49
1:A:76:THR:HG22	1:A:100:HIS:CE1	2.47	0.49
2:D:17:LYS:HB2	2:D:49:TYR:CE1	2.46	0.49
1:E:104:MSE:HB3	1:E:129:PHE:HE1	1.77	0.49
2:L:46:TRP:O	2:L:50:THR:HG22	2.13	0.49
1:K:91:MSE:HE3	1:K:93:THR:CG2	2.41	0.49
1:A:158:MSE:HE1	1:I:27:PRO:HG2	1.95	0.48
1:A:160:MSE:O	1:A:164:ILE:HG13	2.14	0.48
1:A:96:ARG:NH2	2:B:69:ALA:HB2	2.29	0.48
1:E:90:THR:HG22	1:E:113:GLN:HG3	1.94	0.48
1:E:140:LYS:HE3	1:I:65:TRP:CD1	2.48	0.48
1:K:42:ARG:NH2	1:K:52:THR:HG21	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:50:THR:O	2:J:54:ASN:ND2	2.34	0.47
1:A:25:ARG:HA	1:K:163:VAL:HG21	1.94	0.47
3:C:91:MSE:HE2	3:C:93:THR:HG22	1.96	0.47
1:E:160:MSE:O	1:E:164:ILE:HG13	2.15	0.47
2:J:55:ALA:O	2:J:58:VAL:HG22	2.15	0.47
2:J:62:ILE:N	2:J:62:ILE:HD12	2.29	0.47
3:C:74:THR:OG1	3:C:75:GLU:N	2.46	0.46
2:L:61:GLY:N	2:L:62:ILE:HD12	2.31	0.46
1:K:22:PHE:CG	1:K:91:MSE:HE1	2.50	0.46
1:I:90:THR:HG22	1:I:113:GLN:HG3	1.98	0.46
2:D:54:ASN:O	2:D:58:VAL:HG23	2.15	0.45
1:K:42:ARG:HH21	1:K:52:THR:HG21	1.81	0.45
3:C:144:TRP:CZ2	4:G:63:PRO:HG3	2.51	0.45
1:A:20:ARG:NH1	2:B:29:SER:OG	2.44	0.45
2:L:62:ILE:N	2:L:62:ILE:HD12	2.31	0.45
1:K:37:ILE:HG13	1:K:56:LEU:HG	1.99	0.45
2:L:54:ASN:O	2:L:58:VAL:HG23	2.17	0.45
1:I:146:ARG:HD2	1:I:146:ARG:HA	1.59	0.44
2:J:6:SER:HB2	2:J:17:LYS:HZ1	1.82	0.44
2:J:33:LEU:HA	2:J:33:LEU:HD23	1.86	0.44
1:A:70:LEU:HD13	1:A:103:ILE:HD11	1.98	0.44
1:E:44:VAL:HA	1:E:49:ASN:O	2.17	0.44
2:L:60:GLN:C	2:L:62:ILE:H	2.21	0.44
4:G:148:LYS:HD2	4:G:148:LYS:HA	1.80	0.44
4:G:62:LEU:HD12	4:G:70:LEU:O	2.18	0.44
1:A:13:THR:OG1	1:A:14:ASP:N	2.51	0.44
1:I:88:ASN:N	1:I:88:ASN:OD1	2.50	0.44
3:C:94:TYR:OH	3:C:96:ARG:HD3	2.18	0.43
1:E:86:PRO:HB3	2:F:33:LEU:HD23	2.00	0.43
1:E:1:MET:O	1:E:130:SER:HA	2.18	0.43
4:G:37:ILE:HD12	4:G:56:LEU:HG	2.00	0.43
1:K:103:ILE:HG22	1:K:104:MSE:HG2	2.00	0.43
4:G:62:LEU:HA	4:G:62:LEU:HD23	1.90	0.43
4:G:110:THR:HA	4:G:124:ASP:O	2.19	0.43
1:A:166:LYS:HD3	1:A:166:LYS:HA	1.81	0.43
2:F:17:LYS:HB2	2:F:49:TYR:CE1	2.54	0.43
1:A:154:LYS:O	1:A:158:MSE:HG2	2.18	0.42
1:K:91:MSE:HE3	1:K:93:THR:HG21	2.01	0.42
2:L:9:PHE:HZ	2:L:57:LEU:HB2	1.85	0.42
3:C:158:MSE:HE3	4:G:30:TYR:CD1	2.55	0.42
1:K:39:THR:HA	1:K:54:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ARG:HH21	3:C:52:THR:HG21	1.85	0.42
5:H:46:TRP:O	5:H:50:THR:HG22	2.19	0.42
1:K:61:LYS:HG3	1:K:73:ILE:HG22	2.02	0.42
3:C:55:LEU:HD12	3:C:55:LEU:HA	1.84	0.41
2:D:33:LEU:HA	2:D:33:LEU:HD23	1.85	0.41
1:E:76:THR:HG22	1:E:100:HIS:CE1	2.55	0.41
3:C:25:ARG:HA	4:G:163:VAL:HG21	2.01	0.41
4:G:22:PHE:CD2	4:G:91:MSE:HE1	2.55	0.41
1:E:80:GLU:HA	1:E:94:TYR:O	2.21	0.41
4:G:166:LYS:HD3	4:G:166:LYS:HA	1.84	0.41
1:K:94:TYR:OH	1:K:96:ARG:HD3	2.21	0.41
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.90	0.41
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.85	0.41
1:E:62:LEU:HA	1:E:63:PRO:HD3	1.88	0.41
4:G:68:PRO:HB3	4:G:71:ARG:NH2	2.35	0.41
