Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 07:45 PM EDT

PDB ID	:	8F6D
Title	:	Crystal structure of the CNNM2 CBS-pair domain in complex with ARL15
Authors	:	Kozlov, G.; Mahbub, L.; Gehring, K.
Deposited on	:	2022-11-16
Resolution	:	3.20 Å(reported)

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

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

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

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

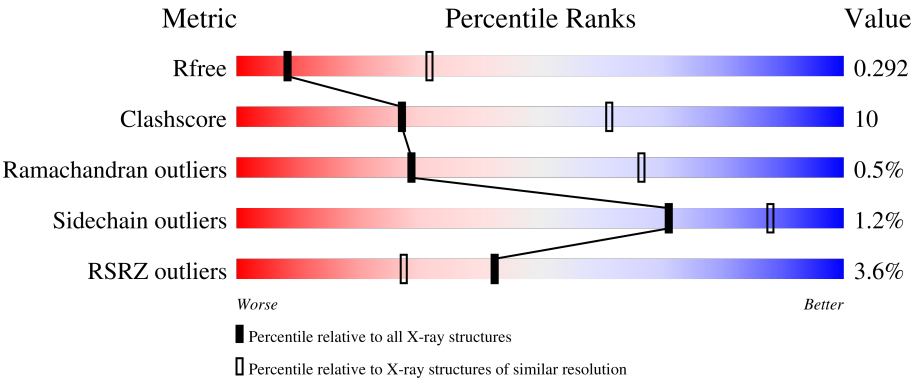
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	156	2% 87% 10%
1	C	156	2% 78% 14% 8%
1	E	156	% 67% 26% 6%
1	G	156	3% 69% 21% 9%
2	B	173	5% 69% 13% 18%

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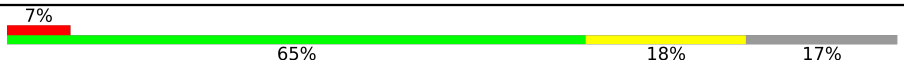
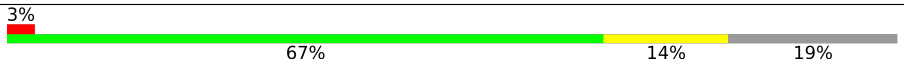
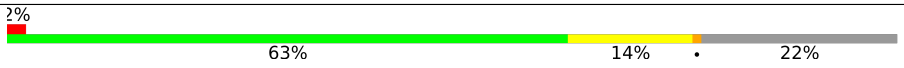
Mol	Chain	Length	Quality of chain
2	D	173	
2	F	173	
2	H	173	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7791 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 Metal transporter CNNM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1094	704	173	211	6			
1	C	144	Total	C	N	O	S	0	0	0
			1015	659	163	189	4			
1	E	146	Total	C	N	O	S	0	0	0
			1026	662	164	195	5			
1	G	142	Total	C	N	O	S	0	0	0
			978	639	155	178	6			

- Molecule 2 is a protein called ADP-ribosylation factor-like protein 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			944	604	162	175	3			
2	D	144	Total	C	N	O	S	0	0	0
			967	613	170	182	2			
2	F	140	Total	C	N	O	S	0	0	0
			957	611	163	179	4			
2	H	135	Total	C	N	O	S	0	0	0
			810	501	149	158	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	MET	-	initiating methionine	UNP Q9NXU5
B	198	HIS	-	expression tag	UNP Q9NXU5
B	199	HIS	-	expression tag	UNP Q9NXU5
B	200	HIS	-	expression tag	UNP Q9NXU5
B	201	HIS	-	expression tag	UNP Q9NXU5
B	202	HIS	-	expression tag	UNP Q9NXU5
B	203	HIS	-	expression tag	UNP Q9NXU5
D	31	MET	-	initiating methionine	UNP Q9NXU5

