Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:16 am BST

PDB ID	:	4CBV
Title	:	X-ray structure of full-length ComE from Streptococcus pneumoniae.
Authors	:	Boudes, M.; Durand, D.; Graille, M.; van Tilbeurgh, H.; Quevillon-Cheruel, S.
Deposited on	:	2013-10-16
Resolution	:	3.39 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:

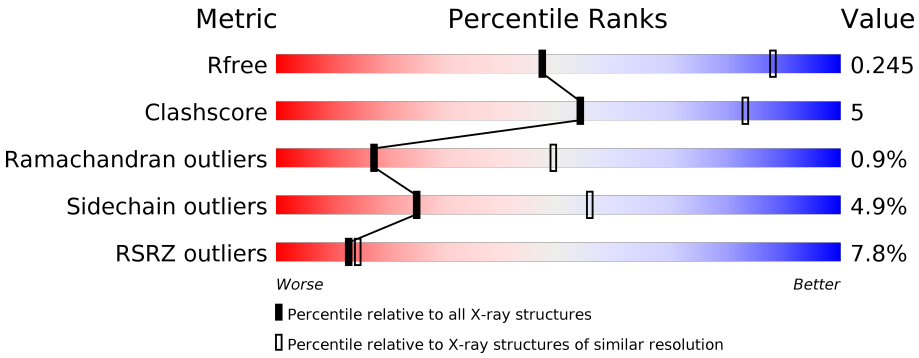
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	256	76% 20%
1	B	256	75% 22%
1	C	256	6% 80% 16%
1	D	256	15% 84% 13%
1	E	256	19% 81% 15%
1	F	256	5% 84% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12732 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 COME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	Se	0	0	0
			2123	1368	355	395	1	4			
1	B	251	Total	C	N	O	S	Se	0	0	0
			2123	1368	355	395	1	4			
1	C	249	Total	C	N	O	S	Se	0	0	0
			2104	1356	350	393	1	4			
1	D	250	Total	C	N	O	S	Se	0	0	0
			2113	1362	352	394	1	4			
1	E	248	Total	C	N	O	S	Se	0	0	0
			2096	1351	349	392	1	3			
1	F	256	Total	C	N	O	S	Se	0	0	0
			2173	1398	370	400	1	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	HIS	-	expression tag	UNP Q79CK7
A	252	HIS	-	expression tag	UNP Q79CK7
A	253	HIS	-	expression tag	UNP Q79CK7
A	254	HIS	-	expression tag	UNP Q79CK7
A	255	HIS	-	expression tag	UNP Q79CK7
A	256	HIS	-	expression tag	UNP Q79CK7
A	58	ALA	ASP	engineered mutation	UNP Q79CK7
B	251	HIS	-	expression tag	UNP Q79CK7
B	252	HIS	-	expression tag	UNP Q79CK7
B	253	HIS	-	expression tag	UNP Q79CK7
B	254	HIS	-	expression tag	UNP Q79CK7
B	255	HIS	-	expression tag	UNP Q79CK7
B	256	HIS	-	expression tag	UNP Q79CK7
B	58	ALA	ASP	engineered mutation	UNP Q79CK7
C	251	HIS	-	expression tag	UNP Q79CK7
C	252	HIS	-	expression tag	UNP Q79CK7
C	253	HIS	-	expression tag	UNP Q79CK7

