Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 10:23 am GMT

PDB ID	:	4UW8
Title	:	Structure of the carboxy-terminal domain of the bacteriophage T5 L- shaped tail fiber with its intra-molecular chaperone domain
Authors	:	Garcia-Doval, C.; Luque, D.; Caston, J.R.; Otero, J.M.; Llamas-Saiz, A.L.; Boulanger, P.; van Raaij, M.J.
Deposited on	:	2014-08-08
Resolution	:	2.52 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 (i)) were used in the production of this report:

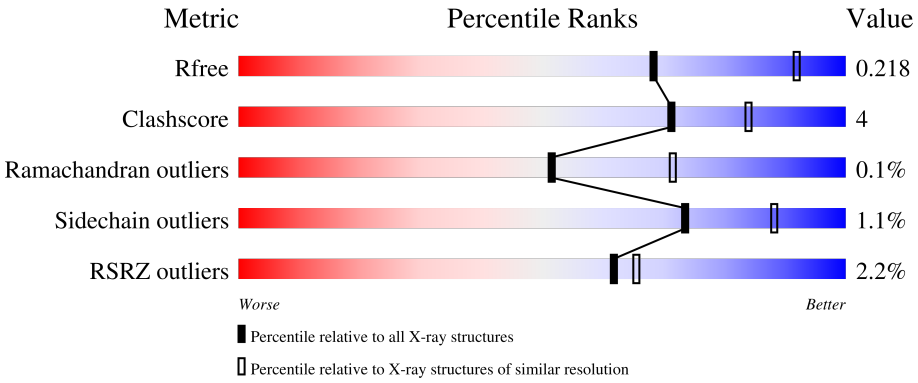
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	427	87% 7% 6%
1	B	427	87% 6% 6%
1	C	427	87% 7% 6%
1	D	427	89% 5% 6%
1	E	427	87% 6% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	427	3% 86% 7% • 6%
1	G	427	3% 87% 6% 6%
1	H	427	4% 87% 6% • 6%
1	I	427	% 88% 5% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	C	2397	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28644 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.

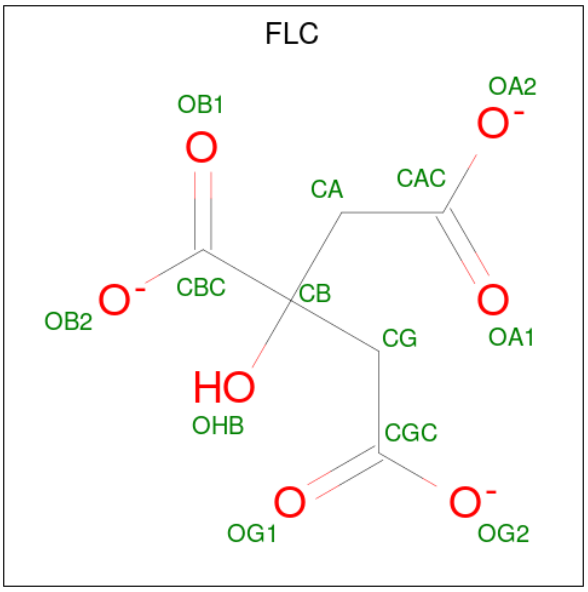
- Molecule 1 is a protein called L-SHAPED TAIL FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	B	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	C	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	D	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	E	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	F	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			
1	G	400	Total	C	N	O	S	0	2	0
			3058	1919	541	585	13			
1	H	401	Total	C	N	O	S	0	3	0
			3071	1928	542	588	13			
1	I	401	Total	C	N	O	S	0	2	0
			3066	1925	542	586	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1264	ALA	SER	engineered mutation	UNP P13390
B	1264	ALA	SER	engineered mutation	UNP P13390
C	1264	ALA	SER	engineered mutation	UNP P13390
D	1264	ALA	SER	engineered mutation	UNP P13390
E	1264	ALA	SER	engineered mutation	UNP P13390
F	1264	ALA	SER	engineered mutation	UNP P13390
G	1264	ALA	SER	engineered mutation	UNP P13390
H	1264	ALA	SER	engineered mutation	UNP P13390
I	1264	ALA	SER	engineered mutation	UNP P13390

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	154	Total O 154 154	0	0
3	B	128	Total O 128 128	0	0
3	C	108	Total O 108 108	0	0

Continued on next page...

Continued from previous page...

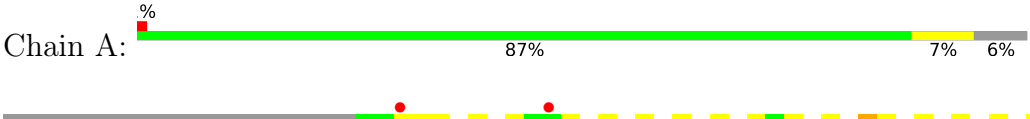
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	136	Total O 136 136	0	0
3	E	122	Total O 122 122	0	0
3	F	65	Total O 65 65	0	0
3	G	90	Total O 90 90	0	0
3	H	63	Total O 63 63	0	0
3	I	70	Total O 70 70	0	0

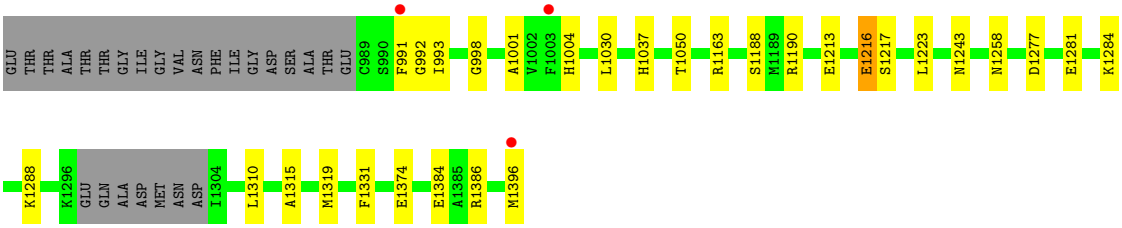
3 Residue-property plots (i)

