



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 06:07 PM JST

PDB ID : 6LP3
Title : Structural basis and functional analysis epo1-bem3p complex for bud growth
Authors : Wang, J.; Li, L.; Ming, Z.H.; Wu, L.J.; Yan, L.M.
Deposited on : 2020-01-08
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

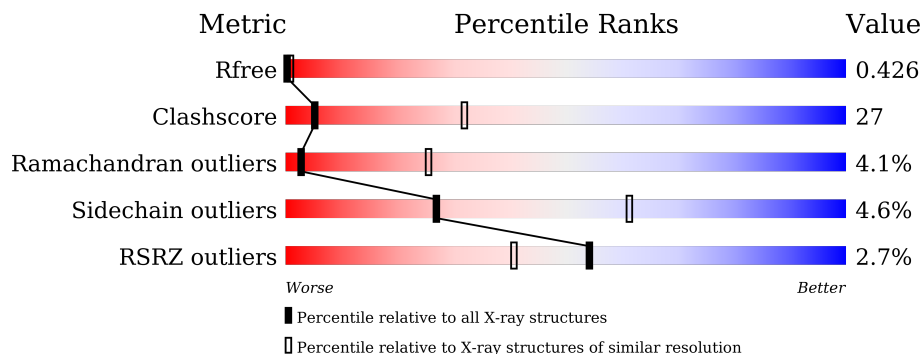
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	198	 2% 30% 26% 40%
1	B	198	 % 35% 22% 39%
1	D	198	 3% 32% 25% 39%
1	E	198	 % 32% 27% 38%
2	C	99	 % 23% 20% 57%
2	F	99	 % 25% 18% 57%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4661 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 Uncharacterized protein YMR124W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	969	602	164	200	3	0	0	0
1	B	120	984	613	167	200	4	0	0	0
1	D	120	984	608	168	205	3	0	0	0
1	E	122	1002	624	170	204	4	0	0	0

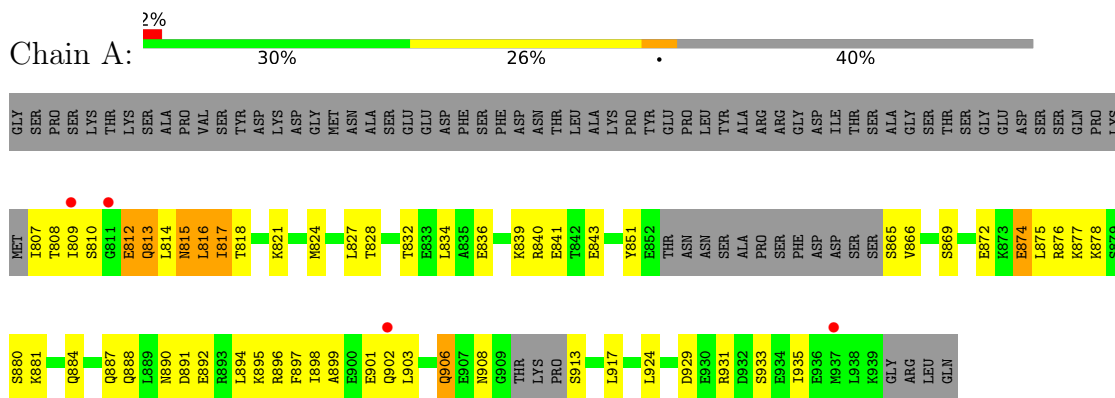
- Molecule 2 is a protein called GTPase-activating protein BEM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	43	361	229	55	76	1	0	0	0
2	F	43	361	229	55	76	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.

