Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 04:27 pm BST

PDB ID	:	4A8J
Title	:	Crystal Structure of the Elongator subcomplex Elp456
Authors	:	Glatt, S.; Mueller, C.W.
Deposited on	:	2011-11-21
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

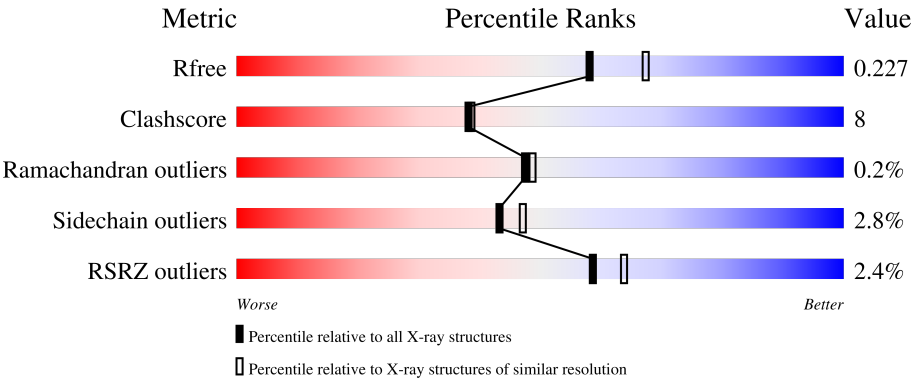
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	361	% 67% 9% • 23%
1	D	361	2% 69% 8% • 22%
2	B	270	4% 62% 18% • 19%
2	E	270	4% 60% 20% • 18%
3	C	280	% 80% 14% 6%

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Mol	Chain	Length	Quality of chain
3	F	280	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13005 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 ELONGATOR COMPLEX PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	Se	26	0	0
			2203	1419	376	399	9			
1	D	280	Total	C	N	O	Se	34	0	0
			2222	1432	379	402	9			

- Molecule 2 is a protein called ELONGATOR COMPLEX PROTEIN 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	Se	28	0	0
			1781	1143	290	341	3	4			
2	E	221	Total	C	N	O	S	Se	30	0	0
			1787	1146	291	343	3	4			

- Molecule 3 is a protein called ELONGATOR COMPLEX PROTEIN 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	Se	25	0	0
			2080	1324	352	397	4	3			
3	F	262	Total	C	N	O	S	Se	14	0	0
			2070	1319	350	394	4	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MSE	-	expression tag	UNP Q04868
C	-5	HIS	-	expression tag	UNP Q04868
C	-4	HIS	-	expression tag	UNP Q04868
C	-3	HIS	-	expression tag	UNP Q04868
C	-2	HIS	-	expression tag	UNP Q04868
C	-1	HIS	-	expression tag	UNP Q04868
C	0	HIS	-	expression tag	UNP Q04868
F	-6	MSE	-	expression tag	UNP Q04868

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	HIS	-	expression tag	UNP Q04868
F	-4	HIS	-	expression tag	UNP Q04868
F	-3	HIS	-	expression tag	UNP Q04868
F	-2	HIS	-	expression tag	UNP Q04868
F	-1	HIS	-	expression tag	UNP Q04868
F	0	HIS	-	expression tag	UNP Q04868

- Molecule 4 is water.