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: L-SHAPED TAIL FIBER PROTEIN

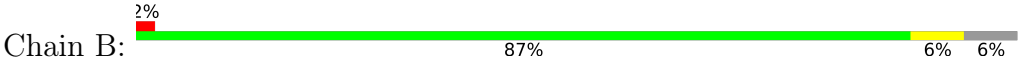
Chain A:

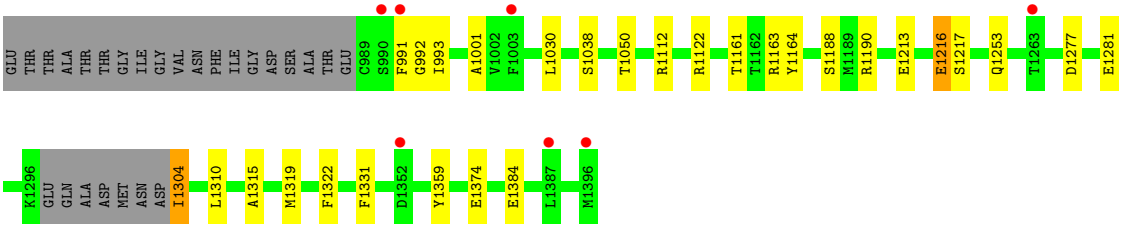




• Molecule 1: L-SHAPED TAIL FIBER PROTEIN

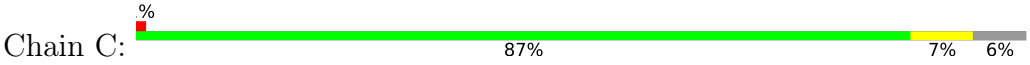
Chain B:

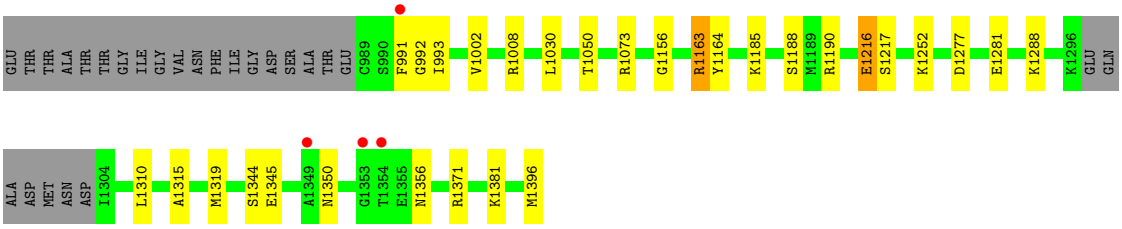




• Molecule 1: L-SHAPED TAIL FIBER PROTEIN

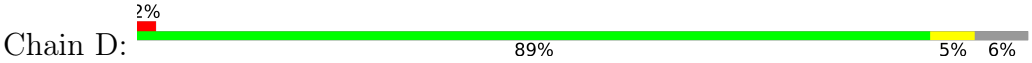
Chain C:

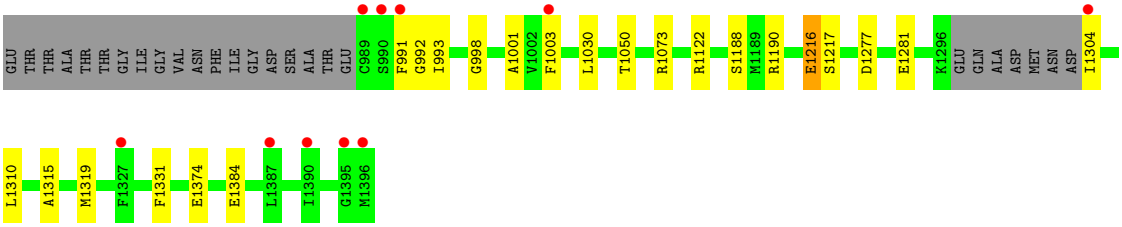




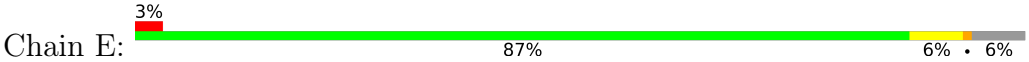
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN

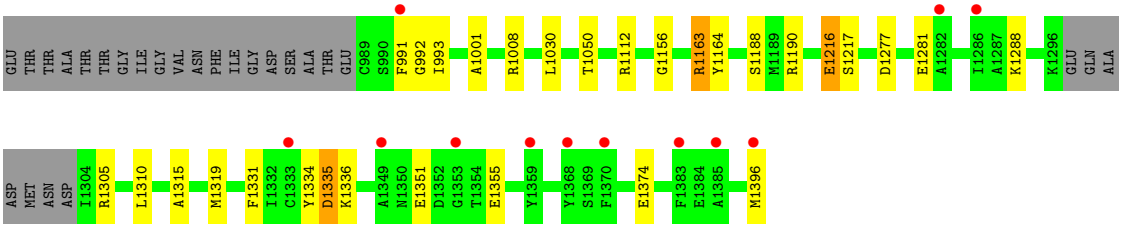
Chain D:



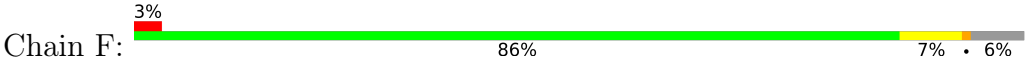


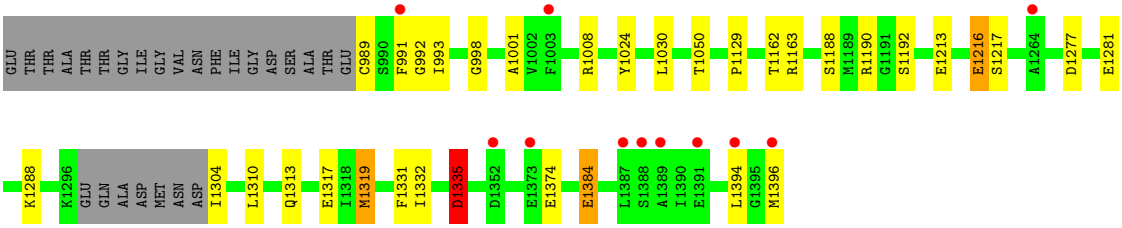
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN