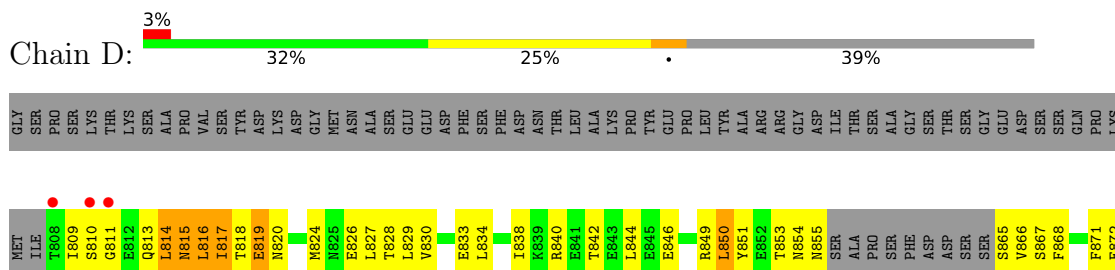
- Molecule 1: Uncharacterized protein YMR124W



- Molecule 1: Uncharacterized protein YMR124W

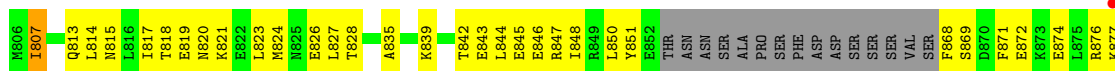
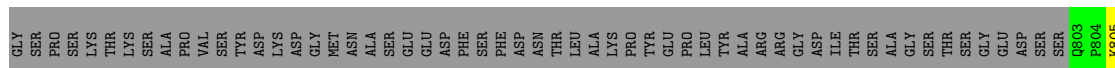
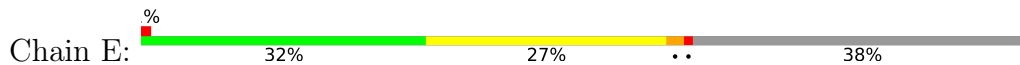


- Molecule 1: Uncharacterized protein YMR124W

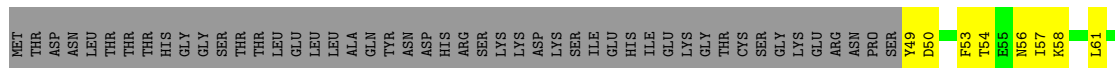




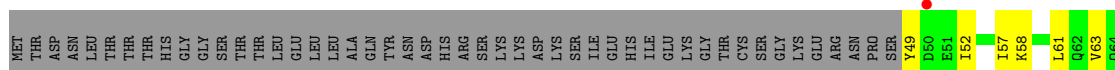
- Molecule 1: Uncharacterized protein YMR124W



- Molecule 2: GTPase-activating protein BEM3



- Molecule 2: GTPase-activating protein BEM3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.41Å 119.41Å 144.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 3.55 46.03 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.03-3.55) 99.7 (46.03-3.55)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.340 , 0.398 0.356 , 0.426	Depositor DCC
R_{free} test set	674 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	124.6	Xtrriage
Anisotropy	0.239	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 112.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.30	0/970	0.49	0/1292
1	B	0.32	0/988	0.51	0/1320
1	D	0.31	0/985	0.52	0/1313
1	E	0.27	0/1006	0.47	0/1343
2	C	0.26	0/363	0.45	0/487
2	F	0.24	0/363	0.36	0/487
All	All	0.29	0/4675	0.49	0/6242

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	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	911	LYS	Peptide
1	E	911	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	993	85	0
1	B	984	0	1010	79	3
1	D	984	0	1002	76	3
1	E	1002	0	1029	65	0
2	C	361	0	362	21	0
2	F	361	0	362	20	0
All	All	4661	0	4758	251	3

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 27.