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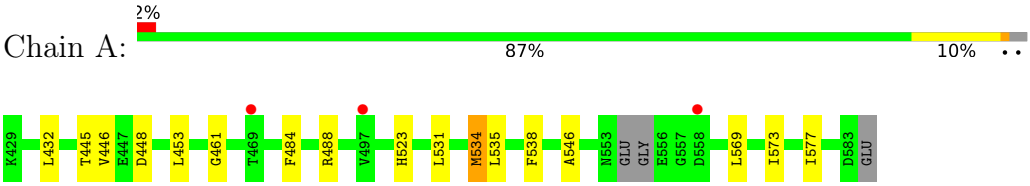
Chain	Residue	Modelled	Actual	Comment	Reference
D	198	HIS	-	expression tag	UNP Q9NXU5
D	199	HIS	-	expression tag	UNP Q9NXU5
D	200	HIS	-	expression tag	UNP Q9NXU5
D	201	HIS	-	expression tag	UNP Q9NXU5
D	202	HIS	-	expression tag	UNP Q9NXU5
D	203	HIS	-	expression tag	UNP Q9NXU5
F	31	MET	-	initiating methionine	UNP Q9NXU5
F	198	HIS	-	expression tag	UNP Q9NXU5
F	199	HIS	-	expression tag	UNP Q9NXU5
F	200	HIS	-	expression tag	UNP Q9NXU5
F	201	HIS	-	expression tag	UNP Q9NXU5
F	202	HIS	-	expression tag	UNP Q9NXU5
F	203	HIS	-	expression tag	UNP Q9NXU5
H	31	MET	-	initiating methionine	UNP Q9NXU5
H	198	HIS	-	expression tag	UNP Q9NXU5
H	199	HIS	-	expression tag	UNP Q9NXU5
H	200	HIS	-	expression tag	UNP Q9NXU5
H	201	HIS	-	expression tag	UNP Q9NXU5
H	202	HIS	-	expression tag	UNP Q9NXU5
H	203	HIS	-	expression tag	UNP Q9NXU5

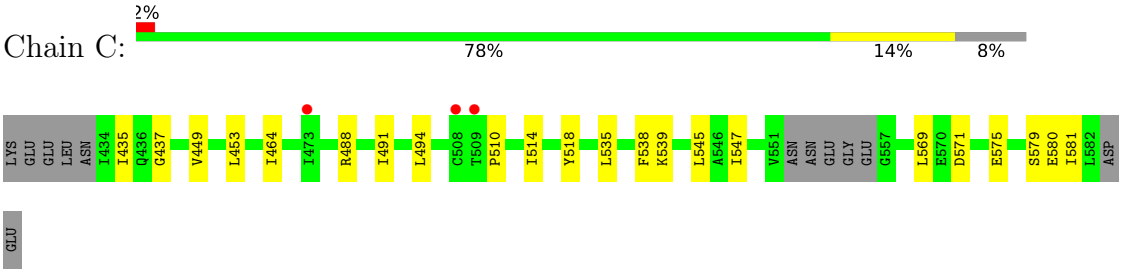
3 Residue-property plots (i)

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.