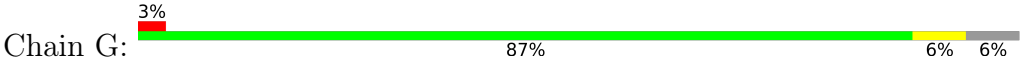


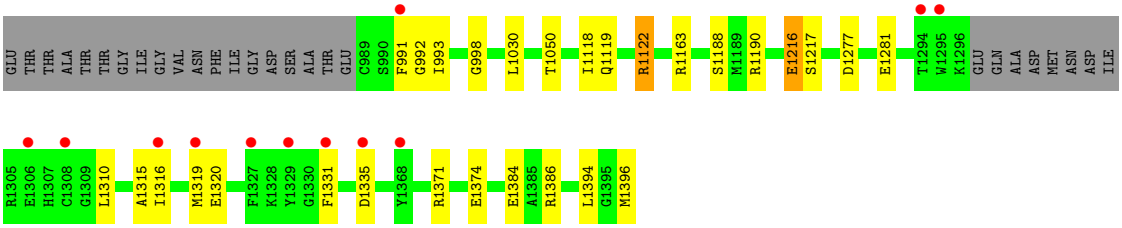
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN



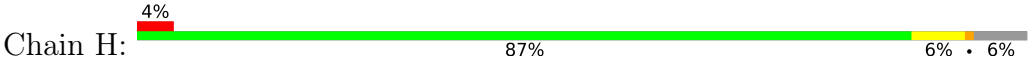


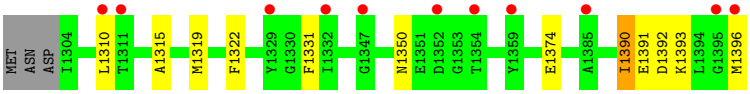
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN





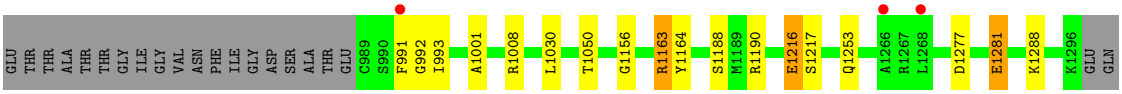
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN





• Molecule 1: L-SHAPED TAIL FIBER PROTEIN

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.85Å 99.29Å 286.23Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	95.38 – 2.52 95.38 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.5 (95.38-2.52) 98.5 (95.38-2.52)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.213 0.190 , 0.218	Depositor DCC
R_{free} test set	2064 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28644	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: FLC

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	0.55	2/3147 (0.1%)	0.72	1/4269 (0.0%)
1	B	0.57	2/3147 (0.1%)	0.74	1/4269 (0.0%)
1	C	0.56	0/3147	0.73	0/4269
1	D	0.52	0/3147	0.72	0/4269
1	E	0.56	2/3147 (0.1%)	0.74	1/4269 (0.0%)
1	F	0.55	0/3147	0.76	4/4269 (0.1%)
1	G	0.50	0/3139	0.76	3/4258 (0.1%)
1	H	0.50	0/3155	0.71	0/4280
1	I	0.54	1/3147 (0.0%)	0.73	3/4269 (0.1%)
All	All	0.54	7/28323 (0.0%)	0.73	13/38421 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1213	GLU	CD-OE1	-5.92	1.19	1.25
1	B	1213	GLU	CD-OE1	-5.86	1.19	1.25
1	E	1355	GLU	CD-OE2	-5.42	1.19	1.25
1	A	1213	GLU	CD-OE2	-5.24	1.19	1.25
1	B	1213	GLU	CD-OE2	-5.21	1.20	1.25
1	I	1281	GLU	CD-OE1	5.21	1.31	1.25
1	E	1335	ASP	CB-CG	5.00	1.62	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1335	ASP	CB-CG-OD2	9.50	126.85	118.30
1	I	1335	ASP	CB-CG-OD2	9.34	126.70	118.30
1	G	1122[A]	ARG	CG-CD-NE	8.76	130.19	111.80
1	G	1122[B]	ARG	CG-CD-NE	8.76	130.19	111.80
1	E	1335	ASP	CB-CG-OD2	8.70	126.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1281	GLU	CG-CD-OE2	-7.23	103.84	118.30
1	F	1384	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	I	1281	GLU	CG-CD-OE1	6.79	131.87	118.30
1	G	1386	ARG	CG-CD-NE	6.66	125.79	111.80
1	F	1319	MET	CG-SD-CE	-5.98	90.64	100.20
1	F	1384	GLU	CG-CD-OE2	5.15	128.60	118.30
1	B	1163	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	1163	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3066	0	2963	26	0
1	B	3066	0	2963	29	0
1	C	3066	0	2963	29	0
1	D	3066	0	2963	24	0
1	E	3066	0	2963	25	0
1	F	3066	0	2963	32	0
1	G	3058	0	2952	26	0
1	H	3071	0	2967	25	0
1	I	3066	0	2963	23	0
2	A	13	0	5	2	0
2	B	13	0	5	2	0
2	C	13	0	5	4	0
2	D	13	0	5	2	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	1	0
2	I	13	0	5	0	0
3	A	154	0	0	0	0
3	B	128	0	0	5	0
3	C	108	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	136	0	0	2	0
3	E	122	0	0	1	0
3	F	65	0	0	3	0
3	G	90	0	0	3	0
3	H	63	0	0	2	0
3	I	70	0	0	0	0
All	All	28644	0	26705	191	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 4.