All (251) 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:D:850:LEU:CD2	1:D:854:ASN:ND2	1.81	1.43
1:A:809:ILE:HG23	1:B:813:GLN:NE2	1.43	1.33
1:D:850:LEU:HD22	1:D:854:ASN:ND2	1.37	1.33
1:A:816:LEU:O	1:A:818:THR:N	1.61	1.31
1:A:810:SER:O	1:A:813:GLN:HG3	1.31	1.30
1:D:896:ARG:NH1	1:D:897:PHE:CZ	1.96	1.30
1:D:851:TYR:O	1:D:855:ASN:ND2	1.68	1.26
1:A:865:SER:HB2	1:B:868:PHE:HD1	1.05	1.14
1:D:883:VAL:HG11	1:E:887:GLN:HB3	1.25	1.13
1:D:820:ASN:ND2	1:E:820:ASN:OD1	1.83	1.12
1:D:931:ARG:NH1	1:E:932:ASP:OD1	1.84	1.10
1:E:936:GLU:O	1:E:939:LYS:HG3	1.53	1.08
1:A:865:SER:HB2	1:B:868:PHE:CD1	1.89	1.07
1:D:851:TYR:HB3	1:E:851:TYR:CE1	1.92	1.04
1:A:810:SER:O	1:A:813:GLN:CG	2.05	1.03
1:D:896:ARG:NH1	1:D:897:PHE:HZ	1.37	1.02
1:D:866:VAL:N	1:E:868:PHE:HD2	1.56	1.01
1:D:850:LEU:HD21	1:D:854:ASN:HD21	1.22	1.01
1:A:812:GLU:O	1:A:813:GLN:O	1.81	0.98
1:D:850:LEU:CD2	1:D:854:ASN:HD21	1.61	0.96
1:D:820:ASN:OD1	1:E:820:ASN:ND2	2.00	0.95
1:D:809:ILE:HG12	1:E:813:GLN:OE1	1.73	0.88
1:A:809:ILE:CG2	1:B:813:GLN:NE2	2.35	0.88
1:A:809:ILE:HG23	1:B:813:GLN:HE22	1.32	0.88
1:A:816:LEU:O	1:A:817:ILE:C	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:LEU:HD22	1:D:854:ASN:HD22	1.08	0.86
1:E:936:GLU:O	1:E:939:LYS:CG	2.23	0.85
1:D:816:LEU:HB2	1:D:898:ILE:HD12	1.57	0.85
1:A:865:SER:O	1:B:868:PHE:N	2.11	0.83
1:A:866:VAL:HG22	1:B:868:PHE:CG	2.14	0.82
1:D:894:LEU:HD11	1:E:897:PHE:HB2	1.60	0.82
1:D:866:VAL:N	1:E:868:PHE:CD2	2.47	0.80
1:A:894:LEU:HB2	1:B:898:ILE:HG22	1.65	0.79
1:D:938:LEU:HD12	1:E:938:LEU:HB3	1.65	0.78
1:B:848:ILE:O	1:B:851:TYR:CD2	2.38	0.77
1:A:865:SER:C	1:B:868:PHE:N	2.38	0.77
1:A:874:GLU:HA	1:A:877:LYS:HE2	1.67	0.76
1:B:848:ILE:O	1:B:851:TYR:N	2.17	0.75
1:A:807:ILE:HG22	1:A:808:THR:N	2.02	0.75
1:D:876:ARG:NH1	2:F:65:GLU:OE1	2.17	0.73
1:D:896:ARG:NH1	1:D:897:PHE:CE1	2.37	0.71
1:A:809:ILE:HG23	1:B:813:GLN:CD	2.11	0.70
1:A:872:GLU:OE2	2:C:58:LYS:NZ	2.25	0.69
1:A:817:ILE:HG22	1:B:820:ASN:HD22	1.57	0.69
1:D:816:LEU:HD12	1:D:894:LEU:HD22	1.74	0.69
1:A:812:GLU:HG3	1:A:813:GLN:H	1.55	0.69
1:E:874:GLU:OE2	2:F:57:ILE:HD11	1.94	0.68
1:D:879:SER:O	1:D:883:VAL:HG23	1.94	0.68
1:A:898:ILE:HA	1:A:901:GLU:HB2	1.74	0.67
1:D:850:LEU:HD23	1:D:854:ASN:ND2	2.03	0.67
1:B:814:LEU:O	1:B:818:THR:OG1	2.12	0.66
1:A:817:ILE:HD11	1:A:895:LYS:HG3	1.76	0.66
1:B:849:ARG:O	1:B:851:TYR:CE2	2.48	0.65
2:C:80:LEU:HD21	2:F:80:LEU:HD23	1.78	0.65
1:A:809:ILE:CG2	1:B:813:GLN:HE22	2.04	0.65
1:B:911:LYS:HE3	1:B:912:PRO:HD2	1.80	0.64
1:A:869:SER:HB2	1:B:873:LYS:HE2	1.78	0.64
1:D:809:ILE:O	1:D:811:GLY:N	2.30	0.64
1:A:812:GLU:C	1:A:813:GLN:O	2.33	0.64
1:B:849:ARG:O	1:B:851:TYR:CD2	2.51	0.64
1:D:849:ARG:O	1:D:853:THR:HG23	1.97	0.64
