Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:19 am BST

PDB ID	:	6FJY
Title	:	Crystal structure of CsuC-CsuE chaperone-tip adhesion subunit pre-assembly complex from archaic chaperone-usher Csu pili of Acinetobacter baumannii
Authors	:	Pakharukova, N.A.; Tuitilla, M.; Paavilainen, S.; Zavialov, A.V.
Deposited on	:	2018-01-23
Resolution	:	2.31 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 ①) were used in the production of this report:

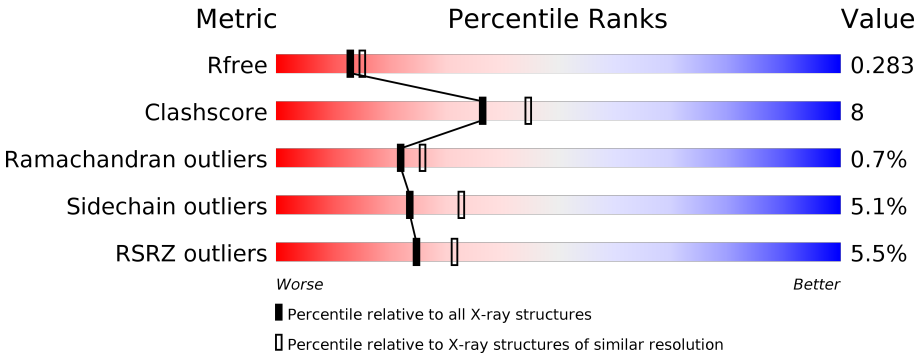
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	250	4% 61% 22% • 14%
1	C	250	8% 66% 12% • 21%
2	B	312	3% 76% 15% • 7%
3	D	312	5% 78% 14% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7724 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 CsuC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1684	1078	286	316	4			
1	C	197	Total	C	N	O	S	0	0	0
			1519	971	261	283	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q6XBY4
A	245	HIS	-	expression tag	UNP Q6XBY4
A	246	HIS	-	expression tag	UNP Q6XBY4
A	247	HIS	-	expression tag	UNP Q6XBY4
A	248	HIS	-	expression tag	UNP Q6XBY4
A	249	HIS	-	expression tag	UNP Q6XBY4
A	250	HIS	-	expression tag	UNP Q6XBY4
C	244	GLY	-	expression tag	UNP Q6XBY4
C	245	HIS	-	expression tag	UNP Q6XBY4
C	246	HIS	-	expression tag	UNP Q6XBY4
C	247	HIS	-	expression tag	UNP Q6XBY4
C	248	HIS	-	expression tag	UNP Q6XBY4
C	249	HIS	-	expression tag	UNP Q6XBY4
C	250	HIS	-	expression tag	UNP Q6XBY4

- Molecule 2 is a protein called Protein CsuE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2220	1405	368	437	10			

- Molecule 3 is a protein called Protein CsuE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	291	Total	C	N	O	S	0	0	0
			2206	1390	365	441	10			

- Molecule 4 is water.

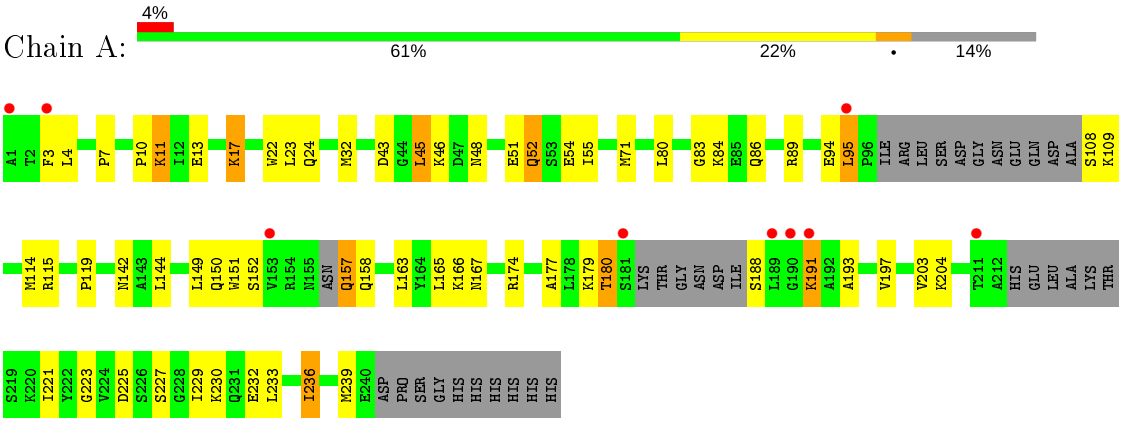
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	45	Total	O	0	0
			45	45		
4	C	11	Total	O	0	0
			11	11		
4	D	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

