



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:08 PM GMT

PDB ID : 4J3O
Title : Crystal structure of the FimD usher traversed by the pilus tip complex assembly composed of FimC:FimF:FimG:FimH
Authors : Geibel, S.; Waksman, G.
Deposited on : 2013-02-06
Resolution : 3.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

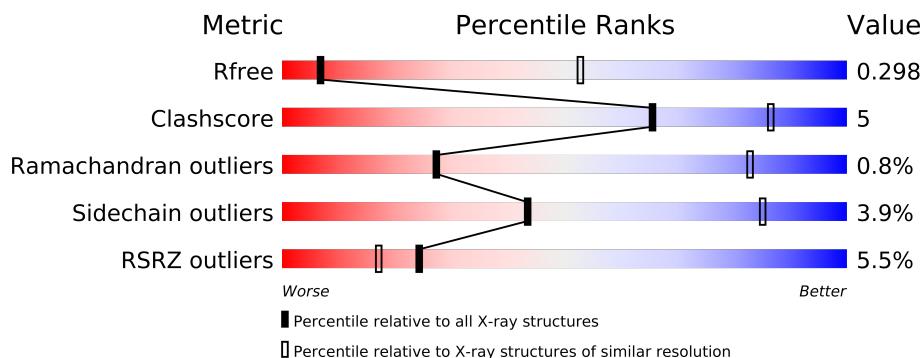
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	G	144	
2	H	279	
3	C	211	
4	F	154	
5	D	843	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11732 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein FimG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	144	Total	C	N	O	S	0	0	0
			1043	640	176	224	3			

- Molecule 2 is a protein called Protein FimH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	279	Total	C	N	O	S	0	0	0
			2051	1297	342	408	4			

- Molecule 3 is a protein called Chaperone protein FimC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	199	Total	C	N	O	S	0	0	0
			1550	981	268	295	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	HIS	-	EXPRESSION TAG	UNP P31697
C	207	HIS	-	EXPRESSION TAG	UNP P31697
C	208	HIS	-	EXPRESSION TAG	UNP P31697
C	209	HIS	-	EXPRESSION TAG	UNP P31697
C	210	HIS	-	EXPRESSION TAG	UNP P31697
C	211	HIS	-	EXPRESSION TAG	UNP P31697

- Molecule 4 is a protein called Protein FimF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	154	Total	C	N	O	S	0	0	0
			1137	711	196	226	4			

- Molecule 5 is a protein called Outer membrane usher protein FimD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	778	Total	C	N	O	S	0	0	0
			5951	3714	1055	1163	19			

There are 11 discrepancies between the modelled and reference sequences:

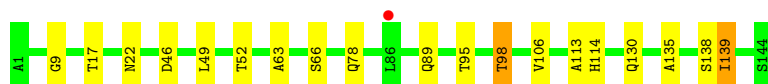
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	PRO	THR	CONFLICT	UNP P30130
D	834	SER	-	EXPRESSION TAG	UNP P30130
D	835	ALA	-	EXPRESSION TAG	UNP P30130
D	836	TRP	-	EXPRESSION TAG	UNP P30130
D	837	SER	-	EXPRESSION TAG	UNP P30130
D	838	HIS	-	EXPRESSION TAG	UNP P30130
D	839	PRO	-	EXPRESSION TAG	UNP P30130
D	840	GLN	-	EXPRESSION TAG	UNP P30130
D	841	PHE	-	EXPRESSION TAG	UNP P30130
D	842	GLU	-	EXPRESSION TAG	UNP P30130
D	843	LYS	-	EXPRESSION TAG	UNP P30130