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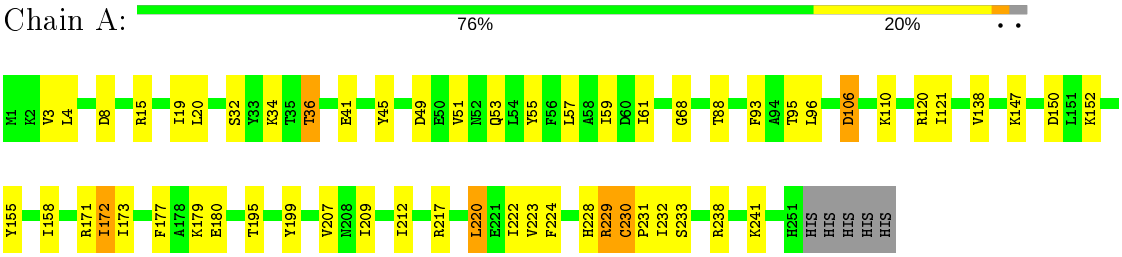
Chain	Residue	Modelled	Actual	Comment	Reference
C	254	HIS	-	expression tag	UNP Q79CK7
C	255	HIS	-	expression tag	UNP Q79CK7
C	256	HIS	-	expression tag	UNP Q79CK7
C	58	ALA	ASP	engineered mutation	UNP Q79CK7
D	251	HIS	-	expression tag	UNP Q79CK7
D	252	HIS	-	expression tag	UNP Q79CK7
D	253	HIS	-	expression tag	UNP Q79CK7
D	254	HIS	-	expression tag	UNP Q79CK7
D	255	HIS	-	expression tag	UNP Q79CK7
D	256	HIS	-	expression tag	UNP Q79CK7
D	58	ALA	ASP	engineered mutation	UNP Q79CK7
E	251	HIS	-	expression tag	UNP Q79CK7
E	252	HIS	-	expression tag	UNP Q79CK7
E	253	HIS	-	expression tag	UNP Q79CK7
E	254	HIS	-	expression tag	UNP Q79CK7
E	255	HIS	-	expression tag	UNP Q79CK7
E	256	HIS	-	expression tag	UNP Q79CK7
E	58	ALA	ASP	engineered mutation	UNP Q79CK7
F	251	HIS	-	expression tag	UNP Q79CK7
F	252	HIS	-	expression tag	UNP Q79CK7
F	253	HIS	-	expression tag	UNP Q79CK7
F	254	HIS	-	expression tag	UNP Q79CK7
F	255	HIS	-	expression tag	UNP Q79CK7
F	256	HIS	-	expression tag	UNP Q79CK7
F	58	ALA	ASP	engineered mutation	UNP Q79CK7

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.

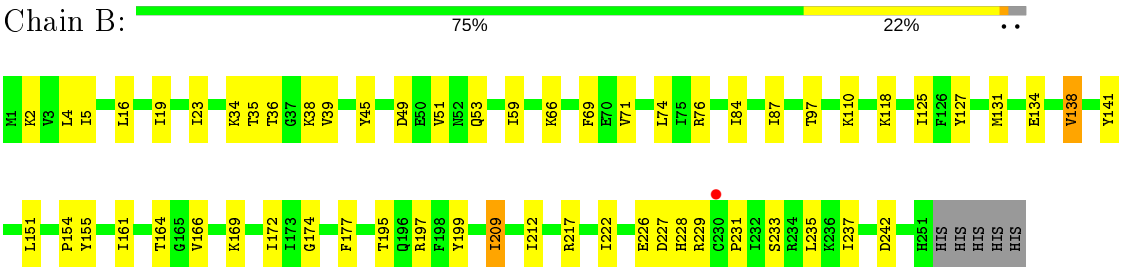
- Molecule 1: COME

Chain A:



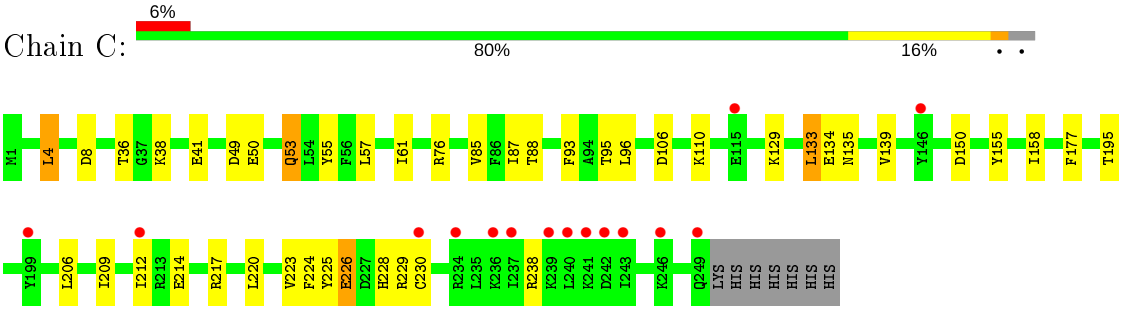
- Molecule 1: COME

Chain B:



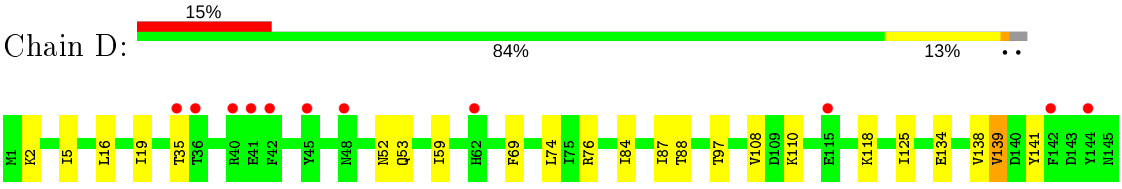
- Molecule 1: COME

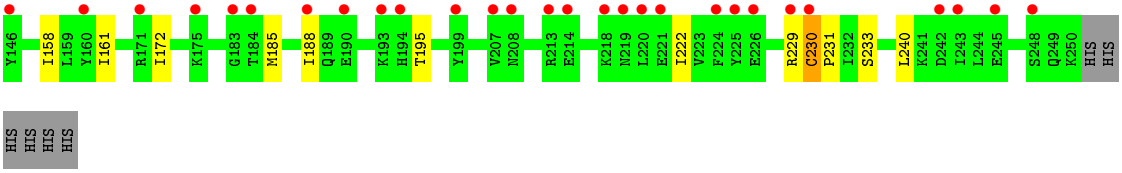
Chain C:



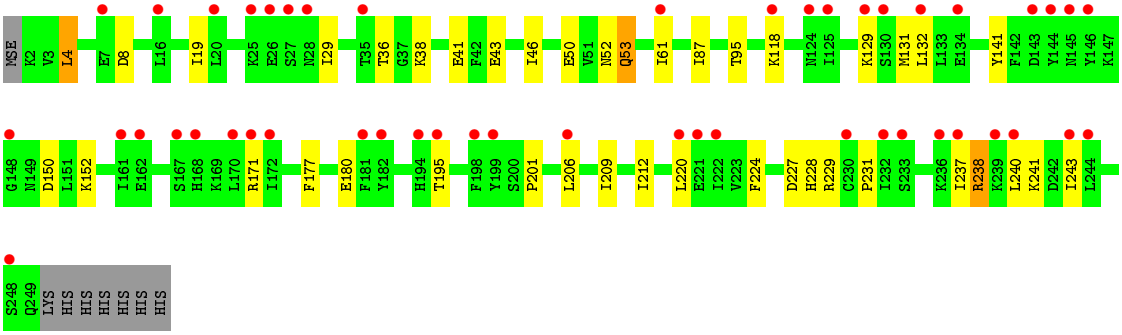
- Molecule 1: COME

Chain D:

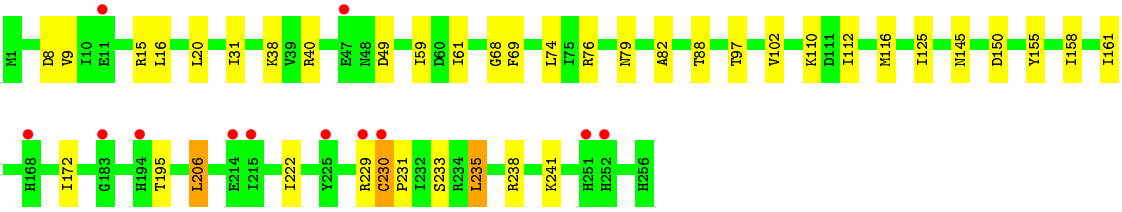




- Molecule 1: COME



- Molecule 1: COME



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	88.89Å 135.00Å 461.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.95 – 3.39 44.45 – 3.39	Depositor EDS
% Data completeness (in resolution range)	96.3 (37.95-3.39) 96.3 (44.45-3.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.196 , 0.223 0.212 , 0.245	Depositor DCC
R_{free} test set	1898 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12732	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.42	0/2163	0.65	0/2903
1	B	0.40	0/2163	0.64	0/2903
1	C	0.39	0/2143	0.59	0/2877
1	D	0.40	0/2152	0.57	0/2888
1	E	0.41	0/2135	0.57	0/2867
1	F	0.39	0/2218	0.58	0/2978
All	All	0.40	0/12974	0.60	0/17416