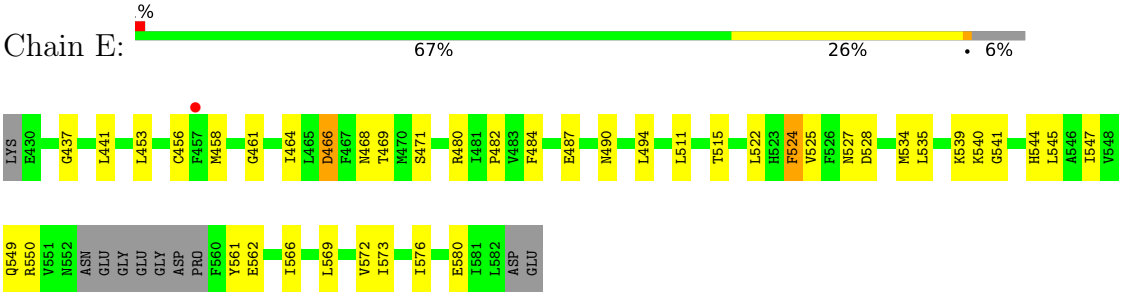
• Molecule 1: Metal transporter CNNM2



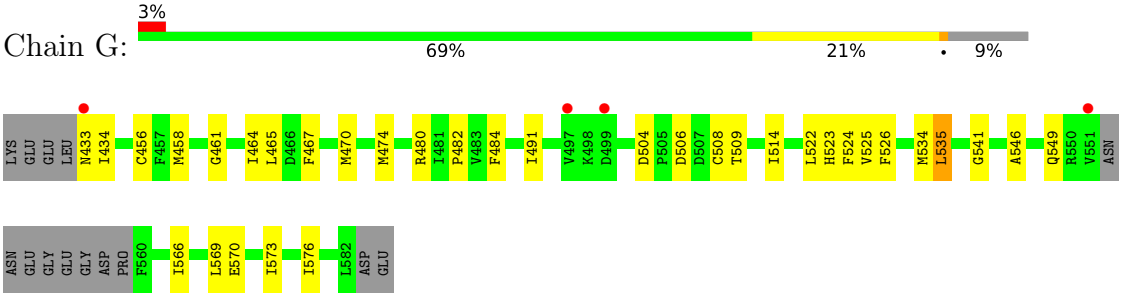
• Molecule 1: Metal transporter CNNM2



• Molecule 1: Metal transporter CNNM2

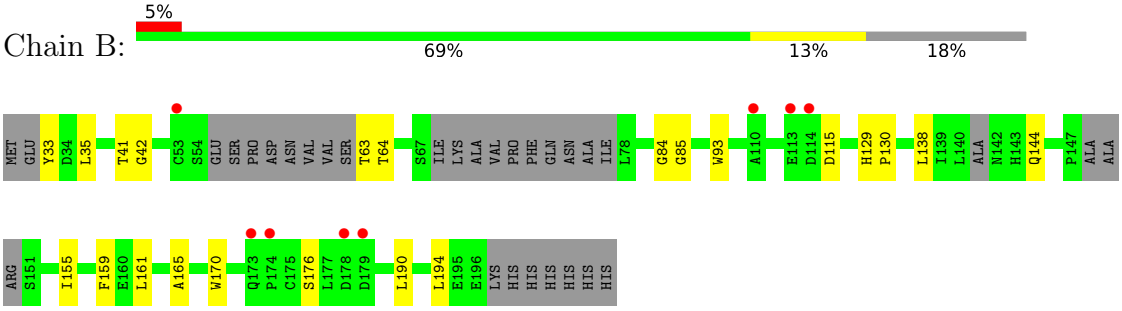


• Molecule 1: Metal transporter CNNM2



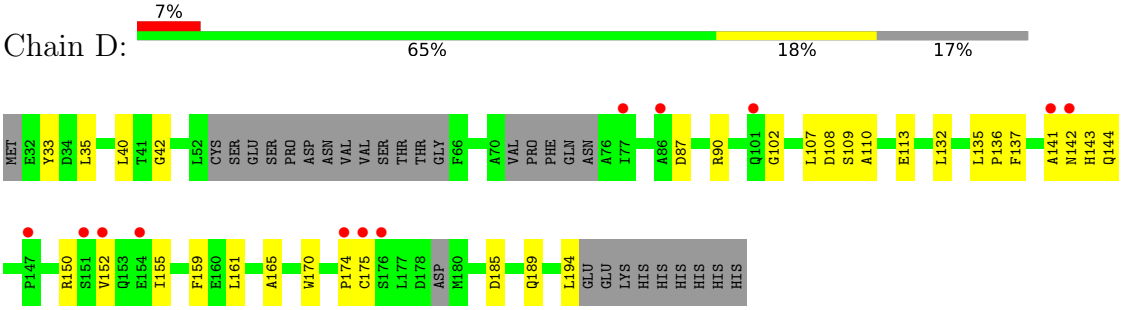
• Molecule 2: ADP-ribosylation factor-like protein 15

Chain B:



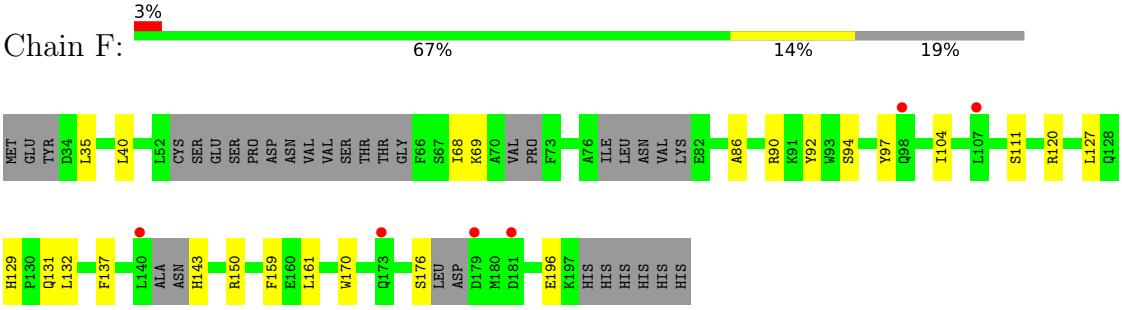
• Molecule 2: ADP-ribosylation factor-like protein 15

Chain D:



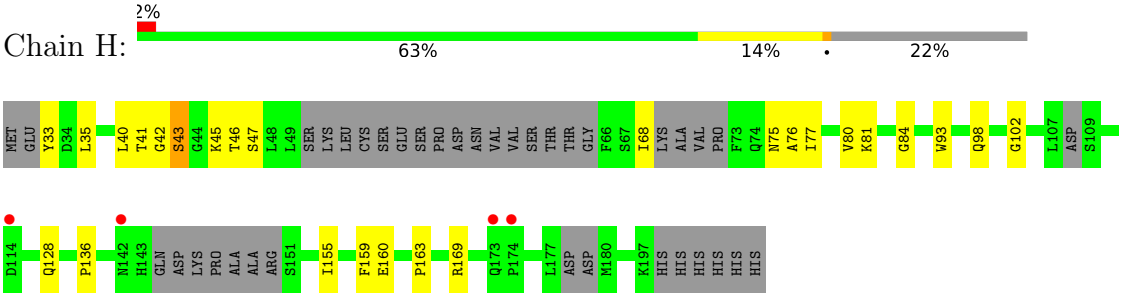
• Molecule 2: ADP-ribosylation factor-like protein 15

Chain F:



• Molecule 2: ADP-ribosylation factor-like protein 15

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.02Å 73.32Å 79.33Å 94.35° 95.50° 115.33°	Depositor
Resolution (Å)	29.53 – 3.20 29.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.53-3.20) 93.8 (29.53-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.264 , 0.293 0.264 , 0.292	Depositor DCC
R_{free} test set	1027 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	114.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 93.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7791	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.25	0/1111	0.48	0/1521
1	C	0.25	0/1032	0.51	0/1417
1	E	0.30	0/1043	0.59	0/1432
1	G	0.28	0/996	0.59	2/1369 (0.1%)
2	B	0.26	0/959	0.46	0/1312
2	D	0.28	0/983	0.54	0/1346
2	F	0.25	0/971	0.52	0/1319
2	H	0.26	0/816	0.47	0/1119
All	All	0.27	0/7911	0.52	2/10835 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	535	LEU	CA-CB-CG	5.56	128.09	115.30
1	G	569	LEU	CA-CB-CG	5.47	127.88	115.30

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	1094	0	1002	11	0
1	C	1015	0	926	13	0
1	E	1026	0	908	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	978	0	846	29	0
2	B	944	0	775	15	0
2	D	967	0	796	21	0
2	F	957	0	801	18	0
2	H	810	0	570	16	0
All	All	7791	0	6624	145	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 10.