1:D:884:GLN:O	1:D:888:GLN:N	2.27	0.63
1:A:865:SER:CB	1:B:868:PHE:CD1	2.77	0.63
1:B:881:LYS:NZ	2:C:65:GLU:OE2	2.32	0.63
1:D:851:TYR:HB3	1:E:851:TYR:CD1	2.32	0.62
1:E:868:PHE:HD1	1:E:869:SER:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:LEU:HD11	1:D:894:LEU:HB3	1.80	0.61
1:D:881:LYS:HD2	1:E:835:ALA:HB2	1.84	0.60
1:B:849:ARG:C	1:B:851:TYR:CD2	2.75	0.60
1:B:849:ARG:C	1:B:851:TYR:HD2	2.04	0.60
1:A:888:GLN:O	1:A:892:GLU:N	2.24	0.60
1:D:851:TYR:CD2	1:E:851:TYR:CD1	2.89	0.60
1:B:913:SER:HB3	1:B:915:MET:HG3	1.83	0.60
1:B:851:TYR:CD2	1:B:851:TYR:N	2.71	0.59
1:D:816:LEU:HD22	1:D:817:ILE:HD13	1.85	0.59
1:B:922:GLU:OE1	1:B:922:GLU:O	2.19	0.59
1:E:883:VAL:O	1:E:887:GLN:HG2	2.01	0.59
1:E:930:GLU:O	1:E:933:SER:OG	2.21	0.59
1:A:816:LEU:HD12	1:A:816:LEU:C	2.23	0.59
1:A:866:VAL:HG23	1:B:868:PHE:CD1	2.39	0.58
1:B:848:ILE:O	1:B:851:TYR:CA	2.51	0.58
1:B:851:TYR:N	1:B:851:TYR:HD2	2.02	0.57
1:D:816:LEU:CD1	1:D:894:LEU:HD22	2.34	0.57
1:D:884:GLN:HA	1:D:887:GLN:HB3	1.85	0.57
1:A:872:GLU:HG2	2:C:58:LYS:HD2	1.85	0.57
2:C:66:TYR:HE2	2:F:63:VAL:HG13	1.68	0.57
1:E:872:GLU:HG3	1:E:876:ARG:NH1	2.19	0.57
1:D:872:GLU:OE2	1:E:877:LYS:NZ	2.36	0.57
1:D:842:THR:O	1:D:846:GLU:HG2	2.05	0.57
1:D:872:GLU:OE2	2:F:58:LYS:HD2	2.05	0.57
1:A:866:VAL:CG2	1:B:868:PHE:CG	2.86	0.57
1:D:934:GLU:HA	1:D:937:MET:HB2	1.85	0.57
1:B:841:GLU:O	1:B:845:GLU:N	2.38	0.57
1:A:881:LYS:HZ3	1:B:834:LEU:C	2.08	0.56
1:E:905:LEU:O	1:E:909:GLY:N	2.37	0.56
1:A:809:ILE:HG22	1:A:809:ILE:O	2.06	0.56
1:A:866:VAL:CG2	1:B:868:PHE:CD1	2.88	0.56
1:E:815:ASN:O	1:E:819:GLU:HG3	2.05	0.55
1:B:926:LYS:O	1:B:930:GLU:N	2.40	0.55
1:A:832:THR:O	1:A:836:GLU:HG2	2.07	0.55
2:F:80:LEU:O	2:F:84:ARG:N	2.27	0.54
1:B:842:THR:HA	1:B:845:GLU:HB3	1.89	0.54
1:D:816:LEU:O	1:D:818:THR:N	2.40	0.54
1:A:876:ARG:O	1:B:884:GLN:NE2	2.41	0.54
1:A:881:LYS:HD3	1:B:835:ALA:HB2	1.89	0.54
1:D:820:ASN:OD1	1:E:820:ASN:CG	2.46	0.54
2:F:76:VAL:O	2:F:80:LEU:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:851:TYR:O	1:D:855:ASN:CG	2.45	0.53
1:D:871:PHE:O	1:D:874:GLU:HG3	2.08	0.53
1:D:871:PHE:CZ	1:E:845:GLU:HB2	2.43	0.53
2:F:87:SER:O	2:F:91:VAL:N	2.42	0.53
1:D:865:SER:C	1:E:868:PHE:HD2	2.12	0.53
1:E:824:MET:O	1:E:828:THR:HG23	2.10	0.52
1:B:885:LEU:HD22	2:C:68:THR:HG21	1.92	0.52
1:E:913:SER:HB2	1:E:916:GLU:HB3	1.92	0.52
1:A:890:ASN:HD21	1:B:895:LYS:HE3	1.75	0.52
2:C:84:ARG:NH2	2:F:84:ARG:HA	2.25	0.51
1:E:842:THR:O	1:E:846:GLU:HG2	2.11	0.51
1:A:866:VAL:HG22	1:B:868:PHE:CD2	2.46	0.51
2:F:61:LEU:O	2:F:65:GLU:HG3	2.11	0.50
1:B:903:LEU:HD11	2:C:84:ARG:HD2	1.92	0.50
1:A:834:LEU:HD13	1:B:834:LEU:HD13	1.92	0.50
1:E:842:THR:O	1:E:845:GLU:HG2	2.12	0.50
1:A:866:VAL:HG23	1:B:868:PHE:CE1	2.46	0.50