All (191) 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:B:1331:PHE:HB3	1:B:1374:GLU:HG2	1.28	1.15
1:F:989:CYS:SG	3:F:2002:HOH:O	2.25	0.92
1:D:1304:ILE:N	3:D:2119:HOH:O	2.08	0.86
1:H:1281:GLU:HB3	1:H:1322:PHE:CE2	2.16	0.80
1:B:1281:GLU:HB3	1:B:1322:PHE:CE2	2.17	0.79
1:F:1335:ASP:OD1	3:F:2054:HOH:O	2.00	0.78
1:G:1335:ASP:OD2	3:G:2080:HOH:O	2.02	0.77
1:C:1073:ARG:HH22	2:C:2397:FLC:CA	1.97	0.76
1:D:993:ILE:HB	1:E:991[B]:PHE:CE1	2.21	0.75
1:B:1164:TYR:CE2	1:E:1112:ARG:HD2	2.21	0.75
1:B:993:ILE:HB	1:C:991[A]:PHE:CE1	2.21	0.74
1:G:991[B]:PHE:CE1	1:I:993:ILE:HB	2.27	0.69
1:F:1313:GLN:O	1:F:1317:GLU:HG2	1.93	0.68
1:D:993:ILE:HD12	1:E:991[B]:PHE:CD1	2.28	0.68
1:G:1394:LEU:HD12	1:G:1396:MET:HE1	1.75	0.68
1:A:993:ILE:HB	1:B:991[A]:PHE:CE1	2.29	0.67
1:I:1313:GLN:O	1:I:1317:GLU:HG2	1.94	0.67
1:F:1162:THR:HG22	3:F:2036:HOH:O	1.95	0.66
1:C:1073:ARG:HH22	2:C:2397:FLC:HA2	1.64	0.63
1:G:1316:ILE:HG22	1:G:1320:GLU:OE2	1.98	0.63
1:F:1192:SER:OG	1:F:1213:GLU:OE1	2.18	0.62
1:G:1316:ILE:CG2	1:G:1320:GLU:OE2	2.48	0.62
1:B:993:ILE:HD12	1:C:991[A]:PHE:CD1	2.36	0.61
1:H:993:ILE:HB	1:I:991[B]:PHE:CE1	2.36	0.60
1:H:1160[A]:ASP:OD1	1:H:1162:THR:O	2.22	0.58
3:B:2056:HOH:O	1:C:1163:ARG:HD2	2.03	0.57
2:F:2397:FLC:OG2	2:F:2397:FLC:CBC	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1185:LYS:HE2	3:C:2065:HOH:O	2.04	0.57
1:G:993:ILE:HB	1:H:991[B]:PHE:CE1	2.39	0.57
1:E:1288:LYS:HG2	1:F:1384:GLU:OE2	2.04	0.56
1:E:993:ILE:HB	1:F:991[B]:PHE:CE1	2.41	0.56
1:H:1390:ILE:O	1:H:1393:LYS:N	2.38	0.55
1:H:993:ILE:HD12	1:I:991[B]:PHE:CD1	2.42	0.55
1:C:1073:ARG:HH22	2:C:2397:FLC:HA1	1.70	0.54
1:B:1161:THR:HG23	3:B:2069:HOH:O	2.07	0.54
2:D:2397:FLC:OA2	2:D:2397:FLC:OHB	2.19	0.54
1:G:1118:ILE:O	1:G:1122[A]:ARG:NH1	2.41	0.54
1:A:991[A]:PHE:CE1	1:C:993:ILE:HB	2.43	0.53
1:C:1156:GLY:HA2	1:C:1164:TYR:CE2	2.43	0.53
1:H:1156:GLY:HA2	1:H:1164:TYR:CE2	2.44	0.53
1:D:993:ILE:HB	1:E:991[B]:PHE:CZ	2.43	0.53
1:G:1394:LEU:HD12	1:G:1396:MET:CE	2.37	0.53
3:H:2026:HOH:O	1:I:1163:ARG:HD2	2.08	0.53
1:F:1394:LEU:HD12	1:F:1396:MET:HE1	1.90	0.52
1:I:1315:ALA:O	1:I:1319:MET:HG2	2.10	0.52
1:A:1216:GLU:HG3	1:A:1217:SER:N	2.25	0.52
1:B:1112:ARG:HD3	3:B:2058:HOH:O	2.09	0.52
1:B:1315:ALA:O	1:B:1319:MET:HG2	2.10	0.52
1:E:1156:GLY:HA2	1:E:1164:TYR:CE2	2.45	0.52
1:G:1384:GLU:OE2	1:I:1288:LYS:HE2	2.10	0.52
1:D:1315:ALA:O	1:D:1319:MET:HG2	2.10	0.51
3:D:2063:HOH:O	1:E:1163:ARG:HD2	2.10	0.51
1:E:1315:ALA:O	1:E:1319:MET:HG2	2.10	0.51
1:B:993:ILE:HB	1:C:991[A]:PHE:CZ	2.45	0.51
1:G:1216:GLU:HG3	1:G:1217:SER:N	2.25	0.51
1:H:1315:ALA:O	1:H:1319:MET:HG2	2.10	0.51
1:B:1277:ASP:O	1:B:1281:GLU:HG2	2.11	0.51
1:C:1315:ALA:O	1:C:1319:MET:HG2	2.11	0.51
1:A:991[A]:PHE:CD1	1:C:993:ILE:HD12	2.46	0.51
1:E:1277:ASP:O	1:E:1281:GLU:HG2	2.11	0.51
1:A:1277:ASP:O	1:A:1281:GLU:HG2	2.11	0.51
1:B:1216:GLU:HG3	1:B:1217:SER:N	2.25	0.51
1:I:1156:GLY:HA2	1:I:1164:TYR:CE2	2.45	0.51
1:A:993:ILE:HD12	1:B:991[A]:PHE:CD1	2.45	0.51
1:B:1359:TYR:HD2	3:B:2123:HOH:O	1.94	0.51
1:G:1315:ALA:O	1:G:1319:MET:HG2	2.10	0.51
1:H:1277:ASP:O	1:H:1281:GLU:HG2	2.11	0.51
1:H:1281:GLU:HB3	1:H:1322:PHE:HE2	1.72	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1277:ASP:O	1:C:1281:GLU:HG2	2.11	0.50
1:F:1277:ASP:O	1:F:1281:GLU:HG2	2.11	0.50
1:G:1277:ASP:O	1:G:1281:GLU:HG2	2.11	0.50
1:A:1223:LEU:HD23	1:C:1345:GLU:HA	1.92	0.50
1:D:1277:ASP:O	1:D:1281:GLU:HG2	2.11	0.50
1:F:1216:GLU:HG3	1:F:1217:SER:N	2.25	0.50
1:H:1350:ASN:HB2	3:H:2059:HOH:O	2.12	0.50
1:E:1216:GLU:HG3	1:E:1217:SER:N	2.26	0.50
1:C:1216:GLU:HG3	1:C:1217:SER:N	2.27	0.50
1:A:1030:LEU:HD23	1:B:1050:THR:HG22	1.92	0.50
1:A:1315:ALA:O	1:A:1319:MET:HG2	2.11	0.50
1:E:1305:ARG:NH2	1:F:1332:ILE:O	2.37	0.49
1:F:1394:LEU:HB2	1:F:1396:MET:HE2	1.94	0.49
1:I:1216:GLU:HG3	1:I:1217:SER:N	2.28	0.49
1:D:991[B]:PHE:CE1	1:F:993:ILE:HB	2.47	0.49
1:D:998:GLY:HA2	1:F:1008:ARG:O	2.12	0.49
1:D:1216:GLU:HG3	1:D:1217:SER:N	2.27	0.48
1:A:1037:HIS:ND1	2:A:2397:FLC:OB2	2.32	0.48
3:B:2102:HOH:O	1:C:1381:LYS:HE2	2.12	0.48
1:A:1050:THR:HG22	1:C:1030:LEU:HD23	1.95	0.48
1:G:1119:GLN:HA	1:G:1122[A]:ARG:CD	2.43	0.48
1:F:1394:LEU:HD12	1:F:1396:MET:CE	2.43	0.47
1:H:1216:GLU:HG3	1:H:1217:SER:N	2.29	0.47
1:D:1122[B]:ARG:NH1	1:F:1129:PRO:O	2.47	0.47
1:E:993:ILE:HD12	1:F:991[B]:PHE:CD1	2.49	0.47
1:D:1030:LEU:HD23	1:E:1050:THR:HG22	1.97	0.47