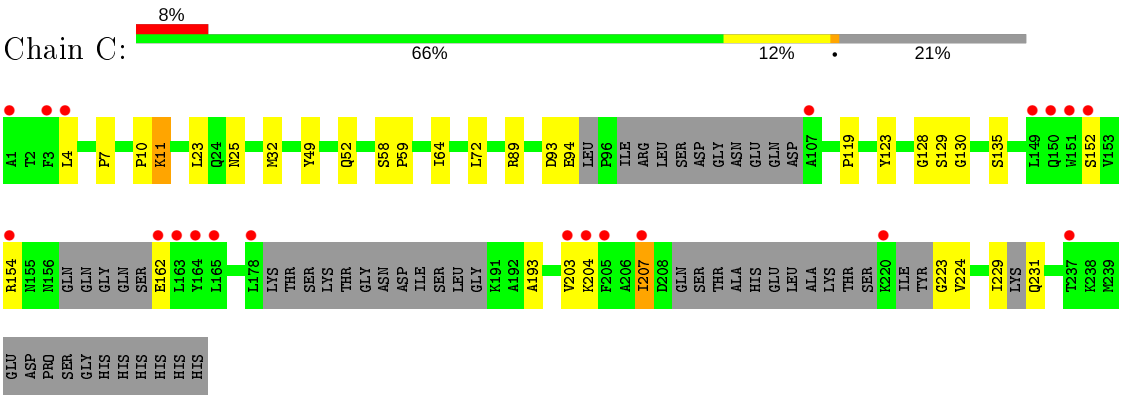
- Molecule 1: CsuC

Chain A:



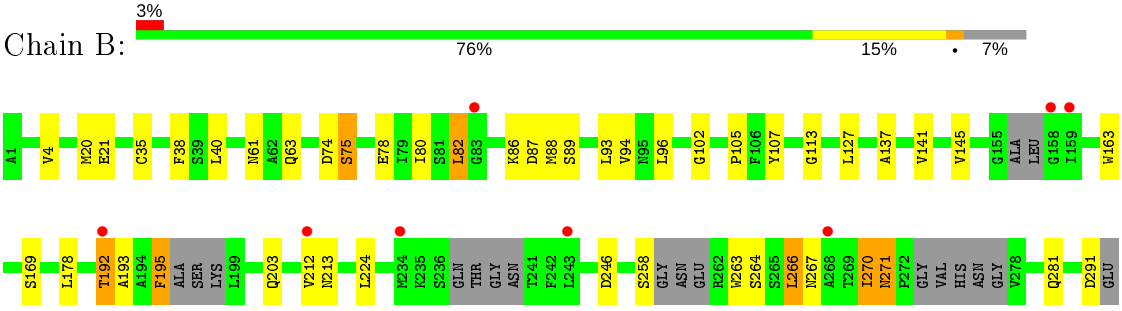
- Molecule 1: CsuC

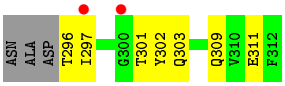
Chain C:



- Molecule 2: Protein CsuE

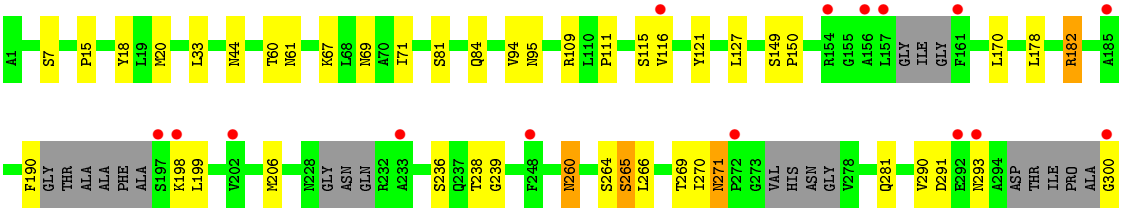
Chain B:





- Molecule 3: Protein CsuE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.84Å 63.85Å 89.25Å 74.65° 79.65° 69.07°	Depositor
Resolution (Å)	53.92 – 2.31 53.92 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.0 (53.92-2.31) 96.0 (53.92-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.216 , 0.272 0.237 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.9	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	0.94	EDS
Total number of atoms	7724	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

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	0.36	0/1712	0.57	0/2303
1	C	0.34	0/1541	0.56	0/2070
2	B	0.37	0/2241	0.57	0/3039
3	D	0.33	0/2248	0.54	0/3048
All	All	0.35	0/7742	0.56	0/10460

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

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	1684	0	1721	46	0
1	C	1519	0	1527	22	0
2	B	2220	0	2150	43	0
3	D	2206	0	2115	23	0
4	A	25	0	0	4	0
4	B	45	0	0	7	0
4	C	11	0	0	3	0
4	D	14	0	0	4	0
All	All	7724	0	7513	120	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 (120) 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:A:13:GLU:OE1	4:A:301:HOH:O	1.85	0.92
1:A:142:ASN:O	4:A:302:HOH:O	1.93	0.86
1:C:52:GLN:O	4:C:301:HOH:O	1.94	0.85
1:A:115:ARG:NH1	2:B:309:GLN:OE1	2.16	0.79
2:B:163:TRP:O	4:B:401:HOH:O	2.01	0.77
3:D:182:ARG:NH2	4:D:403:HOH:O	2.20	0.75
2:B:203:GLN:O	4:B:402:HOH:O	2.03	0.74
1:A:52:GLN:OE1	1:A:55:ILE:N	2.19	0.74
3:D:264:SER:O	3:D:266:LEU:N	2.22	0.73
1:A:191:LYS:HZ2	2:B:264:SER:H	1.38	0.71
2:B:75:SER:HB3	2:B:105:PRO:O	1.91	0.70
3:D:60:THR:HG22	3:D:67:LYS:HG2	1.73	0.69
1:A:51:GLU:OE1	4:A:303:HOH:O	2.10	0.68
1:A:45:LEU:HB3	1:A:204:LYS:HG2	1.75	0.67
2:B:63:GLN:OE1	4:B:405:HOH:O	2.14	0.66
2:B:271:ASN:OD1	2:B:271:ASN:N	2.29	0.65
3:D:44:ASN:O	4:D:402:HOH:O	2.15	0.65
1:C:7:PRO:HB3	3:D:178:LEU:HD13	1.77	0.65
1:A:46:LYS:NZ	1:A:48:ASN:OD1	2.29	0.64
1:C:32:MET:O	1:C:94:GLU:HB2	1.97	0.64
3:D:95:ASN:ND2	4:D:401:HOH:O	2.07	0.64
3:D:71:ILE:HB	3:D:109:ARG:HB3	1.80	0.63
2:B:137:ALA:HB3	2:B:145:VAL:HG13	1.81	0.62
2:B:75:SER:HA	2:B:107:TYR:HE2	1.63	0.61
2:B:74:ASP:O	2:B:75:SER:OG	2.14	0.61
2:B:296:THR:N	4:B:409:HOH:O	2.33	0.61
2:B:87:ASP:OD1	2:B:89:SER:OG	2.17	0.61