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	2123	0	2132	34	0
1	B	2123	0	2132	25	0
1	C	2104	0	2112	21	0
1	D	2113	0	2125	19	0
1	E	2096	0	2100	18	0
1	F	2173	0	2167	19	1
All	All	12732	0	12768	134	1

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 5.

All (134) 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:49:ASP:HB2	1:A:53:GLN:HG3	1.51	0.92
1:A:224:PHE:HE1	1:A:231:PRO:HD2	1.43	0.83
1:A:93:PHE:HA	1:A:96:LEU:HD23	1.67	0.76
1:C:224:PHE:HB2	1:C:228:HIS:HB2	1.72	0.71
1:C:36:THR:HG21	1:C:41:GLU:HB3	1.75	0.68
1:E:220:LEU:HD13	1:E:238:ARG:HH22	1.61	0.65
1:E:36:THR:HG21	1:E:41:GLU:HB3	1.78	0.65
1:A:224:PHE:HE1	1:A:231:PRO:CD	2.10	0.64
1:B:161:ILE:HG12	1:B:172:ILE:HD13	1.80	0.63
1:E:224:PHE:HE1	1:E:231:PRO:HG2	1.64	0.63
1:B:45:TYR:HA	1:B:49:ASP:HB3	1.80	0.62
1:B:59:ILE:HG23	1:B:66:LYS:HA	1.82	0.61
1:D:138:VAL:HG23	1:D:139:VAL:HG22	1.82	0.61
1:A:223:VAL:HG22	1:A:229:ARG:HG2	1.83	0.61
1:B:5:ILE:HB	1:B:35:THR:HG22	1.82	0.61
1:C:55:TYR:HB3	1:C:57:LEU:HD13	1.83	0.61
1:F:230:CYS:H	1:F:231:PRO:HD2	1.66	0.59
1:E:29:ILE:HG21	1:E:129:LYS:HD2	1.85	0.59
1:F:59:ILE:HD12	1:F:88:THR:HG21	1.84	0.59
1:A:199:TYR:HB2	1:A:209:ILE:HD11	1.86	0.57
1:D:230:CYS:H	1:D:231:PRO:HD2	1.69	0.57
1:A:220:LEU:HD13	1:A:238:ARG:HH22	1.70	0.56
1:D:134:GLU:HA	1:D:138:VAL:HG21	1.87	0.56
1:A:55:TYR:HB3	1:A:57:LEU:HD13	1.88	0.56
1:A:222:ILE:HD11	1:A:241:LYS:HE2	1.87	0.55
1:C:36:THR:HG22	1:C:38:LYS:H	1.70	0.55
1:E:209:ILE:HA	1:E:212:ILE:HD12	1.88	0.55
1:A:233:SER:HB3	1:A:238:ARG:HH21	1.70	0.55
1:C:50:GLU:HB2	1:C:53:GLN:HG2	1.87	0.55
1:C:214:GLU:HB3	1:C:223:VAL:HB	1.88	0.55
1:A:59:ILE:HA	1:A:68:GLY:HA3	1.89	0.55
1:C:93:PHE:HA	1:C:96:LEU:HD23	1.89	0.55
1:A:15:ARG:O	1:A:19:ILE:HG12	2.07	0.54
1:D:5:ILE:HB	1:D:35:THR:HG22	1.90	0.54
1:F:112:ILE:HD12	1:F:116:MSE:HB3	1.90	0.54
1:B:199:TYR:HB2	1:B:209:ILE:HD12	1.89	0.54
1:E:50:GLU:HB2	1:E:53:GLN:HG2	1.89	0.54
1:B:222:ILE:HB	1:B:231:PRO:HG2	1.90	0.54
1:A:224:PHE:CE1	1:A:231:PRO:HD2	2.33	0.53