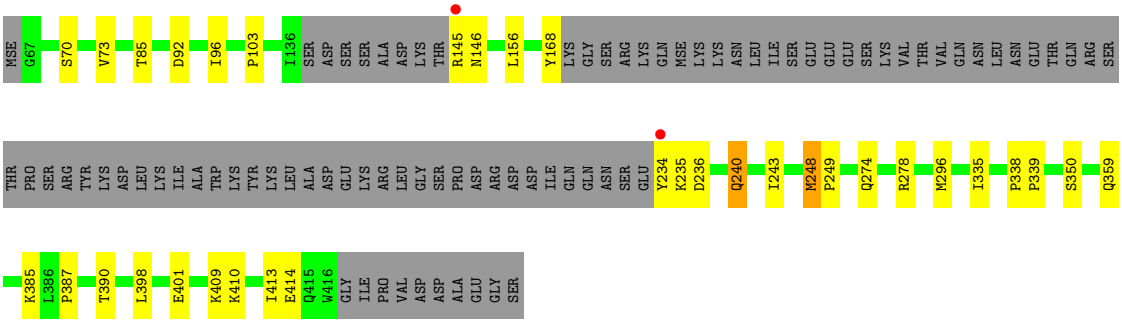
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	213	Total O 213 213	0	0
4	B	113	Total O 113 113	0	0
4	C	131	Total O 131 131	0	0
4	D	187	Total O 187 187	0	0
4	E	96	Total O 96 96	0	0
4	F	122	Total O 122 122	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

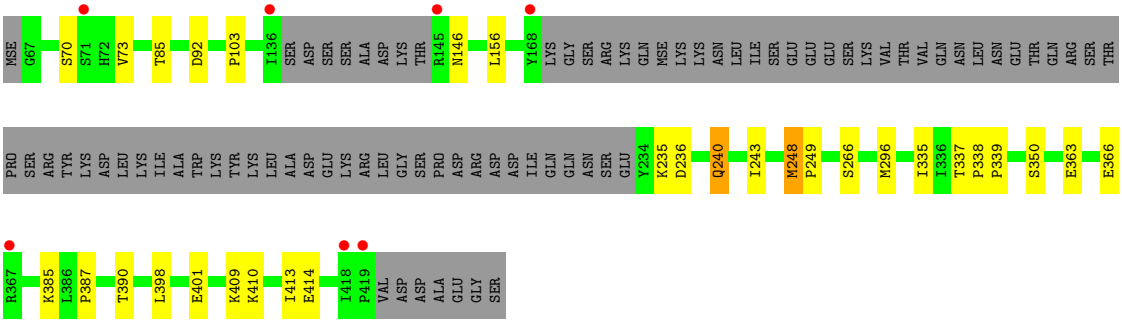
• Molecule 1: ELONGATOR COMPLEX PROTEIN 4

Chain A:



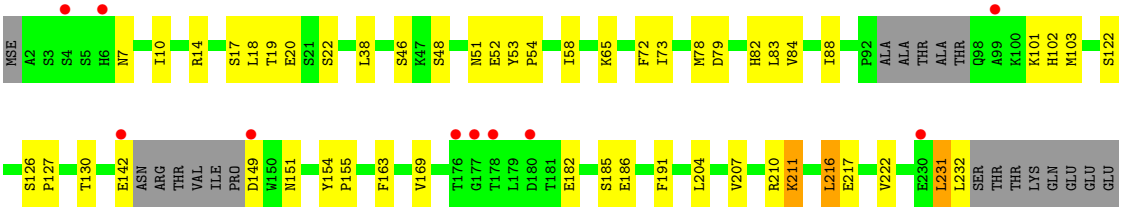
• Molecule 1: ELONGATOR COMPLEX PROTEIN 4

Chain D:

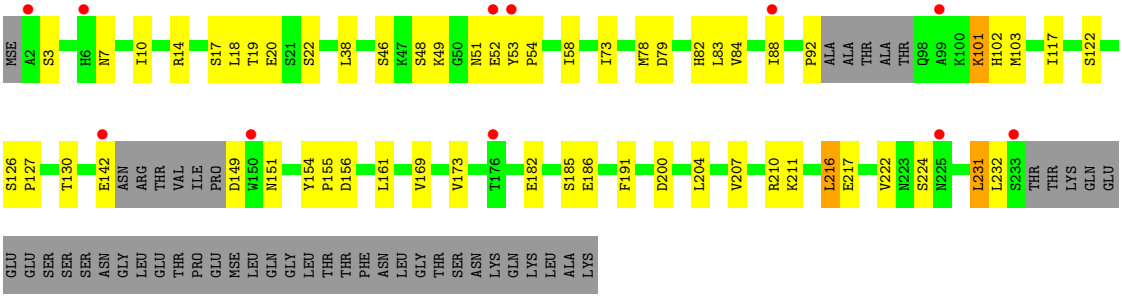


• Molecule 2: ELONGATOR COMPLEX PROTEIN 5

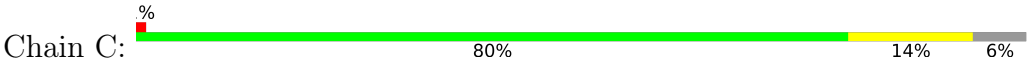
Chain B:

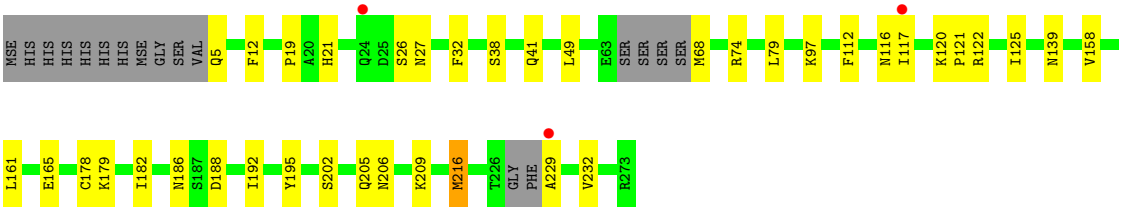


• Molecule 2: ELONGATOR COMPLEX PROTEIN 5

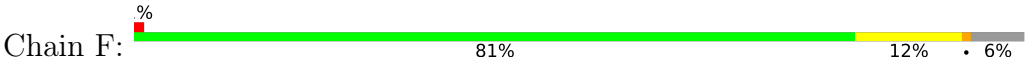


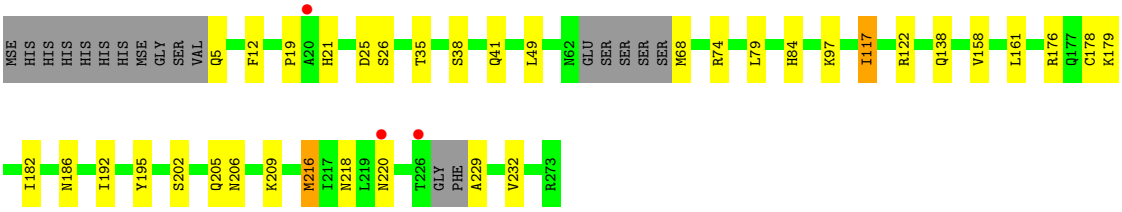
• Molecule 3: ELONGATOR COMPLEX PROTEIN 6





• Molecule 3: ELONGATOR COMPLEX PROTEIN 6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.73Å 124.89Å 146.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.10 46.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.20-2.10) 99.0 (46.20-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.231 0.202 , 0.227	Depositor DCC
R_{free} test set	5606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13005	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5003e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.46	0/2243	0.58	0/3022
1	D	0.46	0/2263	0.58	0/3050
2	B	0.43	0/1812	0.56	1/2451 (0.0%)
2	E	0.42	0/1818	0.55	0/2459
3	C	0.48	1/2120 (0.0%)	0.59	0/2878
3	F	0.50	1/2110 (0.0%)	0.60	0/2865
All	All	0.46	2/12366 (0.0%)	0.58	1/16725 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	178	CYS	CB-SG	-5.45	1.73	1.81
3	F	178	CYS	CB-SG	-5.19	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	211	LYS	CD-CE-NZ	5.70	124.80	111.70

There are no chirality outliers.

There are no planarity outliers.

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	2203	0	2255	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2222	0	2276	22	0
2	B	1781	0	1775	34	0
2	E	1787	0	1780	45	0
3	C	2080	0	2056	30	0
3	F	2070	0	2051	28	0
4	A	213	0	0	8	0
4	B	113	0	0	3	0
4	C	131	0	0	4	0
4	D	187	0	0	4	0
4	E	96	0	0	5	0
4	F	122	0	0	5	0
All	All	13005	0	12193	181	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 8.