1:E:22:PHE:CD1	1:E:91:MSE:HE1	2.57	0.40
1:I:50:LEU:HD12	1:I:50:LEU:HA	1.87	0.40
1:A:26:TYR:HB2	1:A:37:ILE:CD1	2.50	0.40
3:C:63:PRO:O	3:C:66:VAL:HG22	2.22	0.40
3:C:64:THR:HA	3:C:71:ARG:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/189 (89%)	166 (98%)	3 (2%)	0	100	100
1	E	162/189 (86%)	162 (100%)	0	0	100	100
1	I	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
1	K	160/189 (85%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
2	D	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
2	F	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
2	J	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
2	L	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
3	C	169/189 (89%)	166 (98%)	3 (2%)	0	100	100
4	G	167/189 (88%)	165 (99%)	2 (1%)	0	100	100
5	H	67/86 (78%)	66 (98%)	1 (2%)	0	100	100
All	All	1398/1650 (85%)	1374 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	131/170 (77%)	129 (98%)	2 (2%)	65	87
1	E	135/170 (79%)	133 (98%)	2 (2%)	65	87
1	I	127/170 (75%)	124 (98%)	3 (2%)	49	79
1	K	135/170 (79%)	132 (98%)	3 (2%)	52	81
2	B	50/73 (68%)	48 (96%)	2 (4%)	31	65
2	D	60/73 (82%)	60 (100%)	0	100	100
2	F	59/73 (81%)	59 (100%)	0	100	100
2	J	52/73 (71%)	51 (98%)	1 (2%)	57	84
2	L	56/73 (77%)	56 (100%)	0	100	100
3	C	143/169 (85%)	143 (100%)	0	100	100
4	G	148/168 (88%)	146 (99%)	2 (1%)	67	89
5	H	58/72 (81%)	56 (97%)	2 (3%)	37	71
All	All	1154/1454 (79%)	1137 (98%)	17 (2%)	65	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	104	MSE
2	B	43	SER
2	B	58	VAL
1	E	64	THR
1	E	104	MSE
4	G	37	ILE
4	G	104	MSE
5	H	5	MSE
5	H	6	SER
1	I	37	ILE
1	I	88	ASN
1	I	104	MSE
2	J	57	LEU
1	K	104	MSE
1	K	146	ARG
1	K	158	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	K	100	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	167/189 (88%)	-0.20	1 (0%)	89	89	5, 32, 78, 146	0
1	E	162/189 (85%)	0.15	6 (3%)	41	37	4, 46, 90, 163	0
1	I	156/189 (82%)	-0.07	4 (2%)	56	52	8, 40, 79, 118	0
1	K	160/189 (84%)	0.04	2 (1%)	77	77	2, 41, 70, 111	0
2	B	72/86 (83%)	-0.33	0	100	100	7, 31, 70, 144	0
2	D	74/86 (86%)	-0.29	1 (1%)	75	75	7, 29, 59, 82	0
2	F	72/86 (83%)	-0.19	0	100	100	24, 52, 82, 96	0
2	J	71/86 (82%)	-0.04	3 (4%)	36	32	15, 44, 86, 122	0
2	L	71/86 (82%)	-0.22	0	100	100	23, 47, 76, 136	0
3	C	166/189 (87%)	-0.27	0	100	100	2, 23, 63, 101	0
4	G	163/189 (86%)	-0.21	0	100	100	2, 24, 53, 100	0
5	H	70/86 (81%)	-0.47	0	100	100	4, 23, 59, 69	0
All	All	1404/1650 (85%)	-0.14	17 (1%)	79	79	2, 35, 78, 163	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	134	ASN	3.8
1	K	70	LEU	3.3
2	J	33	LEU	3.3
1	E	103	ILE	3.3
2	D	38	VAL	3.0
2	J	61	GLY	3.0
1	A	103	ILE	2.8
1	E	84	VAL	2.8
1	E	3	LEU	2.7
1	I	65	TRP	2.7
1	I	121	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	J	62	ILE	2.4
1	I	129	PHE	2.4
1	E	33	HIS	2.1
1	I	134	ASN	2.1
1	E	102	GLY	2.0
1	K	136	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.