1:C:217:ARG:HH11	1:C:238:ARG:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ILE:HG12	1:D:172:ILE:HD13	1.91	0.52
1:B:164:THR:HG22	1:B:169:LYS:O	2.10	0.51
1:B:87:ILE:HG22	1:B:110:LYS:HD3	1.93	0.51
1:E:50:GLU:H	1:E:53:GLN:HG3	1.75	0.51
1:E:224:PHE:CE1	1:E:231:PRO:HG2	2.46	0.51
1:A:230:CYS:HB2	1:A:231:PRO:HD3	1.93	0.50
1:D:139:VAL:HG23	1:D:141:TYR:CE1	2.46	0.50
1:C:88:THR:HA	1:C:110:LYS:HE3	1.94	0.50
1:F:222:ILE:HB	1:F:231:PRO:HG2	1.93	0.50
1:E:201:PRO:HA	1:E:237:ILE:HG21	1.94	0.49
1:E:4:LEU:HD13	1:E:53:GLN:HE22	1.75	0.49
1:F:155:TYR:HA	1:F:158:ILE:HD12	1.93	0.49
1:A:232:ILE:H	1:A:232:ILE:HD12	1.77	0.49
1:C:49:ASP:HB2	1:C:53:GLN:HG3	1.93	0.49
1:B:212:ILE:HG23	1:B:222:ILE:HG23	1.94	0.49
1:D:59:ILE:HD12	1:D:88:THR:HG21	1.94	0.49
1:B:127:TYR:O	1:B:131:MSE:HG2	2.12	0.49
1:F:20:LEU:HD22	1:F:31:ILE:HG21	1.95	0.49
1:A:51:VAL:HG22	1:A:179:LYS:HG2	1.94	0.49
1:A:8:ASP:HB3	1:A:61:ILE:HG23	1.95	0.49
1:D:19:ILE:HG23	1:D:118:LYS:HG3	1.95	0.49
1:E:224:PHE:HB2	1:E:228:HIS:HB2	1.95	0.49
1:A:158:ILE:HG12	1:A:172:ILE:HD11	1.95	0.48
1:C:223:VAL:HG22	1:C:229:ARG:HG2	1.94	0.48
1:D:76:ARG:HH21	1:D:84:ILE:HG12	1.79	0.48
1:C:209:ILE:HA	1:C:212:ILE:HD12	1.94	0.48
1:D:222:ILE:HB	1:D:231:PRO:HG2	1.94	0.48
1:A:224:PHE:HB2	1:A:228:HIS:HB2	1.95	0.48
1:D:158:ILE:HG23	1:D:172:ILE:HG23	1.96	0.48
1:D:2:LYS:H	1:D:53:GLN:HG2	1.77	0.48
1:E:36:THR:HG22	1:E:38:LYS:H	1.78	0.47
1:F:15:ARG:HH11	1:F:110:LYS:HE3	1.79	0.47
1:C:4:LEU:HD13	1:C:53:GLN:HE22	1.77	0.47
1:E:8:ASP:HB3	1:E:61:ILE:HG23	1.95	0.47
1:F:79:ASN:HB3	1:F:82:ALA:HB2	1.97	0.47
1:C:8:ASP:HB3	1:C:61:ILE:HG23	1.96	0.46
1:E:240:LEU:HD13	1:E:243:ILE:HD11	1.97	0.46
1:E:171:ARG:HG3	1:E:180:GLU:HG2	1.96	0.46
1:F:230:CYS:H	1:F:231:PRO:CD	2.29	0.46
1:F:222:ILE:HG12	1:F:241:LYS:HE3	1.98	0.46
1:B:141:TYR:HA	1:B:154:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ILE:HG12	1:F:172:ILE:HD13	1.97	0.46
1:E:43:GLU:HA	1:E:46:ILE:HD12	1.97	0.46
1:B:69:PHE:HE1	1:B:97:THR:HG22	1.80	0.45
1:F:145:ASN:HD22	1:F:150:ASP:HB3	1.81	0.45
1:B:19:ILE:HG23	1:B:118:LYS:HG3	1.98	0.45
1:F:59:ILE:HA	1:F:68:GLY:HA3	1.98	0.45