All (181) 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:240:GLN:OE1	1:D:410:LYS:HE3	1.56	1.06
1:A:240:GLN:OE1	1:A:410:LYS:HE3	1.55	1.04
2:E:54:PRO:HG2	2:E:102:HIS:ND1	1.74	1.03
3:F:35:THR:OG1	3:F:220:ASN:ND2	1.99	0.94
2:E:92:PRO:HD3	2:E:102:HIS:CD2	2.04	0.92
1:A:168:TYR:O	4:A:2073:HOH:O	1.96	0.82
2:E:156:ASP:OD2	4:E:2063:HOH:O	2.01	0.78
2:E:46:SER:O	2:E:51:ASN:HB2	1.84	0.76
2:E:18:LEU:HD21	2:E:103:MSE:CE	2.17	0.74
3:C:26:SER:HA	3:C:179:LYS:NZ	2.03	0.74
3:F:19:PRO:HB3	3:F:21:HIS:CE1	2.23	0.74
2:E:54:PRO:HG2	2:E:102:HIS:CE1	2.23	0.73
3:C:112:PHE:CE2	3:C:117:ILE:HD11	2.24	0.73
3:F:26:SER:HA	3:F:179:LYS:NZ	2.04	0.73
2:B:46:SER:O	2:B:51:ASN:HB2	1.88	0.73
2:B:18:LEU:HD21	2:B:103:MSE:CE	2.19	0.72
3:C:19:PRO:HB3	3:C:21:HIS:CE1	2.24	0.71
2:E:149:ASP:N	4:E:2055:HOH:O	2.24	0.70
2:B:149:ASP:N	4:B:2066:HOH:O	2.24	0.69
3:C:112:PHE:HE2	3:C:117:ILE:HD11	1.57	0.69
2:E:14:ARG:NH1	2:E:20:GLU:OE1	2.24	0.69
2:E:92:PRO:CD	2:E:102:HIS:CD2	2.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2134:HOH:O	2:B:151:ASN:ND2	2.27	0.68
3:F:41:GLN:NE2	4:F:2018:HOH:O	2.27	0.67
1:D:366:GLU:OE1	2:E:3:SER:HB3	1.94	0.67
3:C:41:GLN:NE2	4:C:2022:HOH:O	2.28	0.66
2:E:92:PRO:HD3	2:E:102:HIS:NE2	2.11	0.65
2:B:54:PRO:HG2	2:B:102:HIS:CE1	2.31	0.65
3:F:25:ASP:O	4:F:2011:HOH:O	2.14	0.65
1:A:234:TYR:N	4:A:2076:HOH:O	2.30	0.65
3:C:165:GLU:OE1	4:C:2076:HOH:O	2.15	0.64
1:A:278:ARG:NH2	4:A:2121:HOH:O	2.17	0.64
2:E:7:ASN:OD1	4:E:2002:HOH:O	2.15	0.64
3:C:139:ASN:ND2	4:C:2068:HOH:O	2.31	0.63
1:A:398:LEU:HG	1:A:401:GLU:HG3	1.80	0.63
2:E:78:MSE:HE3	2:E:83:LEU:HD13	1.80	0.62
2:B:78:MSE:HE3	2:B:83:LEU:HD13	1.81	0.62
3:C:205:GLN:NE2	3:C:206:ASN:OD1	2.33	0.61
3:C:205:GLN:OE1	3:C:209:LYS:NZ	2.28	0.61
4:D:2112:HOH:O	2:E:151:ASN:ND2	2.33	0.61
1:D:398:LEU:HG	1:D:401:GLU:HG3	1.82	0.61
3:F:205:GLN:OE1	3:F:209:LYS:NZ	2.26	0.60
2:B:163:PHE:O	4:B:2076:HOH:O	2.16	0.60
3:F:205:GLN:NE2	3:F:206:ASN:OD1	2.34	0.60
2:B:54:PRO:HG2	2:B:102:HIS:ND1	2.17	0.59
2:E:18:LEU:HD21	2:E:103:MSE:HE2	1.84	0.59
2:E:79:ASP:OD1	2:E:82:HIS:ND1	2.35	0.59
2:B:18:LEU:HD21	2:B:103:MSE:HE2	1.84	0.59
1:A:350:SER:HB3	1:A:387:PRO:HD3	1.85	0.59