1:A:881:LYS:HZ3	1:B:835:ALA:HA	1.77	0.50
1:A:935:ILE:HD11	1:B:935:ILE:HD12	1.94	0.50
1:D:865:SER:C	1:E:868:PHE:HB2	2.33	0.49
1:B:909:GLY:O	1:B:910:THR:OG1	2.28	0.49
1:A:815:ASN:HB3	1:A:898:ILE:HG21	1.94	0.49
1:D:931:ARG:HH12	1:E:932:ASP:CG	2.11	0.49
1:A:881:LYS:NZ	1:B:834:LEU:HG	2.28	0.49
1:B:884:GLN:O	1:B:888:GLN:HG3	2.12	0.49
1:B:922:GLU:OE1	1:B:922:GLU:C	2.51	0.49
2:C:50:ASP:O	2:C:54:THR:HG23	2.12	0.49
1:A:839:LYS:O	1:A:843:GLU:HG3	2.13	0.49
2:C:56:ASN:HD22	2:F:52:ILE:HG23	1.78	0.48
1:A:881:LYS:NZ	1:B:835:ALA:HA	2.27	0.48
1:A:881:LYS:HZ3	1:B:835:ALA:N	2.10	0.48
1:E:844:LEU:O	1:E:848:ILE:HG13	2.13	0.48
1:A:881:LYS:HE3	1:A:881:LYS:HB2	1.59	0.48
2:C:87:SER:O	2:C:91:VAL:HG23	2.14	0.48
1:A:834:LEU:HA	1:B:834:LEU:HD13	1.96	0.48
1:A:810:SER:O	1:A:813:GLN:HG2	2.08	0.48
1:B:806:MET:HG2	1:B:807:ILE:H	1.78	0.48
1:A:807:ILE:HG22	1:A:808:THR:H	1.76	0.48
2:C:82:LYS:NZ	2:C:85:GLU:OE1	2.32	0.48
1:A:816:LEU:O	1:A:816:LEU:HD12	2.14	0.47
1:D:824:MET:O	1:D:828:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ARG:HB2	2:C:76:VAL:HG12	1.96	0.47
1:D:866:VAL:H	1:E:868:PHE:HD2	1.52	0.47
2:C:53:PHE:CE1	2:C:57:ILE:HD11	2.49	0.47
1:D:817:ILE:HG22	1:E:820:ASN:HD22	1.79	0.47
1:E:910:THR:O	1:E:910:THR:OG1	2.33	0.47
1:A:874:GLU:OE1	1:A:874:GLU:O	2.32	0.47
1:B:809:ILE:C	1:B:811:GLY:H	2.18	0.47
2:C:56:ASN:HD22	2:F:52:ILE:HD12	1.79	0.47
1:D:851:TYR:CB	1:E:851:TYR:CE1	2.82	0.47
1:E:847:ARG:HA	1:E:850:LEU:HG	1.95	0.47
1:B:872:GLU:HG2	1:B:876:ARG:HE	1.80	0.47
1:A:896:ARG:HD2	1:B:919:GLY:HA2	1.96	0.47
1:D:865:SER:O	1:E:868:PHE:HB2	2.15	0.46
1:D:809:ILE:C	1:D:811:GLY:H	2.17	0.46
1:A:815:ASN:CB	1:A:898:ILE:HG21	2.46	0.46
1:A:913:SER:O	1:A:917:LEU:HG	2.15	0.46
1:E:885:LEU:HD22	2:F:68:THR:HG21	1.98	0.46
1:B:895:LYS:O	1:B:898:ILE:HG12	2.15	0.46
1:A:809:ILE:HG12	1:B:810:SER:O	2.16	0.46
1:A:841:GLU:HB2	1:B:841:GLU:HG2	1.98	0.46
1:A:876:ARG:HD3	1:B:881:LYS:HD3	1.98	0.46
1:B:848:ILE:O	1:B:851:TYR:HA	2.15	0.46
1:D:814:LEU:HD12	1:D:815:ASN:N	2.30	0.46
1:A:903:LEU:HB3	1:A:908:ASN:O	2.15	0.46
2:C:76:VAL:O	2:C:80:LEU:N	2.49	0.46
1:A:809:ILE:CG2	1:A:809:ILE:O	2.63	0.46
1:A:824:MET:O	1:A:828:THR:HG23	2.15	0.46
1:E:819:GLU:O	1:E:823:LEU:HG	2.16	0.46
2:C:80:LEU:HD21	2:F:80:LEU:CD2	2.46	0.45
1:D:888:GLN:NE2	1:E:827:LEU:HD23	2.31	0.45
1:D:931:ARG:HD3	1:D:931:ARG:HA	1.75	0.45
1:A:881:LYS:O	1:A:884:GLN:N	2.49	0.45
1:B:868:PHE:HB3	1:B:869:SER:H	1.41	0.45
1:D:840:ARG:O	1:D:844:LEU:HG	2.16	0.45
1:D:897:PHE:CE1	1:E:915:MET:HB2	2.51	0.45
1:E:845:GLU:HA	1:E:848:ILE:HD12	1.98	0.45
1:A:872:GLU:HA	1:A:875:LEU:HB2	1.98	0.45
1:A:816:LEU:C	1:A:816:LEU:CD1	2.85	0.45
1:E:911:LYS:HZ2	1:E:912:PRO:HD2	1.82	0.45
1:D:830:VAL:HG21	1:E:827:LEU:HD11	2.00	0.44