3:D:270:ILE:HD13	3:D:281:GLN:HG3	1.81	0.60
1:A:11:LYS:NZ	4:A:307:HOH:O	2.34	0.60
1:A:230:LYS:NZ	2:B:63:GLN:HB2	2.16	0.60
1:C:93:ASP:OD2	4:C:302:HOH:O	2.15	0.59
1:C:23:LEU:HD22	1:C:72:LEU:HD21	1.85	0.59
1:C:11:LYS:HG3	1:C:129:SER:HB3	1.86	0.56
3:D:260:ASN:OD1	3:D:260:ASN:N	2.37	0.56
3:D:271:ASN:N	3:D:271:ASN:OD1	2.38	0.56
1:A:150:GLN:HB3	1:A:239:MET:HG3	1.88	0.55
1:A:191:LYS:NZ	2:B:264:SER:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASP:HB3	2:B:80:ILE:HG22	1.89	0.54
1:A:149:LEU:HB3	1:A:236:ILE:HD12	1.90	0.54
1:A:80:LEU:HD22	1:A:86:GLN:HG3	1.90	0.53
1:A:221:ILE:HB	1:A:236:ILE:HG23	1.91	0.53
1:A:108:SER:HA	2:B:302:TYR:O	2.09	0.52
1:A:193:ALA:HA	2:B:266:LEU:HD22	1.91	0.52
2:B:21:GLU:OE1	4:B:407:HOH:O	2.18	0.52
1:C:23:LEU:HD13	1:C:72:LEU:HG	1.91	0.52
1:A:167:ASN:HB2	1:A:197:VAL:HG12	1.91	0.52
2:B:40:LEU:HD23	2:B:94:VAL:HG13	1.92	0.52
2:B:38:PHE:CD1	2:B:94:VAL:HG22	2.44	0.51
2:B:78:GLU:OE1	4:B:406:HOH:O	2.18	0.51
1:A:22:TRP:CZ3	1:A:71:MET:HB2	2.46	0.51
1:A:179:LYS:HD3	1:A:188:SER:N	2.26	0.50
1:C:10:PRO:HD2	1:C:119:PRO:O	2.11	0.50
2:B:82:LEU:HD12	2:B:82:LEU:H	1.77	0.50
1:C:193:ALA:HB2	3:D:264:SER:HB2	1.93	0.50
3:D:236:SER:OG	3:D:239:GLY:O	2.29	0.50
2:B:75:SER:HA	2:B:107:TYR:CE2	2.46	0.49
1:C:229:ILE:O	1:C:231:GLN:N	2.45	0.49
1:C:128:GLY:HA3	1:C:135:SER:HB2	1.95	0.49
1:A:52:GLN:HG2	1:A:54:GLU:H	1.77	0.48
2:B:74:ASP:HB3	2:B:80:ILE:CG2	2.43	0.48
1:C:129:SER:N	1:C:130:GLY:HA2	2.28	0.48
3:D:206:MET:HE1	3:D:308:VAL:HG11	1.95	0.48
1:A:17:LYS:HB2	1:A:17:LYS:HE3	1.76	0.48
1:A:179:LYS:HG2	1:A:180:THR:H	1.79	0.47
3:D:149:SER:HB2	3:D:150:PRO:HD2	1.96	0.47
1:A:191:LYS:HZ1	2:B:263:TRP:HA	1.80	0.47
1:A:4:LEU:HD22	1:A:24:GLN:HB3	1.97	0.46
1:C:123:TYR:CZ	1:C:129:SER:HA	2.51	0.46
1:A:43:ASP:O	1:A:48:ASN:ND2	2.44	0.46
2:B:192:THR:OG1	2:B:193:ALA:N	2.47	0.45
2:B:78:GLU:HB2	4:B:406:HOH:O	2.16	0.45
1:A:230:LYS:O	1:A:232:GLU:HG2	2.17	0.45
1:A:10:PRO:HD2	1:A:119:PRO:O	2.17	0.45
3:D:190:PHE:HB3	3:D:199:LEU:HD22	1.99	0.45
1:A:151:TRP:HB3	1:A:236:ILE:HD11	1.99	0.45
2:B:61:ASN:HD21	2:B:63:GLN:NE2	2.15	0.45
1:C:4:LEU:HD12	3:D:182:ARG:NH2	2.31	0.45
3:D:238:THR:OG1	3:D:239:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLY:O	1:A:233:LEU:HD12	2.17	0.45