2:E:22:SER:O	2:E:130:THR:HG23	2.04	0.58
3:C:12:PHE:CZ	3:C:216:MSE:HE1	2.39	0.58
1:A:240:GLN:OE1	1:A:410:LYS:CE	2.43	0.57
3:C:26:SER:HA	3:C:179:LYS:HZ3	1.69	0.56
3:F:12:PHE:CZ	3:F:216:MSE:HE1	2.40	0.56
1:A:73:VAL:HG21	1:A:236:ASP:HB2	1.86	0.56
2:E:18:LEU:HD21	2:E:103:MSE:HE3	1.86	0.56
3:F:26:SER:HA	3:F:179:LYS:HZ1	1.68	0.56
2:E:49:LYS:O	4:E:2014:HOH:O	2.18	0.55
2:E:231:LEU:HG	2:E:232:LEU:H	1.70	0.55
1:D:73:VAL:HG21	1:D:236:ASP:HB2	1.88	0.55
2:E:58:ILE:HD12	2:E:58:ILE:N	2.22	0.55
1:A:243:ILE:HD12	1:A:409:LYS:O	2.07	0.54
2:B:58:ILE:HD12	2:B:58:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:SER:OG	2:B:19:THR:HG23	2.09	0.53
1:D:243:ILE:HD12	1:D:409:LYS:O	2.07	0.53
3:F:138:GLN:HG3	4:F:2077:HOH:O	2.09	0.53
3:F:218:ASN:HD21	3:F:220:ASN:HD21	1.56	0.53
2:E:19:THR:OG1	2:E:20:GLU:N	2.41	0.52
2:B:22:SER:O	2:B:130:THR:HG23	2.09	0.52
1:D:266:SER:HB3	3:F:117:ILE:HD12	1.91	0.52
2:B:18:LEU:HD21	2:B:103:MSE:HE3	1.91	0.52
3:C:116:ASN:O	3:C:125:ILE:HG12	2.10	0.52
2:B:79:ASP:OD1	2:B:82:HIS:ND1	2.36	0.52
1:A:338:PRO:HB3	3:C:192:ILE:HG21	1.92	0.52
3:F:26:SER:HA	3:F:179:LYS:HZ2	1.73	0.52
1:A:385:LYS:HG3	1:A:390:THR:HG21	1.91	0.52
2:B:19:THR:OG1	2:B:20:GLU:N	2.43	0.52
1:D:350:SER:HB3	1:D:387:PRO:HD3	1.92	0.52
2:B:231:LEU:HG	2:B:232:LEU:H	1.75	0.51
2:E:173:VAL:O	4:E:2072:HOH:O	2.19	0.51
1:D:338:PRO:HB3	3:F:192:ILE:HG21	1.91	0.51
2:E:17:SER:OG	2:E:19:THR:HG23	2.11	0.51
3:C:26:SER:HA	3:C:179:LYS:HZ1	1.72	0.50
1:A:335:ILE:HD12	4:A:2159:HOH:O	2.10	0.50
2:B:73:ILE:CG2	2:B:78:MSE:HE1	2.41	0.50
3:F:84:HIS:HE1	4:F:2018:HOH:O	1.94	0.50
1:A:274:GLN:OE1	4:A:2119:HOH:O	2.19	0.50
2:B:10:ILE:O	2:B:14:ARG:HG3	2.11	0.50
1:A:85:THR:HA	1:A:103:PRO:HA	1.94	0.49
2:B:84:VAL:O	2:B:88:ILE:HG13	2.12	0.49
1:D:85:THR:HA	1:D:103:PRO:HA	1.95	0.49
3:F:49:LEU:HD13	3:F:182:ILE:HD13	1.95	0.49
1:D:73:VAL:HG21	1:D:236:ASP:CB	2.43	0.48
2:E:126:SER:OG	2:E:127:PRO:HD2	2.14	0.48
1:D:235:LYS:O	1:D:236:ASP:HB2	2.12	0.48
2:E:231:LEU:HG	2:E:232:LEU:N	2.28	0.48
2:E:18:LEU:CD2	2:E:103:MSE:HE3	2.44	0.48
2:E:10:ILE:O	2:E:14:ARG:HG3	2.13	0.48
2:B:182:GLU:O	2:B:186:GLU:HG2	2.14	0.48
3:C:38:SER:HB3	3:C:186:ASN:HD21	1.79	0.48
3:F:38:SER:HB3	3:F:186:ASN:HD21	1.79	0.47