All (145) 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:E:525:VAL:HG11	1:E:534:MET:HE1	1.51	0.91
1:G:433:ASN:HB3	1:G:434:ILE:HD12	1.66	0.78
2:B:63:THR:HG23	2:B:64:THR:HG23	1.64	0.77
1:E:573:ILE:HD12	1:G:535:LEU:HD11	1.65	0.77
1:E:544:HIS:HD2	1:G:541:GLY:HA3	1.53	0.74
1:E:544:HIS:O	1:E:544:HIS:ND1	2.22	0.72
2:H:136:PRO:HB3	2:H:169:ARG:HB2	1.73	0.70
2:H:33:TYR:N	2:H:77:ILE:O	2.25	0.70
1:A:446:VAL:HG11	1:A:534:MET:HG3	1.74	0.69
1:E:522:LEU:HB3	1:E:524:PHE:HE1	1.57	0.68
2:F:111:SER:O	2:F:150:ARG:NH1	2.25	0.68
2:D:152:VAL:HG21	2:D:174:PRO:HG3	1.75	0.67
1:E:540:LYS:O	1:G:480:ARG:NH2	2.28	0.67
2:B:165:ALA:HA	2:B:170:TRP:HZ3	1.59	0.67
1:E:480:ARG:HB3	1:E:494:LEU:HD21	1.77	0.67
2:B:155:ILE:O	2:B:159:PHE:HB2	1.95	0.66
1:E:573:ILE:HD12	1:G:535:LEU:CD1	2.25	0.66
2:B:35:LEU:HD21	2:B:194:LEU:HD21	1.78	0.66
1:C:453:LEU:O	1:C:488:ARG:NH2	2.27	0.66
2:D:165:ALA:O	2:D:170:TRP:NE1	2.29	0.66
1:E:535:LEU:HD22	1:G:573:ILE:CG2	2.27	0.64
1:E:524:PHE:CZ	1:E:547:ILE:HD11	2.32	0.64
2:F:159:PHE:HB3	2:F:161:LEU:HD13	1.79	0.64
1:E:544:HIS:CD2	1:G:541:GLY:HA3	2.32	0.64
1:E:545:LEU:HD11	1:E:566:ILE:HD12	1.79	0.63
2:D:142:ASN:OD1	2:D:143:HIS:N	2.32	0.63
1:A:538:PHE:HB3	1:A:569:LEU:HD12	1.80	0.63
1:G:573:ILE:HA	1:G:576:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:HIS:HD2	2:B:130:PRO:HD2	1.63	0.62
2:F:143:HIS:HA	2:F:176:SER:HA	1.81	0.62
2:H:75:ASN:OD1	2:H:76:ALA:N	2.34	0.61
1:A:445:THR:OG1	1:A:448:ASP:OD1	2.16	0.61
1:E:547:ILE:HG22	1:E:566:ILE:HG22	1.82	0.61
2:D:142:ASN:OD1	2:D:143:HIS:ND1	2.35	0.60
1:G:458:MET:HG2	1:G:482:PRO:HG2	1.84	0.59
2:H:84:GLY:O	2:H:93:TRP:NE1	2.31	0.59
1:E:522:LEU:O	2:F:94:SER:OG	2.21	0.59
1:E:569:LEU:O	1:E:573:ILE:HG12	2.03	0.59
2:F:86:ALA:O	2:F:90:ARG:HG3	2.02	0.59
2:D:87:ASP:HA	2:D:90:ARG:HG3	1.85	0.59
1:E:535:LEU:HD22	1:G:573:ILE:HG21	1.85	0.59
2:F:94:SER:HA	2:F:97:TYR:CD2	2.38	0.58
2:H:40:LEU:O	2:H:42:GLY:N	2.36	0.58
1:E:458:MET:HG2	1:E:482:PRO:HG2	1.86	0.58
1:C:494:LEU:HD21	1:C:545:LEU:HD22	1.86	0.58
2:H:155:ILE:O	2:H:159:PHE:HB2	2.04	0.57
2:B:165:ALA:HA	2:B:170:TRP:CZ3	2.40	0.57
2:D:35:LEU:HD21	2:D:194:LEU:HD21	1.86	0.57
2:D:132:LEU:O	2:D:135:LEU:HB2	2.05	0.56
1:C:449:VAL:HG22	1:C:571:ASP:HB3	1.87	0.56
1:A:453:LEU:O	1:A:488:ARG:NH2	2.38	0.55