1:A:1223:LEU:HD22	1:C:1344:SER:O	2.15	0.47
1:B:1281:GLU:HB3	1:B:1322:PHE:HE2	1.74	0.47
1:A:1004:HIS:NE2	2:C:2397:FLC:OG2	2.44	0.47
1:D:1073:ARG:NH2	2:D:2397:FLC:OG1	2.47	0.47
1:A:1384:GLU:OE2	1:C:1288:LYS:HE2	2.14	0.46
1:A:991[B]:PHE:CD1	1:A:992:GLY:N	2.84	0.46
1:A:1288:LYS:HE2	1:B:1384:GLU:OE2	2.16	0.46
1:H:1030:LEU:HD23	1:I:1050:THR:HG22	1.98	0.46
1:H:1390:ILE:O	1:H:1392:ASP:N	2.49	0.46
1:D:993:ILE:HD12	1:E:991[B]:PHE:HD1	1.79	0.46
1:G:991[B]:PHE:CD1	1:I:993:ILE:HD12	2.50	0.46
1:G:1050:THR:HG22	1:I:1030:LEU:HD23	1.98	0.46
3:G:2035:HOH:O	1:H:1163:ARG:HD2	2.15	0.46
1:B:1281:GLU:CB	1:B:1322:PHE:CE2	2.97	0.46
1:E:991[A]:PHE:CD1	1:E:992:GLY:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:991[B]:PHE:CD1	1:C:992:GLY:N	2.84	0.46
1:I:1277:ASP:O	1:I:1281:GLU:HG2	2.16	0.46
1:B:991[B]:PHE:CD1	1:B:992:GLY:N	2.85	0.45
2:B:2397:FLC:HG1	1:C:1002:VAL:HG11	1.99	0.45
1:E:1030:LEU:HD23	1:F:1050:THR:HG22	1.98	0.45
1:C:1350:ASN:OD1	1:C:1356:ASN:OD1	2.35	0.45
1:I:991[A]:PHE:CD1	1:I:992:GLY:N	2.85	0.45
1:F:1162:THR:HG23	1:F:1162:THR:O	2.17	0.45
1:H:991[A]:PHE:CD1	1:H:992:GLY:N	2.85	0.44
2:A:2397:FLC:OB2	2:A:2397:FLC:CGC	2.63	0.44
1:D:991[A]:PHE:CD1	1:D:992:GLY:N	2.85	0.44
1:B:1188:SER:OG	1:B:1190:ARG:NH1	2.51	0.44
1:D:1050:THR:HG22	1:F:1030:LEU:HD23	1.98	0.44
1:H:1188:SER:OG	1:H:1190:ARG:NH1	2.50	0.44
1:G:991[B]:PHE:CZ	1:I:993:ILE:HB	2.53	0.44
1:A:998:GLY:HA2	1:C:1008:ARG:O	2.17	0.44
1:A:1188:SER:OG	1:A:1190:ARG:NH1	2.51	0.44
1:F:1188:SER:OG	1:F:1190:ARG:NH1	2.50	0.43
1:G:1394:LEU:HB2	1:G:1396:MET:HE2	1.99	0.43
1:B:1030:LEU:HD23	1:C:1050:THR:HG22	2.00	0.43
1:H:1160[A]:ASP:OD2	1:H:1164:TYR:HE1	2.01	0.43
1:D:991[B]:PHE:CZ	1:F:993:ILE:HB	2.53	0.43
1:F:991[A]:PHE:CD1	1:F:992:GLY:N	2.86	0.43
1:G:991[A]:PHE:CD1	1:G:992:GLY:N	2.86	0.43
1:I:1188:SER:OG	1:I:1190:ARG:NH1	2.51	0.43
1:E:1008:ARG:O	1:F:998:GLY:HA2	2.19	0.42
2:H:2397:FLC:OA2	2:H:2397:FLC:OHB	2.32	0.42
1:C:1188:SER:OG	1:C:1190:ARG:NH1	2.51	0.42
1:H:1281:GLU:CB	1:H:1322:PHE:CE2	2.95	0.42
1:H:1331:PHE:HB3	1:H:1374:GLU:HB3	2.02	0.42
1:E:1188:SER:OG	1:E:1190:ARG:NH1	2.52	0.42
1:A:1243:ASN:OD1	1:C:1252:LYS:HB3	2.20	0.42
1:B:993:ILE:HG13	1:B:1001:ALA:HB1	2.01	0.42
1:E:1334:TYR:HE2	1:E:1336:LYS:HE3	1.84	0.42
1:G:1030:LEU:HD23	1:H:1050:THR:HG22	2.02	0.42
1:E:993:ILE:HG13	1:E:1001:ALA:HB1	2.02	0.42
1:G:1188:SER:OG	1:G:1190:ARG:NH1	2.52	0.42
1:G:1371:ARG:NH1	1:I:1253:GLN:OE1	2.42	0.42
1:A:993:ILE:HG13	1:A:1001:ALA:HB1	2.02	0.41
1:E:1331:PHE:HB3	1:E:1374:GLU:HB3	2.02	0.41
1:F:993:ILE:HG13	1:F:1001:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:993:ILE:HG13	1:D:1001:ALA:HB1	2.01	0.41
1:I:1331:PHE:HB3	1:I:1374:GLU:HB3	2.02	0.41
1:D:991[B]:PHE:CD1	1:F:993:ILE:HD12	2.56	0.41
1:B:1304:ILE:HG13	1:B:1304:ILE:O	2.20	0.41
1:G:1163:ARG:HD2	3:G:2048:HOH:O	2.20	0.41
1:I:993:ILE:HG13	1:I:1001:ALA:HB1	2.01	0.41
1:D:1003:PHE:CD1	1:F:1024:TYR:CE2	3.09	0.41
1:D:1384:GLU:OE2	1:F:1288:LYS:HE2	2.20	0.41
1:G:1331:PHE:HB3	1:G:1374:GLU:HB3	2.02	0.41
1:H:993:ILE:HG13	1:H:1001:ALA:HB1	2.03	0.41
1:A:1223:LEU:CD2	1:C:1345:GLU:HB3	2.50	0.41
1:A:1331:PHE:HB3	1:A:1374:GLU:HB3	2.03	0.41
1:E:1351:GLU:HG2	3:E:2110:HOH:O	2.20	0.41
1:G:998:GLY:HA2	1:I:1008:ARG:O	2.21	0.41
1:A:1258:ASN:HB2	1:B:1253:GLN:HB3	2.03	0.41
1:A:1284:LYS:HD3	1:A:1386:ARG:CG	2.51	0.41
1:D:1331:PHE:HB3	1:D:1374:GLU:HB3	2.02	0.41
1:B:1122[B]:ARG:HA	1:B:1122[B]:ARG:HD3	1.80	0.40
1:B:1253:GLN:OE1	1:C:1371:ARG:NH1	2.47	0.40
1:B:1038:SER:HB2	2:B:2397:FLC:OB2	2.21	0.40
1:D:1188:SER:OG	1:D:1190:ARG:NH1	2.53	0.40
1:F:1331:PHE:HB3	1:F:1374:GLU:HB3	2.04	0.40
1:F:1304:ILE:HG22	1:F:1304:ILE:O	2.22	0.40
1:H:1288:LYS:HE2	1:I:1384:GLU:OE2	2.22	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	399/427 (93%)	390 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	399/427 (93%)	389 (98%)	10 (2%)	0	100	100
1	C	399/427 (93%)	390 (98%)	9 (2%)	0	100	100
1	D	399/427 (93%)	390 (98%)	9 (2%)	0	100	100
1	E	399/427 (93%)	390 (98%)	9 (2%)	0	100	100
1	F	399/427 (93%)	390 (98%)	9 (2%)	0	100	100
1	G	398/427 (93%)	389 (98%)	9 (2%)	0	100	100
1	H	400/427 (94%)	388 (97%)	10 (2%)	2 (0%)	29	47
1	I	399/427 (93%)	390 (98%)	9 (2%)	0	100	100
All	All	3591/3843 (93%)	3506 (98%)	83 (2%)	2 (0%)	51	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1390	ILE
1	H	1391	GLU