3:C:12:PHE:HZ	3:C:216:MSE:HE1	1.78	0.47
2:E:92:PRO:HD3	2:E:102:HIS:HD2	1.69	0.47
2:B:231:LEU:HG	2:B:232:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:ILE:CG2	2:E:78:MSE:HE1	2.44	0.47
3:F:202:SER:HA	3:F:205:GLN:HG3	1.97	0.47
3:C:179:LYS:HA	3:C:179:LYS:HD2	1.65	0.47
2:B:73:ILE:CG2	2:B:78:MSE:CE	2.93	0.47
2:E:18:LEU:N	2:E:18:LEU:HD22	2.29	0.46
1:A:73:VAL:CG2	1:A:236:ASP:HB2	2.44	0.46
1:D:73:VAL:CG2	1:D:236:ASP:HB2	2.45	0.46
2:B:53:TYR:CD1	2:B:101:LYS:HB3	2.51	0.46
1:D:338:PRO:HB2	1:D:339:PRO:HD3	1.97	0.46
2:B:126:SER:OG	2:B:127:PRO:HD2	2.16	0.46
2:E:53:TYR:CD1	2:E:101:LYS:HB3	2.51	0.46
1:A:235:LYS:O	1:A:236:ASP:HB2	2.15	0.46
1:A:73:VAL:HG21	1:A:236:ASP:CB	2.46	0.46
1:D:385:LYS:HG3	1:D:390:THR:HG21	1.96	0.46
2:E:182:GLU:O	2:E:186:GLU:HG2	2.16	0.45
2:B:18:LEU:HD22	2:B:18:LEU:N	2.31	0.45
2:E:84:VAL:O	2:E:88:ILE:HG13	2.16	0.45
3:F:202:SER:HA	3:F:205:GLN:CG	2.47	0.45
3:F:12:PHE:HZ	3:F:216:MSE:HE1	1.80	0.45
1:D:240:GLN:OE1	1:D:410:LYS:CE	2.45	0.45
2:E:154:TYR:CD1	2:E:155:PRO:HD2	2.52	0.44
1:A:338:PRO:HB2	1:A:339:PRO:HD3	1.98	0.44
2:E:73:ILE:CG2	2:E:78:MSE:CE	2.95	0.44
2:B:38:LEU:HD21	2:B:169:VAL:HG11	2.00	0.44
3:C:122:ARG:HG3	3:C:158:VAL:HG11	2.00	0.43
1:D:335:ILE:HD12	4:D:2131:HOH:O	2.16	0.43
4:B:2016:HOH:O	3:F:176:ARG:NH2	2.17	0.43
3:C:202:SER:HA	3:C:205:GLN:HG3	2.00	0.43
3:F:122:ARG:HG3	3:F:158:VAL:HG11	2.00	0.43
3:C:229:ALA:HB3	3:C:232:VAL:HG12	2.01	0.43
2:B:154:TYR:CD1	2:B:155:PRO:HD2	2.54	0.43
1:D:248:MSE:HA	1:D:249:PRO:HA	1.87	0.43
1:A:92:ASP:HB3	1:A:413:ILE:HB	2.00	0.43
1:A:359:GLN:HG3	2:B:216:LEU:HD23	2.01	0.43
3:C:38:SER:OG	3:C:188:ASP:OD2	2.31	0.43
2:E:200:ASP:O	2:E:224:SER:OG	2.36	0.43
3:C:49:LEU:HD13	3:C:182:ILE:HD13	2.01	0.43
2:E:38:LEU:HD21	2:E:169:VAL:HG11	2.01	0.43
2:B:7:ASN:HB3	2:B:10:ILE:HD12	2.01	0.43
2:B:18:LEU:CD2	2:B:103:MSE:HE3	2.49	0.42
3:C:120:LYS:HA	3:C:121:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:HD12	1:D:296:MSE:HG3	2.00	0.42
2:E:54:PRO:CG	2:E:102:HIS:CE1	2.99	0.42
1:A:274:GLN:NE2	4:A:2120:HOH:O	2.25	0.42
1:A:248:MSE:HA	1:A:249:PRO:HA	1.88	0.42
3:F:179:LYS:HA	3:F:179:LYS:HD2	1.72	0.42