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

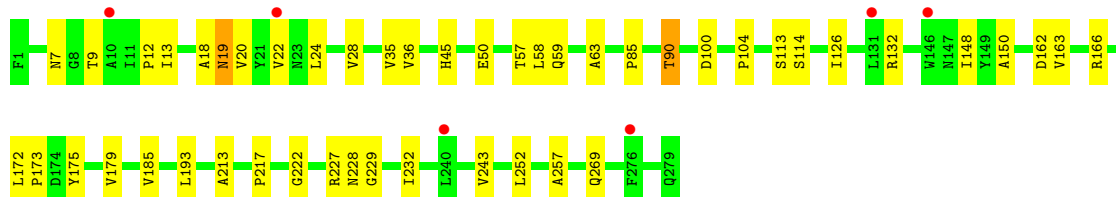
- Molecule 1: Protein FimG

Chain G: 



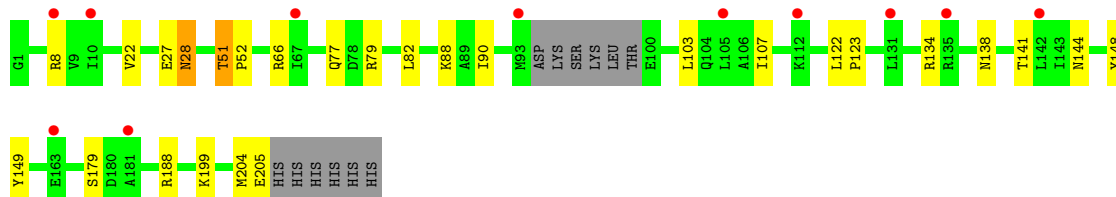
- Molecule 2: Protein FimH

Chain H: 



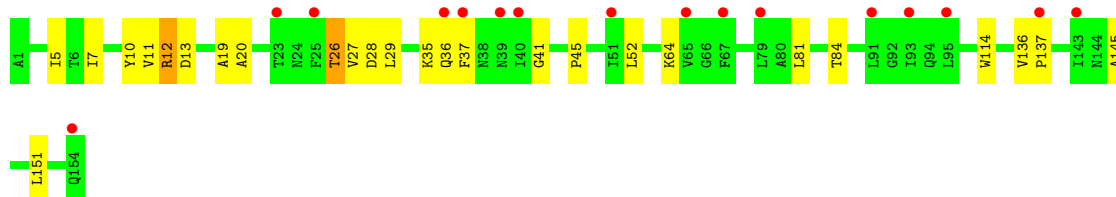
- Molecule 3: Chaperone protein FimC

Chain C: 



- Molecule 4: Protein FimF

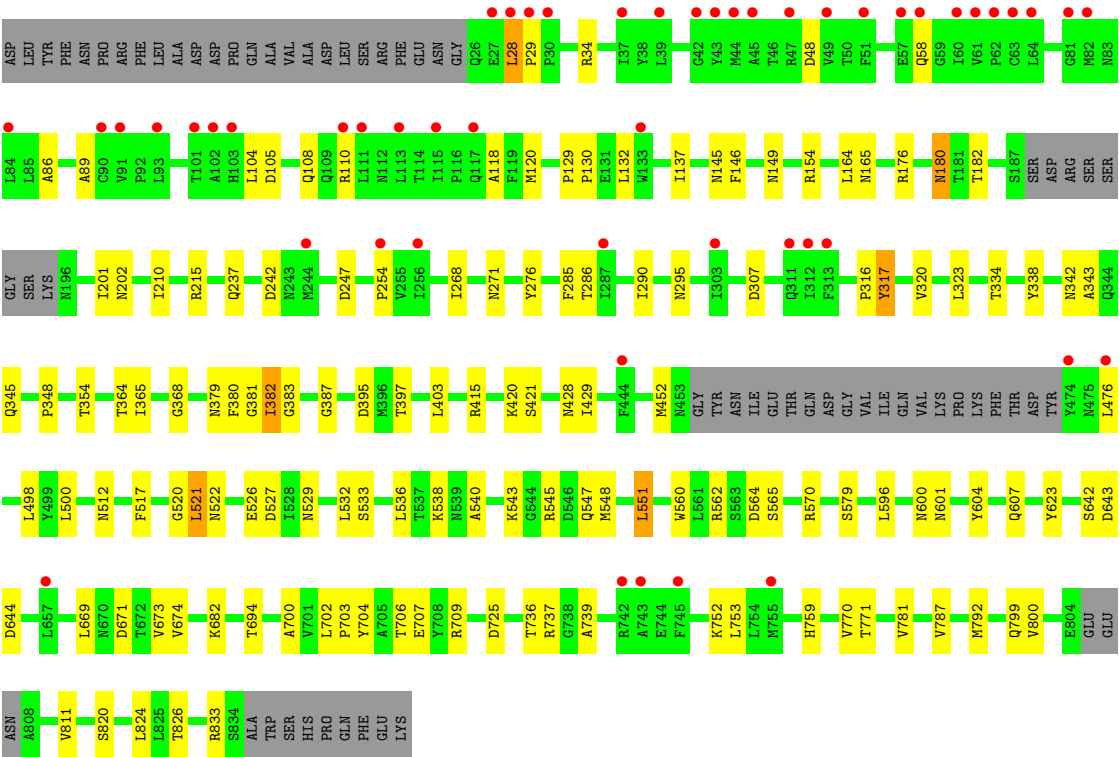
Chain F: 