1:A:149:LEU:HA	1:A:166:LYS:O	2.16	0.44
1:A:152:SER:HB3	1:A:239:MET:HB2	1.99	0.44
1:A:225:ASP:OD2	1:A:227:SER:OG	2.27	0.44
2:B:270:ILE:HB	2:B:281:GLN:HG3	1.99	0.44
1:C:25:ASN:HB2	1:C:64:ILE:HG22	2.00	0.44
3:D:61:ASN:HB2	3:D:121:TYR:CE2	2.53	0.44
3:D:69:ASN:O	3:D:111:PRO:HD2	2.18	0.44
1:A:3:PHE:CZ	1:A:23:LEU:HD22	2.53	0.44
1:A:174:ARG:N	1:A:225:ASP:OD1	2.46	0.44
1:A:7:PRO:HB3	2:B:178:LEU:HD13	2.00	0.44
2:B:291:ASP:OD2	2:B:297:ILE:HG12	2.18	0.44
2:B:93:LEU:HD12	2:B:96:LEU:HD12	2.00	0.43
1:A:177:ALA:O	1:A:223:GLY:HA2	2.18	0.43
2:B:61:ASN:HD21	2:B:63:GLN:HE22	1.66	0.43
1:C:152:SER:OG	1:C:154:ARG:NH1	2.51	0.43
1:C:4:LEU:HD12	3:D:182:ARG:HH22	1.83	0.43
1:A:94:GLU:HB3	1:A:114:MET:HB2	2.00	0.43
1:A:230:LYS:HB2	1:A:230:LYS:HE3	1.83	0.43
1:C:223:GLY:N	4:C:304:HOH:O	2.50	0.43
2:B:86:LYS:HE2	2:B:88:MET:HG2	2.01	0.43
2:B:4:VAL:HG13	2:B:169:SER:HB3	2.01	0.43
2:B:88:MET:O	2:B:93:LEU:HD22	2.18	0.43
1:C:49:TYR:CE1	1:C:89:ARG:HG3	2.53	0.43
1:A:83:GLY:O	1:A:84:LYS:HD2	2.19	0.43
2:B:20:MET:O	2:B:113:GLY:HA2	2.19	0.43
1:A:109:LYS:HG2	2:B:303:GLN:HG2	2.01	0.42
1:A:89:ARG:NH2	2:B:311:GLU:HG3	2.33	0.42
3:D:20:MET:HG3	3:D:115:SER:HB2	2.01	0.42
1:A:157:GLN:CD	1:A:158:GLN:H	2.22	0.42
2:B:195:PHE:HB3	2:B:297:ILE:O	2.19	0.42
1:A:163:LEU:O	1:A:204:LYS:HA	2.20	0.41
2:B:212:VAL:HG13	2:B:213:ASN:N	2.36	0.41
3:D:15:PRO:HG2	3:D:18:TYR:HB3	2.02	0.41
1:A:32:MET:O	1:A:95:LEU:HG	2.21	0.41
2:B:35:CYS:O	2:B:102:GLY:HA3	2.21	0.41
3:D:300:GLY:N	4:D:408:HOH:O	2.53	0.41
1:A:83:GLY:C	1:A:84:LYS:HD2	2.41	0.41
1:C:207:ILE:O	1:C:207:ILE:HG13	2.21	0.41
1:C:58:SER:HA	1:C:59:PRO:HA	1.93	0.41
2:B:267:ASN:HA	2:B:267:ASN:HD22	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:HA	1:C:207:ILE:HG12	2.03	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	206/250 (82%)	195 (95%)	11 (5%)	0	100	100
1	C	183/250 (73%)	176 (96%)	6 (3%)	1 (0%)	29	35
2	B	275/312 (88%)	256 (93%)	16 (6%)	3 (1%)	14	15
3	D	279/312 (89%)	259 (93%)	17 (6%)	3 (1%)	14	15
All	All	943/1124 (84%)	886 (94%)	50 (5%)	7 (1%)	22	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	ILE
3	D	265	SER
2	B	192	THR
3	D	293	ASN
3	D	269	THR
2	B	75	SER
2	B	301	THR