2:B:207:VAL:HG22	2:B:217:GLU:HG3	2.01	0.42
3:C:122:ARG:HD2	3:C:161:LEU:HA	2.02	0.42
3:F:12:PHE:CE1	3:F:216:MSE:HE1	2.55	0.42
2:B:204:LEU:HD22	2:B:222:VAL:HG21	2.02	0.42
3:C:202:SER:HA	3:C:205:GLN:CG	2.50	0.42
1:A:156:LEU:HD12	1:A:296:MSE:HG3	2.02	0.42
1:A:235:LYS:HA	4:A:2081:HOH:O	2.19	0.42
3:F:122:ARG:HD2	3:F:161:LEU:HA	2.02	0.42
1:D:92:ASP:HB3	1:D:413:ILE:HB	2.02	0.41
2:E:78:MSE:HE3	2:E:83:LEU:CD1	2.46	0.41
2:E:92:PRO:HD3	2:E:102:HIS:HE2	1.83	0.41
2:B:210:ARG:NE	2:B:216:LEU:HD13	2.35	0.41
1:D:337:THR:HG23	4:D:2132:HOH:O	2.20	0.41
2:E:204:LEU:HD22	2:E:222:VAL:HG21	2.02	0.41
1:A:235:LYS:HG2	1:A:236:ASP:OD2	2.21	0.41
2:E:210:ARG:NE	2:E:216:LEU:HD13	2.35	0.41
1:A:350:SER:HB3	1:A:387:PRO:CD	2.48	0.41
2:B:65:LYS:HG3	2:B:72:PHE:CD1	2.56	0.41
3:C:26:SER:O	3:C:27:ASN:HB2	2.20	0.41
3:C:12:PHE:CE1	3:C:216:MSE:HE1	2.56	0.41
3:C:32:PHE:HB2	3:C:182:ILE:HG12	2.02	0.41
2:E:117:ILE:HD12	2:E:161:LEU:HD21	2.03	0.41
3:F:229:ALA:HB3	3:F:232:VAL:HG12	2.03	0.41
3:C:122:ARG:HG3	3:C:158:VAL:CG1	2.51	0.40
1:D:156:LEU:H	1:D:296:MSE:SE	2.54	0.40
1:D:363:GLU:HB3	4:D:2151:HOH:O	2.21	0.40
3:F:122:ARG:HG3	3:F:158:VAL:CG1	2.52	0.40
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.89	0.40
3:F:5:GLN:O	4:F:2001:HOH:O	2.22	0.40
3:C:5:GLN:O	4:C:2001:HOH:O	2.22	0.40
2:E:207:VAL:HG22	2:E:217:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/361 (75%)	260 (96%)	11 (4%)	0	100	100
1	D	274/361 (76%)	263 (96%)	11 (4%)	0	100	100
2	B	214/270 (79%)	207 (97%)	7 (3%)	0	100	100
2	E	215/270 (80%)	208 (97%)	7 (3%)	0	100	100
3	C	257/280 (92%)	245 (95%)	11 (4%)	1 (0%)	34	32
3	F	256/280 (91%)	246 (96%)	8 (3%)	2 (1%)	19	15
All	All	1487/1822 (82%)	1429 (96%)	55 (4%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	195	TYR
3	C	195	TYR
3	F	117	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	250/315 (79%)	244 (98%)	6 (2%)	49	53
1	D	252/315 (80%)	247 (98%)	5 (2%)	55	60
2	B	207/246 (84%)	198 (96%)	9 (4%)	29	29
2	E	208/246 (85%)	198 (95%)	10 (5%)	25	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	244/257 (95%)	239 (98%)	5 (2%)	55 60
3	F	243/257 (95%)	238 (98%)	5 (2%)	53 59
All	All	1404/1636 (86%)	1364 (97%)	40 (3%)	43 47