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	318/336 (95%)	315 (99%)	3 (1%)	78	91
1	B	318/336 (95%)	315 (99%)	3 (1%)	78	91
1	C	318/336 (95%)	314 (99%)	4 (1%)	69	86
1	D	318/336 (95%)	316 (99%)	2 (1%)	86	94
1	E	318/336 (95%)	313 (98%)	5 (2%)	62	82
1	F	318/336 (95%)	313 (98%)	5 (2%)	62	82
1	G	317/336 (94%)	315 (99%)	2 (1%)	86	94
1	H	319/336 (95%)	315 (99%)	4 (1%)	69	86
1	I	318/336 (95%)	314 (99%)	4 (1%)	69	86
All	All	2862/3024 (95%)	2830 (99%)	32 (1%)	73	88

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1216	GLU
1	A	1310	LEU
1	A	1396	MET
1	B	1216	GLU
1	B	1304	ILE
1	B	1310	LEU
1	C	1163	ARG
1	C	1216	GLU
1	C	1310	LEU
1	C	1396	MET
1	D	1216	GLU
1	D	1310	LEU
1	E	1163	ARG
1	E	1216	GLU
1	E	1310	LEU
1	E	1335	ASP
1	E	1396	MET
1	F	1163	ARG
1	F	1216	GLU
1	F	1310	LEU
1	F	1319	MET
1	F	1335	ASP
1	G	1216	GLU
1	G	1310	LEU
1	H	1163	ARG
1	H	1216	GLU
1	H	1310	LEU
1	H	1396	MET
1	I	1163	ARG
1	I	1216	GLU
1	I	1310	LEU
1	I	1335	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands 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	FLC	A	2397	-	12,12,12	1.32	1 (8%)	17,17,17	1.32	4 (23%)
2	FLC	D	2397	-	12,12,12	1.38	1 (8%)	17,17,17	1.83	4 (23%)
2	FLC	H	2397	-	12,12,12	1.48	1 (8%)	17,17,17	1.23	1 (5%)
2	FLC	C	2397	-	12,12,12	1.61	1 (8%)	17,17,17	1.23	2 (11%)
2	FLC	G	2397	-	12,12,12	1.40	1 (8%)	17,17,17	1.30	2 (11%)
2	FLC	I	2397	-	12,12,12	1.02	0	17,17,17	1.41	1 (5%)
2	FLC	F	2397	-	12,12,12	1.43	1 (8%)	17,17,17	1.48	3 (17%)
2	FLC	B	2397	-	12,12,12	1.27	1 (8%)	17,17,17	1.17	2 (11%)
2	FLC	E	2397	-	12,12,12	1.36	1 (8%)	17,17,17	1.32	1 (5%)