- Molecule 5: Outer membrane usher protein FimD

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.36Å 122.36Å 328.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.67 – 3.80 83.67 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (83.67-3.80) 86.0 (83.67-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.248 , 0.299 0.251 , 0.298	Depositor DCC
R_{free} test set	1074 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	159.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 123.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 25474 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11732	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	G	0.21	0/1057	0.39	0/1445
2	H	0.21	0/2096	0.38	0/2881
3	C	0.20	0/1578	0.38	0/2146
4	F	0.22	0/1157	0.40	0/1584
5	D	0.20	0/6079	0.36	0/8276
All	All	0.21	0/11967	0.37	0/16332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1043	0	1009	12	0
2	H	2051	0	2007	26	0
3	C	1550	0	1582	13	0
4	F	1137	0	1126	13	0
5	D	5951	0	5656	66	0
All	All	11732	0	11380	120	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (120) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:D:562:ARG:HG2	5:D:564:ASP:H	1.53	0.72
5:D:165:ASN:HA	5:D:182:THR:HG22	1.74	0.69
2:H:12:PRO:HA	2:H:18:ALA:HB2	1.75	0.68
5:D:538:LYS:HD2	5:D:545:ARG:HG2	1.76	0.68
2:H:163:VAL:HG12	2:H:185:VAL:HG22	1.76	0.67
4:F:26:THR:O	4:F:28:ASP:N	2.28	0.66
1:G:78:GLN:NE2	5:D:526:GLU:O	2.30	0.65
5:D:154:ARG:NH1	5:D:644:ASP:OD2	2.30	0.64
2:H:35:VAL:HG12	2:H:36:VAL:HG23	1.79	0.64
5:D:517:PHE:HB3	5:D:536:LEU:HB3	1.80	0.63
2:H:57:THR:OG1	2:H:90:THR:O	2.16	0.63
2:H:58:LEU:H	2:H:90:THR:HG22	1.64	0.63
5:D:403:LEU:HD22	5:D:476:LEU:HD13	1.82	0.62
2:H:126:ILE:HD11	2:H:150:ALA:HB2	1.80	0.61
5:D:338:TYR:HB3	5:D:348:PRO:HD2	1.82	0.61
5:D:379:ASN:ND2	5:D:397:THR:OG1	2.31	0.61
5:D:548:MET:SD	5:D:579:SER:OG	2.59	0.60
1:G:106:VAL:HA	1:G:113:ALA:HB2	1.83	0.60
2:H:59:GLN:HE21	2:H:132:ARG:HD2	1.67	0.60
5:D:770:VAL:HG22	5:D:800:VAL:HG22	1.82	0.60
3:C:88:LYS:HE2	3:C:90:ILE:HD11	1.84	0.59
2:H:172:LEU:HD23	2:H:179:VAL:HG22	1.85	0.58
5:D:295:ASN:ND2	5:D:428:ASN:OD1	2.37	0.57
1:G:22:ASN:ND2	5:D:604:TYR:O	2.38	0.57
5:D:176:ARG:HH21	5:D:739:ALA:HB2	1.71	0.56
4:F:35:LYS:HA	4:F:36:GLN:HB2	1.89	0.55