1:E:525:VAL:HG21	1:E:534:MET:HE2	1.87	0.55
2:B:144:GLN:HA	2:B:176:SER:HB3	1.87	0.55
2:F:35:LEU:HD13	2:F:104:ILE:HD12	1.89	0.55
1:C:435:ILE:O	1:C:437:GLY:N	2.38	0.55
1:G:523:HIS:HB3	1:G:546:ALA:HA	1.89	0.54
1:E:453:LEU:HA	1:E:456:CYS:SG	2.46	0.54
1:E:550:ARG:N	1:E:562:GLU:O	2.31	0.54
2:B:161:LEU:O	2:B:165:ALA:HB3	2.07	0.54
2:B:33:TYR:HD2	2:B:194:LEU:HD23	1.72	0.54
2:D:102:GLY:HA2	2:D:136:PRO:HD2	1.91	0.53
2:H:42:GLY:O	2:H:45:LYS:N	2.42	0.53
2:D:107:LEU:HD11	2:D:155:ILE:HD13	1.89	0.53
1:C:579:SER:O	1:C:581:ILE:HG13	2.08	0.53
1:G:525:VAL:HG11	1:G:534:MET:SD	2.49	0.53
1:G:525:VAL:HA	2:H:98:GLN:OE1	2.08	0.53
2:F:97:TYR:CE1	2:F:132:LEU:HD11	2.45	0.52
2:D:113:GLU:OE1	2:D:113:GLU:N	2.34	0.52
1:E:511:LEU:O	1:E:515:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:PHE:HB2	2:F:170:TRP:CD1	2.45	0.52
2:B:159:PHE:HB3	2:B:161:LEU:HG	1.92	0.52
2:H:43:SER:O	2:H:47:SER:OG	2.14	0.51
2:B:129:HIS:CD2	2:B:130:PRO:HD2	2.46	0.51
2:H:42:GLY:O	2:H:46:THR:N	2.29	0.51
2:H:35:LEU:HB2	2:H:80:VAL:HG22	1.94	0.50
2:D:108:ASP:OD1	2:D:110:ALA:N	2.44	0.50
1:G:456:CYS:SG	1:G:566:ILE:HG12	2.52	0.50
1:E:527:ASN:OD1	1:E:528:ASP:N	2.45	0.49
1:E:524:PHE:HB3	1:E:549:GLN:HE21	1.77	0.49
2:F:94:SER:HA	2:F:97:TYR:CE2	2.48	0.49
2:B:84:GLY:O	2:B:93:TRP:NE1	2.41	0.48
2:D:185:ASP:O	2:D:189:GLN:HG3	2.14	0.48
1:E:466:ASP:OD1	1:E:468:ASN:N	2.45	0.48
1:E:437:GLY:O	1:E:441:LEU:HD13	2.14	0.48
1:E:535:LEU:HD23	1:E:535:LEU:O	2.14	0.48
1:G:522:LEU:HD13	1:G:524:PHE:HE1	1.80	0.47
1:E:461:GLY:N	1:E:484:PHE:O	2.45	0.47
1:E:535:LEU:HD22	1:G:573:ILE:HG23	1.95	0.47
2:B:41:THR:O	2:B:41:THR:OG1	2.32	0.47
2:B:138:LEU:HB2	2:B:190:LEU:HD13	1.97	0.47
1:C:538:PHE:HB3	1:C:569:LEU:HD12	1.96	0.47
1:G:461:GLY:N	1:G:484:PHE:O	2.47	0.47
1:A:531:LEU:O	1:A:535:LEU:HB2	2.14	0.47
1:G:482:PRO:HB2	1:G:491:ILE:HD13	1.95	0.47
2:D:107:LEU:HD11	2:D:155:ILE:CD1	2.45	0.47
2:F:97:TYR:CD1	2:F:132:LEU:HD11	2.49	0.47
2:F:68:ILE:O	2:F:69:LYS:HG3	2.15	0.46
1:A:573:ILE:HD12	1:C:539:LYS:HA	1.96	0.46
1:G:506:ASP:C	1:G:508:CYS:H	2.19	0.46
2:D:33:TYR:CG	2:D:194:LEU:HD23	2.50	0.46
1:A:573:ILE:HD13	1:C:535:LEU:HG	1.97	0.46
2:D:141:ALA:O	2:D:144:GLN:NE2	2.49	0.46
1:E:539:LYS:CD	1:G:570:GLU:HA	2.46	0.46
1:G:434:ILE:HD12	1:G:434:ILE:H	1.81	0.46
1:E:464:ILE:O	1:E:469:THR:OG1	2.29	0.45