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	FLC	A	2397	-	-	8/16/16/16	-
2	FLC	D	2397	-	-	6/16/16/16	-
2	FLC	H	2397	-	-	2/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	C	2397	-	-	4/16/16/16	-
2	FLC	G	2397	-	-	5/16/16/16	-
2	FLC	I	2397	-	-	7/16/16/16	-
2	FLC	F	2397	-	-	2/16/16/16	-
2	FLC	B	2397	-	-	9/16/16/16	-
2	FLC	E	2397	-	-	2/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2397	FLC	CB-CBC	-3.89	1.49	1.53
2	H	2397	FLC	CB-CBC	-3.85	1.49	1.53
2	F	2397	FLC	CB-CBC	-3.69	1.49	1.53
2	D	2397	FLC	CB-CBC	-3.67	1.49	1.53
2	G	2397	FLC	CB-CBC	-3.52	1.49	1.53
2	A	2397	FLC	CB-CBC	-3.26	1.50	1.53
2	E	2397	FLC	CB-CBC	-3.13	1.50	1.53
2	B	2397	FLC	CB-CBC	-2.60	1.50	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2397	FLC	OB1-CBC-CB	-4.81	115.45	122.25
2	I	2397	FLC	OB2-CBC-CB	4.10	120.17	113.05
2	D	2397	FLC	OB2-CBC-CB	3.84	119.71	113.05
2	F	2397	FLC	OB1-CBC-CB	-3.61	117.15	122.25
2	C	2397	FLC	OB1-CBC-CB	-3.13	117.82	122.25
2	A	2397	FLC	OB2-CBC-CB	2.60	117.56	113.05
2	E	2397	FLC	OB1-CBC-CB	-2.53	118.67	122.25
2	H	2397	FLC	OB1-CBC-CB	-2.53	118.67	122.25
2	G	2397	FLC	OHB-CB-CBC	-2.44	105.44	108.86
2	C	2397	FLC	OB2-CBC-CB	2.36	117.14	113.05
2	B	2397	FLC	OHB-CB-CBC	-2.30	105.63	108.86
2	F	2397	FLC	OG1-CGC-CG	-2.29	116.25	122.94
2	G	2397	FLC	OB1-CBC-CB	-2.23	119.09	122.25
2	B	2397	FLC	OB2-CBC-CB	2.23	116.92	113.05
2	D	2397	FLC	OHB-CB-CBC	-2.18	105.81	108.86
2	A	2397	FLC	OG2-CGC-CG	2.10	121.11	114.35
2	A	2397	FLC	OG1-CGC-CG	-2.06	116.92	122.94
2	D	2397	FLC	OG1-CGC-CG	-2.05	116.97	122.94
2	F	2397	FLC	OB2-CBC-CB	2.01	116.54	113.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2397	FLC	OB1-CBC-CB	-2.01	119.41	122.25

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2397	FLC	CG-CB-CBC-OB1
2	A	2397	FLC	CG-CB-CBC-OB2
2	A	2397	FLC	OHB-CB-CBC-OB1
2	A	2397	FLC	OHB-CB-CBC-OB2
2	B	2397	FLC	CA-CB-CBC-OB1
2	B	2397	FLC	CA-CB-CBC-OB2
2	B	2397	FLC	OHB-CB-CBC-OB1
2	B	2397	FLC	OHB-CB-CBC-OB2
2	B	2397	FLC	CA-CB-CG-CGC
2	B	2397	FLC	CBC-CB-CG-CGC
2	B	2397	FLC	OHB-CB-CG-CGC
2	G	2397	FLC	CA-CB-CG-CGC
2	G	2397	FLC	OHB-CB-CG-CGC
2	I	2397	FLC	CG-CB-CBC-OB1
2	I	2397	FLC	OHB-CB-CBC-OB1
2	I	2397	FLC	OHB-CB-CBC-OB2
2	D	2397	FLC	CAC-CA-CB-OHB
2	G	2397	FLC	CBC-CB-CG-CGC
2	I	2397	FLC	CG-CB-CBC-OB2
2	D	2397	FLC	CAC-CA-CB-CBC
2	D	2397	FLC	CB-CA-CAC-OA2
2	D	2397	FLC	CB-CA-CAC-OA1
2	D	2397	FLC	CAC-CA-CB-CG
2	A	2397	FLC	CA-CB-CBC-OB1
2	A	2397	FLC	CA-CB-CBC-OB2
2	A	2397	FLC	CB-CA-CAC-OA1
2	A	2397	FLC	CB-CA-CAC-OA2
2	G	2397	FLC	CB-CA-CAC-OA2
2	C	2397	FLC	CG-CB-CBC-OB1
2	C	2397	FLC	CG-CB-CBC-OB2
2	G	2397	FLC	CB-CA-CAC-OA1
2	I	2397	FLC	CB-CA-CAC-OA2
2	C	2397	FLC	OHB-CB-CG-CGC
2	H	2397	FLC	CB-CA-CAC-OA2
2	E	2397	FLC	CAC-CA-CB-CBC
2	I	2397	FLC	CB-CA-CAC-OA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	2397	FLC	CAC-CA-CB-OHB
2	H	2397	FLC	CB-CA-CAC-OA1
2	C	2397	FLC	CBC-CB-CG-CGC
2	F	2397	FLC	CB-CA-CAC-OA1
2	F	2397	FLC	CB-CA-CAC-OA2
2	D	2397	FLC	CBC-CB-CG-CGC
2	I	2397	FLC	CA-CB-CBC-OB2
2	B	2397	FLC	CB-CA-CAC-OA1
2	B	2397	FLC	CB-CA-CAC-OA2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2397	FLC	2	0
2	D	2397	FLC	2	0
2	H	2397	FLC	1	0
2	C	2397	FLC	4	0
2	F	2397	FLC	1	0
2	B	2397	FLC	2	0