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	145	ARG
1	A	146	ASN
1	A	240	GLN
1	A	248	MSE
1	A	414	GLU
2	B	48	SER
2	B	52	GLU
2	B	122	SER
2	B	142	GLU
2	B	185	SER
2	B	191	PHE
2	B	211	LYS
2	B	216	LEU
2	B	231	LEU
3	C	68	MSE
3	C	74	ARG
3	C	79	LEU
3	C	97	LYS
3	C	216	MSE
1	D	70	SER
1	D	146	ASN
1	D	240	GLN
1	D	248	MSE
1	D	414	GLU
2	E	48	SER
2	E	52	GLU
2	E	101	LYS
2	E	122	SER
2	E	142	GLU
2	E	185	SER
2	E	191	PHE
2	E	211	LYS
2	E	216	LEU

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Mol	Chain	Res	Type
2	E	231	LEU
3	F	68	MSE
3	F	74	ARG
3	F	79	LEU
3	F	97	LYS
3	F	216	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	220	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	268/361 (74%)	-0.39	2 (0%)	87	89	20, 33, 56, 88	8 (2%)
1	D	271/361 (75%)	-0.30	7 (2%)	56	61	21, 35, 61, 106	12 (4%)
2	B	216/270 (80%)	-0.03	10 (4%)	32	38	27, 43, 75, 124	9 (4%)
2	E	217/270 (80%)	0.04	11 (5%)	28	33	27, 44, 80, 144	9 (4%)
3	C	260/280 (92%)	-0.10	3 (1%)	79	82	22, 35, 75, 190	7 (2%)
3	F	259/280 (92%)	-0.08	3 (1%)	79	82	22, 34, 76, 208	7 (2%)
All	All	1491/1822 (81%)	-0.15	36 (2%)	59	64	20, 36, 73, 208	52 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	142	GLU	7.6
1	D	419	PRO	5.2
2	B	6	HIS	5.1
2	B	142	GLU	5.1
1	D	418	ILE	4.0
2	E	52	GLU	3.7
2	B	99	ALA	3.5
2	B	176	THR	3.4
3	F	220	ASN	3.2
2	E	2	ALA	3.1
2	B	4	SER	3.0
2	B	180	ASP	3.0
2	E	150	TRP	2.7
1	D	145	ARG	2.7
2	E	99	ALA	2.7
3	C	229	ALA	2.7
3	F	226	THR	2.6
3	C	24	GLN	2.6
3	C	117	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	6	HIS	2.5
1	D	71	SER	2.5
2	B	230	GLU	2.5
2	B	178	THR	2.4
2	E	53	TYR	2.4
1	A	145	ARG	2.4
2	E	176	THR	2.4
2	B	149	ASP	2.4
2	E	88	ILE	2.3
2	B	177	GLY	2.3
1	D	136	ILE	2.2
1	A	234	TYR	2.2
3	F	20	ALA	2.1
1	D	367	ARG	2.1
2	E	233	SER	2.0
2	E	225	ASN	2.0
1	D	168	TYR	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.