5:D:317:TYR:O	5:D:421:SER:OG	2.16	0.55
5:D:108:GLN:HB2	5:D:110:ARG:HD2	1.89	0.55
5:D:820:SER:HB2	5:D:826:THR:HG21	1.89	0.54
4:F:37:PHE:HD2	4:F:41:GLY:HA2	1.71	0.54
5:D:118:ALA:HB2	5:D:285:PHE:HA	1.90	0.54
4:F:19:ALA:HB3	4:F:52:LEU:HB3	1.90	0.53
5:D:532:LEU:HD13	5:D:551:LEU:HB3	1.91	0.53
5:D:381:GLY:HA2	5:D:395:ASP:HB3	1.91	0.53
2:H:193:LEU:HD12	2:H:243:VAL:HG21	1.91	0.53
5:D:771:THR:HG23	5:D:799:GLN:HB3	1.90	0.52
2:H:227:ARG:O	2:H:229:GLY:N	2.42	0.52
2:H:227:ARG:HG2	2:H:232:ILE:HD11	1.91	0.52
2:H:213:ALA:HB3	2:H:217:PRO:HB3	1.92	0.52
3:C:66:ARG:NH2	5:D:725:ASP:OD2	2.42	0.52
5:D:694:THR:HA	5:D:700:ALA:HB2	1.91	0.52
3:C:28:ASN:OD1	3:C:28:ASN:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:D:354:THR:HA	5:D:368:GLY:HA3	1.92	0.52
1:G:130:GLN:HG3	4:F:11:VAL:O	2.10	0.51
5:D:753:LEU:HD11	5:D:792:MET:HG3	1.92	0.51
5:D:642:SER:O	5:D:644:ASP:N	2.42	0.51
2:H:126:ILE:HB	2:H:148:ILE:HB	1.93	0.51
4:F:36:GLN:HE21	4:F:137:PRO:HB3	1.76	0.51
1:G:63:ALA:HB1	1:G:139:ILE:HD11	1.92	0.51
1:G:89:GLN:HG2	1:G:95:THR:HA	1.93	0.50
5:D:86:ALA:HB3	5:D:89:ALA:HB2	1.92	0.50
5:D:320:VAL:H	5:D:323:LEU:HD12	1.76	0.50
5:D:215:ARG:NH2	5:D:737:ARG:HB3	2.27	0.50
5:D:58:GLN:NE2	5:D:104:LEU:O	2.45	0.49
5:D:180:ASN:HB3	5:D:201:ILE:HB	1.92	0.49
3:C:138:ASN:OD1	3:C:179:SER:OG	2.28	0.49
5:D:176:ARG:NH2	5:D:736:THR:OG1	2.45	0.49
5:D:682:LYS:O	5:D:694:THR:OG1	2.27	0.48
5:D:34:ARG:NH2	5:D:48:ASP:OD2	2.47	0.48
5:D:565:SER:O	5:D:570:ARG:NH1	2.47	0.48
1:G:135:ALA:HB3	4:F:7:ILE:HB	1.96	0.48
2:H:45:HIS:ND1	2:H:100:ASP:OD2	2.44	0.47
5:D:725:ASP:HB2	5:D:752:LYS:HE2	1.96	0.47
1:G:49:LEU:HD21	4:F:5:ILE:HD11	1.95	0.47
5:D:512:ASN:HB3	5:D:540:ALA:HB1	1.97	0.47
5:D:342:ASN:OD1	5:D:343:ALA:N	2.48	0.47
3:C:144:ASN:ND2	3:C:148:TYR:O	2.47	0.46
5:D:180:ASN:N	5:D:202:ASN:O	2.44	0.46
5:D:674:VAL:HB	5:D:702:LEU:HB2	1.98	0.46
4:F:64:LYS:HE3	4:F:114:TRP:CE2	2.51	0.46
2:H:63:ALA:HB2	2:H:85:PRO:HB3	1.98	0.45
5:D:364:THR:N	5:D:383:GLY:O	2.49	0.45
5:D:210:ILE:HD12	5:D:210:ILE:H	1.81	0.45
5:D:811:VAL:HB	5:D:833:ARG:HB3	1.98	0.45
3:C:82:LEU:HB2	3:C:149:TYR:CZ	2.52	0.44
5:D:145:ASN:HB3	5:D:165:ASN:HB2	1.99	0.44
5:D:674:VAL:HB	5:D:702:LEU:HD12	1.99	0.44
3:C:27:GLU:N	3:C:27:GLU:OE1	2.46	0.44
1:G:66:SER:N	1:G:138:SER:O	2.49	0.44
2:H:162:ASP:OD2	2:H:166:ARG:NH2	2.51	0.44