1:D:894:LEU:HD11	1:E:897:PHE:CB	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:GLU:HB3	1:A:902:GLN:NE2	2.33	0.44
1:A:865:SER:OG	1:A:866:VAL:N	2.50	0.44
1:A:836:GLU:HB2	1:A:840:ARG:NH2	2.32	0.44
1:E:888:GLN:HE21	2:F:69:GLU:HB2	1.83	0.44
1:A:809:ILE:HG12	1:B:813:GLN:OE1	2.18	0.44
1:D:888:GLN:HE21	1:E:827:LEU:HD23	1.83	0.44
1:A:881:LYS:HZ3	1:B:835:ALA:CA	2.31	0.43
1:B:881:LYS:HG3	2:C:61:LEU:HB3	2.00	0.43
1:D:834:LEU:O	1:D:838:ILE:HG13	2.17	0.43
1:E:814:LEU:O	1:E:818:THR:OG1	2.23	0.43
1:E:935:ILE:O	1:E:939:LYS:N	2.52	0.43
1:A:881:LYS:CE	1:B:834:LEU:HG	2.48	0.43
2:C:67:GLU:OE2	2:F:66:TYR:CZ	2.72	0.43
1:E:894:LEU:O	1:E:898:ILE:HG22	2.19	0.43
1:D:906:GLN:HB3	1:D:907:GLU:H	1.54	0.43
1:E:817:ILE:O	1:E:821:LYS:HE2	2.18	0.43
1:E:839:LYS:O	1:E:843:GLU:HB2	2.19	0.43
1:D:829:LEU:O	1:D:833:GLU:N	2.40	0.43
1:E:931:ARG:HA	1:E:931:ARG:HD3	1.56	0.42
1:D:872:GLU:HB3	1:E:877:LYS:HE2	2.01	0.42
1:B:805:LYS:O	1:B:807:ILE:HG13	2.18	0.42
1:D:876:ARG:HG2	1:E:880:SER:HB3	2.00	0.42
1:D:896:ARG:H	1:D:896:ARG:HG3	1.66	0.42
1:D:907:GLU:HG3	1:D:908:ASN:H	1.84	0.42
1:A:887:GLN:O	1:A:891:ASP:HB2	2.19	0.42
1:D:872:GLU:OE1	2:F:58:LYS:NZ	2.27	0.42
1:B:848:ILE:C	1:B:851:TYR:H	2.19	0.42
1:D:818:THR:HG22	1:D:819:GLU:H	1.85	0.42
1:D:888:GLN:OE1	1:E:824:MET:HG3	2.20	0.42
1:D:894:LEU:HG	1:E:898:ILE:HA	2.00	0.42
1:E:805:LYS:O	1:E:807:ILE:HG12	2.20	0.42
1:B:849:ARG:HA	1:B:851:TYR:CE2	2.54	0.42
1:B:873:LYS:HB2	1:B:873:LYS:HE3	1.90	0.41
1:A:874:GLU:OE1	1:A:874:GLU:C	2.58	0.41
1:B:911:LYS:HB2	1:B:912:PRO:CD	2.50	0.41
1:D:826:GLU:O	1:D:830:VAL:HG23	2.19	0.41
1:B:881:LYS:HD2	2:C:65:GLU:OE1	2.21	0.41
1:A:903:LEU:HA	1:A:906:GLN:HB2	2.01	0.41
1:D:824:MET:H	1:D:824:MET:HG3	1.74	0.41
1:A:899:ALA:O	1:A:903:LEU:HG	2.20	0.41
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:ARG:O	1:B:851:TYR:HE2	1.99	0.41
1:D:820:ASN:CG	1:E:820:ASN:OD1	2.54	0.41
1:D:932:ASP:O	1:D:936:GLU:HG2	2.20	0.41
2:F:75:LYS:HA	2:F:75:LYS:HD3	1.92	0.41
1:A:812:GLU:CG	1:A:813:GLN:H	2.26	0.41
1:A:865:SER:CB	1:B:868:PHE:HD1	1.98	0.41
1:B:806:MET:CG	1:B:807:ILE:H	2.32	0.41
1:E:911:LYS:NZ	1:E:911:LYS:HB2	2.36	0.41
1:A:880:SER:OG	1:A:881:LYS:N	2.54	0.41
1:E:871:PHE:H	1:E:871:PHE:HD1	1.69	0.41
1:E:911:LYS:HB2	1:E:912:PRO:CD	2.51	0.41
2:F:73:LEU:O	2:F:76:VAL:HG22	2.21	0.40
1:A:897:PHE:HZ	1:B:915:MET:HB3	1.86	0.40
2:C:87:SER:O	2:C:91:VAL:N	2.43	0.40
1:A:872:GLU:HA	1:A:875:LEU:HD12	2.03	0.40
1:D:888:GLN:HG3	1:E:828:THR:HG22	2.03	0.40
1:A:878:LYS:HG2	1:B:838:ILE:HG21	2.02	0.40
1:A:929:ASP:O	1:A:933:SER:OG	2.24	0.40
1:B:878:LYS:HE3	1:B:878:LYS:HB2	1.76	0.40
1:A:836:GLU:HB2	1:A:840:ARG:HH21	1.87	0.40
2:F:52:ILE:HD13	2:F:52:ILE:HA	1.91	0.40