1:D:87:ILE:HG13	1:D:108:VAL:HB	1.98	0.45
1:F:38:LYS:HE3	1:F:40:ARG:HG3	1.98	0.45
1:B:226:GLU:O	1:B:228:HIS:N	2.50	0.45
1:B:2:LYS:H	1:B:53:GLN:HG2	1.82	0.45
1:F:235:LEU:HD12	1:F:238:ARG:HH22	1.80	0.45
1:A:34:LYS:HB3	1:A:45:TYR:CE2	2.53	0.44
1:B:76:ARG:NH2	1:B:84:ILE:HG12	2.32	0.44
1:D:87:ILE:HG23	1:D:110:LYS:HD3	1.99	0.44
1:A:220:LEU:HA	1:A:238:ARG:NH2	2.32	0.44
1:B:38:LYS:HZ2	1:B:39:VAL:H	1.64	0.44
1:C:226:GLU:HG3	1:D:134:GLU:HB2	2.00	0.44
1:F:76:ARG:HD2	1:F:102:VAL:HA	2.00	0.44
1:A:106:ASP:OD1	1:A:120:ARG:NH2	2.51	0.44
1:D:69:PHE:HE1	1:D:97:THR:HG22	1.81	0.44
1:A:220:LEU:HD13	1:A:238:ARG:HH12	1.82	0.43
1:F:69:PHE:HE1	1:F:97:THR:HG22	1.84	0.43
1:A:232:ILE:N	1:A:232:ILE:HD12	2.33	0.43
1:B:4:LEU:HD23	1:B:34:LYS:HB3	2.00	0.43
1:C:129:LYS:HE3	1:C:133:LEU:HD13	1.99	0.43
1:C:155:TYR:HA	1:C:158:ILE:HD12	2.00	0.43
1:A:138:VAL:HG21	1:A:152:LYS:HE3	2.01	0.43
1:F:8:ASP:HB3	1:F:61:ILE:HG23	2.01	0.43
1:C:220:LEU:HD13	1:C:238:ARG:HH12	1.84	0.42
1:A:36:THR:HG21	1:A:41:GLU:HB3	2.01	0.42
1:A:4:LEU:HD21	1:A:45:TYR:HB3	2.01	0.42
1:B:134:GLU:HA	1:B:138:VAL:CG2	2.49	0.42
1:C:85:VAL:HG13	1:C:106:ASP:HB3	2.00	0.42
1:A:217:ARG:HD2	1:A:238:ARG:HD2	2.01	0.42
1:B:69:PHE:CE1	1:B:97:THR:HG22	2.54	0.42
1:E:52:ASN:HD21	1:E:152:LYS:H	1.66	0.42
1:F:161:ILE:HD12	1:F:206:LEU:HD12	2.01	0.42
1:D:222:ILE:HD11	1:D:233:SER:HB2	2.02	0.42
1:A:155:TYR:HA	1:A:158:ILE:HD12	2.02	0.41
1:A:88:THR:HA	1:A:110:LYS:HE3	2.02	0.41
1:B:166:VAL:HG13	1:B:169:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLY:HA3	1:B:177:PHE:CE1	2.55	0.41
1:E:19:ILE:HG23	1:E:118:LYS:HG3	2.02	0.41
1:B:134:GLU:HA	1:B:138:VAL:HG22	2.02	0.41
1:B:155:TYR:CZ	1:B:197:ARG:HD3	2.56	0.41
1:A:171:ARG:NH1	1:A:180:GLU:OE2	2.54	0.41
1:A:3:VAL:HG11	1:A:20:LEU:HD21	2.03	0.41
1:D:185:MSE:HA	1:D:188:ILE:HD12	2.04	0.40
1:C:93:PHE:HD1	1:C:96:LEU:HD23	1.86	0.40
1:C:225:TYR:HB3	1:D:134:GLU:O	2.20	0.40
1:A:207:VAL:HG12	1:A:231:PRO:HG2	2.03	0.40
1:A:209:ILE:HA	1:A:212:ILE:HD12	2.03	0.40
1:B:38:LYS:HA	1:B:38:LYS:HZ3	1.87	0.40