5:D:28:LEU:HG	5:D:29:PRO:HD2	1.99	0.44
2:H:20:VAL:HG22	2:H:22:VAL:HG13	2.00	0.44
5:D:365:ILE:HG22	5:D:382:ILE:HD13	1.99	0.44
1:G:46:ASP:HB2	5:D:704:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:10:TYR:HB3	4:F:12:ARG:NH1	2.33	0.43
2:H:213:ALA:HA	2:H:269:GLN:HB3	1.99	0.43
2:H:28:VAL:HG21	2:H:162:ASP:HB2	1.99	0.43
5:D:129:PRO:HD2	5:D:132:LEU:HD12	2.01	0.43
5:D:146:PHE:HD1	5:D:164:LEU:HB2	1.84	0.43
1:G:17:THR:OG1	1:G:52:THR:O	2.33	0.43
5:D:237:GLN:HG3	5:D:334:THR:HG22	2.00	0.43
2:H:222:GLY:N	2:H:257:ALA:O	2.35	0.43
1:G:9:GLY:HA2	2:H:172:LEU:HB2	2.01	0.42
3:C:107:ILE:HD11	4:F:20:ALA:HB2	2.01	0.42
5:D:420:LYS:HB3	5:D:429:ILE:HB	2.02	0.42
3:C:134:ARG:HB3	3:C:141:THR:HB	2.00	0.42
5:D:254:PRO:HD3	5:D:317:TYR:CE1	2.55	0.42
2:H:19:ASN:N	2:H:19:ASN:OD1	2.53	0.42
2:H:227:ARG:HB3	2:H:252:LEU:HD23	2.02	0.42
3:C:188:ARG:HG2	3:C:199:LYS:HA	2.02	0.42
2:H:113:SER:OG	2:H:114:SER:N	2.53	0.42
5:D:781:VAL:HG22	5:D:787:VAL:HB	2.02	0.41
2:H:24:LEU:HG	2:H:36:VAL:HG22	2.02	0.41
5:D:342:ASN:HB3	5:D:345:GLN:HG3	2.02	0.41
5:D:316:PRO:HB2	5:D:387:GLY:HA3	2.03	0.41
5:D:673:VAL:HG22	5:D:703:PRO:HA	2.03	0.41
2:H:173:PRO:HD3	2:H:179:VAL:HG13	2.01	0.41
5:D:129:PRO:HA	5:D:130:PRO:HD3	1.83	0.41
3:C:103:LEU:HD13	4:F:145:ALA:HB3	2.02	0.41
5:D:307:ASP:OD1	5:D:307:ASP:N	2.49	0.41
5:D:268:ILE:HB	5:D:276:TYR:HB3	2.02	0.41
5:D:596:LEU:O	5:D:600:ASN:HA	2.20	0.41
5:D:669:LEU:HD22	5:D:673:VAL:HG21	2.02	0.41
5:D:247:ASP:OD2	5:D:709:ARG:NH1	2.54	0.41
5:D:607:GLN:HG3	5:D:623:TYR:HB2	2.02	0.41
5:D:520:GLY:HA2	5:D:533:SER:HA	2.03	0.40
4:F:81:LEU:HD23	4:F:145:ALA:HB2	2.02	0.40
3:C:122:LEU:HD12	3:C:123:PRO:HD2	2.03	0.40
5:D:498:LEU:HD13	5:D:521:LEU:HG	2.02	0.40
3:C:51:THR:HA	3:C:52:PRO:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	G	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	30	84
2	H	277/279 (99%)	250 (90%)	23 (8%)	4 (1%)	16	74
3	C	195/211 (92%)	181 (93%)	14 (7%)	0	100	100
4	F	152/154 (99%)	135 (89%)	15 (10%)	2 (1%)	18	76
5	D	770/843 (91%)	701 (91%)	64 (8%)	5 (1%)	33	86
All	All	1536/1631 (94%)	1397 (91%)	127 (8%)	12 (1%)	27	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	27	VAL
2	H	228	ASN
1	G	98	THR
2	H	7	ASN
5	D	452	MET
5	D	643	ASP
5	D	671	ASP
4	F	45	PRO
5	D	382	ILE
5	D	290	ILE
2	H	175	TYR
2	H	104	PRO