All (3) 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:B:833:GLU:OE1	1:D:854:ASN:OD1[5_445]	1.63	0.57
1:B:833:GLU:OE2	1:D:854:ASN:OD1[5_445]	2.01	0.19
1:B:833:GLU:CD	1:D:854:ASN:OD1[5_445]	2.06	0.14

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	112/198 (57%)	98 (88%)	9 (8%)	5 (4%)	2	23
1	B	116/198 (59%)	101 (87%)	10 (9%)	5 (4%)	2	24
1	D	114/198 (58%)	100 (88%)	7 (6%)	7 (6%)	1	17
1	E	118/198 (60%)	105 (89%)	8 (7%)	5 (4%)	3	24
2	C	41/99 (41%)	40 (98%)	1 (2%)	0	100	100
2	F	41/99 (41%)	40 (98%)	1 (2%)	0	100	100
All	All	542/990 (55%)	484 (89%)	36 (7%)	22 (4%)	3	25

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	813	GLN
1	A	817	ILE
1	B	912	PRO
1	D	906	GLN
1	E	912	PRO
1	A	814	LEU
1	A	906	GLN
1	B	807	ILE
1	E	911	LYS
1	E	913	SER
1	B	810	SER
1	D	815	ASN
1	B	911	LYS
1	D	810	SER
1	D	813	GLN
1	D	817	ILE
1	D	819	GLU
1	A	812	GLU
1	B	908	ASN
1	D	816	LEU
1	E	910	THR
1	E	807	ILE