All (1) 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:F:116:MSE:CE	1:F:116:MSE:CE[3_655]	0.63	1.57

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	249/256 (97%)	236 (95%)	11 (4%)	2 (1%)	19	51
1	B	249/256 (97%)	235 (94%)	12 (5%)	2 (1%)	19	51
1	C	247/256 (96%)	231 (94%)	12 (5%)	4 (2%)	9	34
1	D	248/256 (97%)	239 (96%)	8 (3%)	1 (0%)	34	67
1	E	246/256 (96%)	232 (94%)	12 (5%)	2 (1%)	19	51
1	F	254/256 (99%)	242 (95%)	10 (4%)	2 (1%)	19	51
All	All	1493/1536 (97%)	1415 (95%)	65 (4%)	13 (1%)	17	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	VAL
1	B	227	ASP
1	C	134	GLU
1	A	229	ARG
1	F	49	ASP
1	A	230	CYS
1	E	131	MSE
1	C	135	ASN
1	C	226	GLU
1	F	230	CYS
1	C	139	VAL
1	D	230	CYS
1	E	227	ASP

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	237/238 (100%)	225 (95%)	12 (5%)	24	54
1	B	237/238 (100%)	221 (93%)	16 (7%)	16	45
1	C	235/238 (99%)	224 (95%)	11 (5%)	26	57
1	D	236/238 (99%)	228 (97%)	8 (3%)	37	65
1	E	234/238 (98%)	221 (94%)	13 (6%)	21	51
1	F	242/238 (102%)	233 (96%)	9 (4%)	34	62
All	All	1421/1428 (100%)	1352 (95%)	69 (5%)	25	55

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	36	THR
1	A	95	THR
1	A	106	ASP

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Mol	Chain	Res	Type
1	A	121	ILE
1	A	147	LYS
1	A	150	ASP
1	A	172	ILE
1	A	173	ILE
1	A	177	PHE
1	A	195	THR
1	A	220	LEU
1	B	16	LEU
1	B	23	ILE
1	B	36	THR
1	B	71	VAL
1	B	74	LEU
1	B	125	ILE
1	B	138	VAL
1	B	151	LEU
1	B	195	THR
1	B	209	ILE
1	B	217	ARG
1	B	229	ARG
1	B	233	SER
1	B	235	LEU
1	B	237	ILE
1	B	242	ASP
1	C	4	LEU
1	C	53	GLN
1	C	76	ARG
1	C	87	ILE
1	C	95	THR
1	C	133	LEU
1	C	150	ASP
1	C	177	PHE
1	C	195	THR
1	C	206	LEU
1	C	230	CYS
1	D	16	LEU
1	D	52	ASN
1	D	74	LEU
1	D	125	ILE
1	D	139	VAL
1	D	195	THR
1	D	229	ARG