1:A:573:ILE:O	1:A:577:ILE:HG12	2.16	0.45
2:F:94:SER:HA	2:F:97:TYR:HD2	1.80	0.45
2:H:40:LEU:O	2:H:43:SER:N	2.49	0.45
1:E:541:GLY:HA3	1:G:480:ARG:NH2	2.31	0.45
2:D:109:SER:HG	2:D:150:ARG:H	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:GLU:O	2:H:163:PRO:HD2	2.17	0.44
1:G:465:LEU:HB2	1:G:509:THR:O	2.18	0.44
1:E:549:GLN:OE1	1:E:561:TYR:HB3	2.17	0.44
1:E:572:VAL:O	1:E:576:ILE:HG13	2.18	0.44
1:A:523:HIS:HB3	1:A:546:ALA:HA	2.01	0.43
1:C:514:ILE:HD11	1:C:518:TYR:HE2	1.83	0.43
2:D:109:SER:OG	2:D:150:ARG:N	2.24	0.43
2:D:159:PHE:HB3	2:D:161:LEU:HG	2.00	0.43
2:H:68:ILE:HA	2:H:81:LYS:HA	2.01	0.43
2:D:107:LEU:HD22	2:D:159:PHE:CZ	2.53	0.42
1:E:490:ASN:CG	2:F:92:TYR:HH	2.19	0.42
1:G:434:ILE:HD12	1:G:434:ILE:N	2.34	0.42
1:A:461:GLY:N	1:A:484:PHE:O	2.52	0.42
1:E:453:LEU:HD12	1:E:456:CYS:SG	2.60	0.42
2:H:40:LEU:C	2:H:42:GLY:N	2.73	0.42
1:E:468:ASN:O	1:E:471:SER:OG	2.38	0.42
1:A:432:LEU:CD1	1:G:514:ILE:HD12	2.50	0.41
2:B:42:GLY:HA3	2:B:85:GLY:H	1.85	0.41
1:C:464:ILE:HD12	1:C:510:PRO:HA	2.03	0.41
1:C:571:ASP:O	1:C:575:GLU:HG2	2.20	0.41
1:E:524:PHE:HB3	1:E:549:GLN:NE2	2.36	0.41
2:F:129:HIS:CE1	2:F:131:GLN:HB2	2.56	0.41
1:G:464:ILE:HD11	1:G:508:CYS:HB3	2.02	0.41
1:G:526:PHE:HA	1:G:549:GLN:O	2.21	0.41
2:D:142:ASN:HA	2:D:175:CYS:O	2.21	0.41
2:F:127:LEU:HD12	2:F:137:PHE:CE2	2.56	0.41
1:C:494:LEU:HD23	1:C:494:LEU:HA	1.92	0.40
1:G:470:MET:O	1:G:474:MET:HG2	2.21	0.40
1:E:487:GLU:HA	1:E:487:GLU:OE1	2.21	0.40
2:F:40:LEU:HD12	2:F:40:LEU:HA	1.85	0.40
2:D:40:LEU:HA	2:D:40:LEU:HD12	1.90	0.40
2:H:102:GLY:HA2	2:H:136:PRO:HD2	2.04	0.40
1:C:491:ILE:HD12	1:C:547:ILE:HG12	2.03	0.40
2:F:120:ARG:HD3	2:F:159:PHE:HA	2.03	0.40
1:G:504:ASP:C	1:G:506:ASP:H	2.24	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	149/156 (96%)	149 (100%)	0	0	100 100
1	C	140/156 (90%)	136 (97%)	3 (2%)	1 (1%)	22 61
1	E	142/156 (91%)	138 (97%)	3 (2%)	1 (1%)	22 61
1	G	138/156 (88%)	135 (98%)	3 (2%)	0	100 100
2	B	132/173 (76%)	129 (98%)	3 (2%)	0	100 100
2	D	136/173 (79%)	133 (98%)	2 (2%)	1 (1%)	22 61
2	F	128/173 (74%)	126 (98%)	2 (2%)	0	100 100
2	H	123/173 (71%)	120 (98%)	1 (1%)	2 (2%)	9 43
All	All	1088/1316 (83%)	1066 (98%)	17 (2%)	5 (0%)	29 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	580	GLU
1	E	580	GLU
2	H	41	THR
2	H	43	SER
2	D	42	GLY