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	113/181 (62%)	106 (94%)	7 (6%)	18	52
1	B	114/181 (63%)	107 (94%)	7 (6%)	18	53
1	D	115/181 (64%)	110 (96%)	5 (4%)	29	63
1	E	116/181 (64%)	114 (98%)	2 (2%)	60	83
2	C	42/93 (45%)	40 (95%)	2 (5%)	25	60
2	F	42/93 (45%)	40 (95%)	2 (5%)	25	60
All	All	542/910 (60%)	517 (95%)	25 (5%)	27	61

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	ASN
1	A	816	LEU
1	A	821	LYS
1	A	827	LEU
1	A	851	TYR
1	A	874	GLU
1	A	931	ARG
1	B	837	SER
1	B	847	ARG
1	B	850	LEU
1	B	851	TYR
1	B	868	PHE
1	B	903	LEU
1	B	933	SER
2	C	49	TYR
2	C	74	GLU
1	D	814	LEU
1	D	827	LEU
1	D	850	LEU
1	D	867	SER
1	D	868	PHE
1	E	826	GLU
1	E	881	LYS
2	F	49	TYR
2	F	89	GLU

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

Mol	Chain	Res	Type
1	A	890	ASN
1	A	902	GLN
1	B	820	ASN
1	D	854	ASN
1	E	888	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	118/198 (59%)	0.21	4 (3%) 45 33	59, 113, 209, 241	0
1	B	120/198 (60%)	0.16	2 (1%) 70 57	77, 107, 198, 336	0
1	D	120/198 (60%)	0.34	6 (5%) 28 20	58, 110, 205, 239	0
1	E	122/198 (61%)	0.03	2 (1%) 72 59	76, 107, 165, 341	0
2	C	43/99 (43%)	0.10	0 100 100	90, 114, 167, 178	0
2	F	43/99 (43%)	0.06	1 (2%) 60 46	93, 120, 166, 186	0
All	All	566/990 (57%)	0.17	15 (2%) 54 41	58, 110, 201, 341	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	937	MET	5.0
2	F	50	ASP	3.8
1	A	809	ILE	3.4
1	A	937	MET	3.4
1	D	808	THR	3.3
1	E	888	GLN	3.3
1	A	811	GLY	3.0
1	D	810	SER	2.8
1	B	938	LEU	2.4
1	D	935	ILE	2.2
1	D	939	LYS	2.2
1	A	902	GLN	2.2
1	D	811	GLY	2.1
1	D	936	GLU	2.1
1	E	877	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.