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Mol	Chain	Res	Type
1	D	240	LEU
1	E	4	LEU
1	E	53	GLN
1	E	87	ILE
1	E	95	THR
1	E	132	LEU
1	E	141	TYR
1	E	150	ASP
1	E	177	PHE
1	E	195	THR
1	E	206	LEU
1	E	229	ARG
1	E	238	ARG
1	E	241	LYS
1	F	9	VAL
1	F	16	LEU
1	F	74	LEU
1	F	125	ILE
1	F	195	THR
1	F	206	LEU
1	F	229	ARG
1	F	233	SER
1	F	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	B	53	GLN
1	B	77	HIS
1	B	228	HIS
1	D	145	ASN
1	D	176	ASN
1	E	52	ASN
1	F	48	ASN
1	F	145	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 carbohydrates 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	247/256 (96%)	-0.05	0 100 100	35, 60, 104, 150	0
1	B	247/256 (96%)	0.09	1 (0%) 92 92	35, 67, 109, 184	0
1	C	245/256 (95%)	0.41	15 (6%) 21 22	74, 116, 163, 206	0
1	D	246/256 (96%)	0.87	39 (15%) 1 2	86, 140, 185, 212	0
1	E	245/256 (95%)	1.03	48 (19%) 1 1	119, 158, 192, 220	0
1	F	252/256 (98%)	0.47	12 (4%) 30 31	94, 125, 159, 171	0
All	All	1482/1536 (96%)	0.47	115 (7%) 13 14	35, 118, 179, 220	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	GLU	7.9
1	D	225	TYR	5.6
1	D	144	TYR	5.3
1	E	199	TYR	5.1
1	E	168	HIS	4.9
1	E	182	TYR	4.1
1	E	240	LEU	4.1
1	D	199	TYR	4.0
1	F	47	GLU	4.0
1	D	230	CYS	3.9
1	E	230	CYS	3.9
1	E	146	TYR	3.9
1	D	171	ARG	3.8
1	D	40	ARG	3.7
1	E	144	TYR	3.7
1	D	213	ARG	3.6
1	E	148	GLY	3.6
1	C	230	CYS	3.5
1	D	142	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	236	LYS	3.4
1	D	243	ILE	3.4
1	E	26	GLU	3.4
1	E	132	LEU	3.3
1	D	229	ARG	3.3
1	E	194	HIS	3.3
1	D	36	THR	3.3
1	D	214	GLU	3.3
1	E	161	ILE	3.2
1	E	16	LEU	3.2
1	E	124	ASN	3.2
1	D	242	ASP	3.2
1	E	239	LYS	3.2
1	E	220	LEU	3.2
1	D	219	ASN	3.2
1	D	48	ASN	3.1
1	B	230	CYS	3.1
1	D	218	LYS	3.1
1	C	236	LYS	3.1
1	F	214	GLU	3.1
1	D	35	THR	3.1
1	E	35	THR	3.0
1	D	194	HIS	3.0
1	F	230	CYS	3.0
1	C	146	TYR	3.0
1	D	188	ILE	3.0
1	D	41	GLU	3.0
1	E	167	SER	2.9
1	E	222	ILE	2.9
1	F	229	ARG	2.9
1	E	145	ASN	2.9
1	E	25	LYS	2.8
1	C	246	LYS	2.8
1	E	28	ASN	2.8
1	F	225	TYR	2.8
1	D	184	THR	2.8
1	E	195	THR	2.8
1	D	146	TYR	2.7
1	C	241	LYS	2.7
1	E	7	GLU	2.7
1	D	175	LYS	2.7
1	F	183	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	199	TYR	2.7
1	D	207	VAL	2.7
1	D	224	PHE	2.6
1	D	62	HIS	2.6
1	D	226	GLU	2.6
1	E	118	LYS	2.5
1	D	245	GLU	2.5
1	C	212	ILE	2.5
1	E	61	ILE	2.4
1	D	160	TYR	2.4
1	E	232	ILE	2.4
1	E	198	PHE	2.4
1	D	190	GLU	2.4
1	F	251	HIS	2.4
1	F	194	HIS	2.4
1	D	193	LYS	2.4
1	F	215	ILE	2.4
1	D	220	LEU	2.3
1	F	168	HIS	2.3
1	D	115	GLU	2.3
1	C	242	ASP	2.3
1	C	234	ARG	2.3
1	D	248	SER	2.3
1	D	183	GLY	2.3
1	C	115	GLU	2.3
1	E	125	ILE	2.3
1	E	181	PHE	2.3
1	D	208	ASN	2.3
1	E	129	LYS	2.2
1	D	42	PHE	2.2
1	E	237	ILE	2.2
1	D	45	TYR	2.2
1	C	249	GLN	2.2
1	E	20	LEU	2.2
1	E	170	LEU	2.2
1	C	237	ILE	2.2
1	F	11	GLU	2.2
1	C	239	LYS	2.1
1	C	243	ILE	2.1
1	E	27	SER	2.1
1	D	221	GLU	2.1
1	E	206	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	244	LEU	2.1
1	E	143	ASP	2.1
1	F	252	HIS	2.1
1	E	243	ILE	2.1
1	E	248	SER	2.1
1	E	134	GLU	2.1
1	E	130	SER	2.0
1	E	172	ILE	2.0
1	E	233	SER	2.0
1	C	240	LEU	2.0
1	E	162	GLU	2.0
1	E	171	ARG	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 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.