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	108/143 (76%)	107 (99%)	1 (1%)	78 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	95/143 (66%)	95 (100%)	0	100 100
1	E	95/143 (66%)	93 (98%)	2 (2%)	53 79
1	G	84/143 (59%)	83 (99%)	1 (1%)	71 88
2	B	72/152 (47%)	71 (99%)	1 (1%)	67 86
2	D	74/152 (49%)	73 (99%)	1 (1%)	67 86
2	F	74/152 (49%)	73 (99%)	1 (1%)	67 86
2	H	45/152 (30%)	44 (98%)	1 (2%)	52 79
All	All	647/1180 (55%)	639 (99%)	8 (1%)	71 88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	MET
2	B	115	ASP
2	D	137	PHE
1	E	466	ASP
1	E	524	PHE
2	F	196	GLU
1	G	467	PHE
2	H	128	GLN

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

Mol	Chain	Res	Type
2	B	129	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

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	153/156 (98%)	-0.21	3 (1%) 65 51	59, 96, 142, 166	0
1	C	144/156 (92%)	-0.26	3 (2%) 63 49	58, 103, 152, 192	0
1	E	146/156 (93%)	-0.45	1 (0%) 87 81	64, 101, 137, 147	0
1	G	142/156 (91%)	-0.30	4 (2%) 53 37	71, 114, 144, 162	0
2	B	142/173 (82%)	0.30	8 (5%) 24 13	74, 137, 177, 196	0
2	D	144/173 (83%)	0.19	12 (8%) 11 6	75, 132, 162, 176	0
2	F	140/173 (80%)	-0.04	6 (4%) 35 22	58, 120, 156, 164	0
2	H	135/173 (78%)	-0.14	4 (2%) 50 34	87, 139, 174, 187	0
All	All	1146/1316 (87%)	-0.11	41 (3%) 42 27	58, 117, 163, 196	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	ALA	5.6
2	B	110	ALA	4.0
2	F	173	GLN	3.9
2	F	140	LEU	3.7
1	C	508	CYS	3.6
2	F	179	ASP	3.5
2	B	178	ASP	3.4
2	B	114	ASP	3.3
2	B	174	PRO	3.1
1	C	509	THR	3.0
2	H	174	PRO	2.9
1	G	499	ASP	2.9
2	B	53	CYS	2.9
1	A	558	ASP	2.8
2	D	151	SER	2.8
2	D	101	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	173	GLN	2.8
1	A	497	VAL	2.6
2	H	142	ASN	2.6
2	D	77	ILE	2.5
1	G	551	VAL	2.5
2	D	174	PRO	2.5
2	F	181	ASP	2.5
2	D	152	VAL	2.4
2	D	176	SER	2.3
2	F	107	LEU	2.3
2	B	113	GLU	2.3
2	B	173	GLN	2.3
2	D	86	ALA	2.3
1	G	497	VAL	2.3
1	E	457	PHE	2.2
2	F	98	GLN	2.2
1	C	473	ILE	2.2
2	D	175	CYS	2.1
1	G	433	ASN	2.1
2	B	179	ASP	2.1
2	D	142	ASN	2.1
2	D	154	GLU	2.1
2	D	147	PRO	2.1
1	A	469	THR	2.0
2	H	114	ASP	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.