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	182/214 (85%)	169 (93%)	13 (7%)	14	19
1	C	160/214 (75%)	156 (98%)	4 (2%)	47	64
2	B	247/261 (95%)	237 (96%)	10 (4%)	31	44
3	D	247/263 (94%)	231 (94%)	16 (6%)	17	22
All	All	836/952 (88%)	793 (95%)	43 (5%)	24	33

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	17	LYS
1	A	45	LEU
1	A	52	GLN
1	A	95	LEU
1	A	144	LEU
1	A	157	GLN
1	A	165	LEU
1	A	180	THR
1	A	191	LYS
1	A	203	VAL
1	A	229	ILE
1	A	236	ILE
2	B	82	LEU
2	B	127	LEU
2	B	141	VAL
2	B	195	PHE
2	B	224	LEU
2	B	246	ASP
2	B	258	SER
2	B	266	LEU
2	B	270	ILE
2	B	271	ASN
1	C	11	LYS
1	C	203	VAL
1	C	204	LYS
1	C	224	VAL
3	D	7	SER
3	D	33	LEU
3	D	81	SER

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Mol	Chain	Res	Type
3	D	84	GLN
3	D	94	VAL
3	D	116	VAL
3	D	127	LEU
3	D	170	LEU
3	D	182	ARG
3	D	198	LYS
3	D	260	ASN
3	D	265	SER
3	D	271	ASN
3	D	290	VAL
3	D	291	ASP
3	D	301	THR

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

Mol	Chain	Res	Type
2	B	267	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLY	B	49	2	9,10,11	0.73	0	6,11,13	0.78	0
2	MLY	B	67	2	9,10,11	0.66	0	6,11,13	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	49	2	-	2/8/9/11	-
2	MLY	B	67	2	-	1/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	67	MLY	CG-CD-CE-NZ
2	B	49	MLY	CA-CB-CG-CD
2	B	49	MLY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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, 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	216/250 (86%)	0.57	9 (4%) 36 43	44, 69, 120, 142	0
1	C	197/250 (78%)	0.65	20 (10%) 6 10	52, 78, 119, 151	0
2	B	289/312 (92%)	0.51	10 (3%) 44 51	46, 64, 106, 132	0
3	D	291/312 (93%)	0.64	16 (5%) 25 31	56, 80, 113, 145	0
All	All	993/1124 (88%)	0.59	55 (5%) 25 31	44, 73, 115, 151	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	157	LEU	5.7
3	D	197	SER	5.3
1	C	163	LEU	4.4
1	C	152	SER	4.1
3	D	292	GLU	4.0
1	C	107	ALA	3.8
1	C	150	GLN	3.8
2	B	297	ILE	3.5
3	D	161	PHE	3.5
1	A	190	GLY	3.4
2	B	300	GLY	3.4
1	C	164	TYR	3.3
3	D	198	LYS	3.2
1	A	211	THR	3.1
2	B	192	THR	3.1
1	C	165	LEU	3.0
1	C	154	ARG	3.0
2	B	158	GLY	3.0
3	D	202	VAL	3.0
1	C	149	LEU	2.9
2	B	268	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	156	ALA	2.8
2	B	83	GLY	2.8
1	A	153	VAL	2.7
1	C	237	THR	2.7
1	C	3	PHE	2.7
1	C	151	TRP	2.6
3	D	272	PRO	2.6
1	C	1	ALA	2.5
1	A	3	PHE	2.5
1	C	4	LEU	2.4
1	C	203	VAL	2.4
1	C	162	GLU	2.4
3	D	293	ASN	2.4
3	D	300	GLY	2.3
1	A	189	LEU	2.3
3	D	116	VAL	2.3
1	A	1	ALA	2.3
1	C	204	LYS	2.2
2	B	234	MET	2.2
1	C	205	PHE	2.2
3	D	233	ALA	2.2
1	C	178	LEU	2.2
3	D	301	THR	2.2
1	A	181	SER	2.2
1	C	207	ILE	2.2
1	A	95	LEU	2.2
2	B	243	LEU	2.1
3	D	248	PHE	2.1
1	A	191	LYS	2.1
2	B	159	ILE	2.0
3	D	185	ALA	2.0
2	B	212	VAL	2.0
1	C	220	LYS	2.0
3	D	154	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLY	B	49	11/12	0.86	0.23	52,63,81,82	0
2	MLY	B	67	11/12	0.91	0.17	45,62,93,94	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.