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	401/427 (93%)	0.14	3 (0%) 87 89	19, 34, 68, 91	0
1	B	401/427 (93%)	0.12	7 (1%) 70 73	20, 34, 73, 93	0
1	C	401/427 (93%)	0.09	4 (0%) 82 84	20, 33, 68, 94	0
1	D	401/427 (93%)	0.13	10 (2%) 57 61	21, 36, 83, 115	0
1	E	401/427 (93%)	0.26	12 (2%) 50 54	20, 36, 86, 111	0
1	F	401/427 (93%)	0.15	11 (2%) 54 58	21, 36, 72, 106	0
1	G	400/427 (93%)	0.23	12 (3%) 50 54	25, 40, 85, 105	0
1	H	401/427 (93%)	0.35	16 (3%) 38 42	24, 42, 90, 120	0
1	I	401/427 (93%)	0.15	5 (1%) 79 81	27, 40, 74, 121	0
All	All	3608/3843 (93%)	0.18	80 (2%) 62 65	19, 37, 82, 121	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	991[A]	PHE	5.8
1	I	1396	MET	4.9
1	F	1396	MET	4.6
1	D	1396	MET	4.5
1	F	1264	ALA	4.4
1	E	1282	ALA	4.3
1	D	991[A]	PHE	4.2
1	A	991[A]	PHE	4.1
1	E	1359	TYR	4.1
1	I	991[A]	PHE	3.9
1	H	1354	THR	3.9
1	E	991[A]	PHE	3.9
1	H	1395	GLY	3.8
1	E	1333	CYS	3.7
1	G	1329	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	1281	GLU	3.6
1	H	1396	MET	3.5
1	H	991[A]	PHE	3.5
1	E	1385	ALA	3.5
1	B	1003	PHE	3.4
1	E	1349	ALA	3.4
1	C	991[A]	PHE	3.4
1	F	991[A]	PHE	3.2
1	H	1329	TYR	3.2
1	A	1003	PHE	3.2
1	E	1353	GLY	3.2
1	I	1268	LEU	3.1
1	E	1396	MET	3.0
1	H	1310	LEU	2.9
1	H	1292	PHE	2.9
1	C	1353	GLY	2.9
1	G	1327	PHE	2.9
1	H	1311	THR	2.8
1	G	1316	ILE	2.7
1	G	991[A]	PHE	2.7
1	G	1295	TRP	2.7
1	I	1266	ALA	2.7
1	D	1395	GLY	2.7
1	D	990	SER	2.6
1	H	1385	ALA	2.6
1	F	1387	LEU	2.6
1	E	1383	PHE	2.6
1	B	990	SER	2.6
1	E	1286	ILE	2.6
1	F	1389	ALA	2.6
1	B	1396	MET	2.6
1	G	1319	MET	2.5
1	D	1387	LEU	2.5
1	H	1352	ASP	2.4
1	D	1304	ILE	2.4
1	G	1331	PHE	2.4
1	D	989	CYS	2.4
1	H	1347	GLY	2.4
1	G	1335	ASP	2.4
1	A	1396	MET	2.3
1	C	1354	THR	2.3
1	H	989	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1327	PHE	2.3
1	B	1263	THR	2.3
1	F	1373	GLU	2.3
1	E	1368	TYR	2.3
1	B	1352	ASP	2.3
1	I	1393	LYS	2.3
1	B	1387	LEU	2.3
1	C	1349	ALA	2.2
1	G	1368	TYR	2.2
1	H	1359	TYR	2.2
1	E	1370	PHE	2.2
1	H	1332	ILE	2.2
1	F	1391	GLU	2.2
1	F	1388	SER	2.2
1	F	1352	ASP	2.1
1	D	1003	PHE	2.1
1	F	1003	PHE	2.1
1	G	1306	GLU	2.1
1	D	1390	ILE	2.1
1	G	1294	THR	2.0
1	H	1282	ALA	2.0
1	G	1308	CYS	2.0
1	F	1394	LEU	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)

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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FLC	I	2397	13/13	0.89	0.31	69,75,88,90	0
2	FLC	C	2397	13/13	0.90	0.28	66,79,90,90	0
2	FLC	H	2397	13/13	0.91	0.25	74,88,92,94	0
2	FLC	F	2397	13/13	0.91	0.32	58,78,90,95	0
2	FLC	B	2397	13/13	0.92	0.26	62,74,87,87	0
2	FLC	A	2397	13/13	0.94	0.38	80,87,97,101	0
2	FLC	G	2397	13/13	0.94	0.32	71,76,96,98	0
2	FLC	D	2397	13/13	0.94	0.19	61,79,88,88	0
2	FLC	E	2397	13/13	0.94	0.26	53,72,81,85	0

6.5 Other polymers (i)

There are no such residues in this entry.