5.3.2 Protein sidechains ⓘ

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	G	115/115 (100%)	112 (97%)	3 (3%)	59	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	226/226 (100%)	221 (98%)	5 (2%)	64	91
3	C	170/182 (93%)	162 (95%)	8 (5%)	36	82
4	F	124/124 (100%)	117 (94%)	7 (6%)	30	78
5	D	621/694 (90%)	595 (96%)	26 (4%)	40	84
All	All	1256/1341 (94%)	1207 (96%)	49 (4%)	43	85

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	98	THR
1	G	114	HIS
1	G	139	ILE
2	H	9	THR
2	H	13	ILE
2	H	19	ASN
2	H	50	GLU
2	H	90	THR
3	C	8	ARG
3	C	22	VAL
3	C	28	ASN
3	C	51	THR
3	C	77	GLN
3	C	79	ARG
3	C	204	MET
3	C	205	GLU
4	F	12	ARG
4	F	13	ASP
4	F	26	THR
4	F	29	LEU
4	F	84	THR
4	F	136	VAL
4	F	151	LEU
5	D	28	LEU
5	D	105	ASP
5	D	120	MET
5	D	137	ILE
5	D	149	ASN
5	D	180	ASN
5	D	242	ASP
5	D	271	ASN
5	D	286	THR

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Mol	Chain	Res	Type
5	D	317	TYR
5	D	380	PHE
5	D	415	ARG
5	D	500	LEU
5	D	521	LEU
5	D	522	ASN
5	D	527	ASP
5	D	529	ASN
5	D	543	LYS
5	D	547	GLN
5	D	551	LEU
5	D	560	TRP
5	D	601	ASN
5	D	706	THR
5	D	707	GLU
5	D	759	HIS
5	D	824	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	78	GLN
2	H	59	GLN
5	D	295	ASN
5	D	428	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 95th 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	G	144/144 (100%)	0.28	1 (0%) 84 67	119, 153, 181, 201	1 (0%)
2	H	279/279 (100%)	0.20	6 (2%) 59 39	118, 187, 225, 290	2 (0%)
3	C	199/211 (94%)	0.40	11 (5%) 24 17	138, 202, 249, 262	1 (0%)
4	F	154/154 (100%)	0.49	16 (10%) 7 8	136, 211, 304, 331	0
5	D	778/843 (92%)	0.42	51 (6%) 18 14	110, 180, 318, 369	2 (0%)
All	All	1554/1631 (95%)	0.37	85 (5%) 24 17	110, 184, 289, 369	6 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	102	ALA	11.8
5	D	474	TYR	9.4
5	D	62	PRO	8.7
5	D	64	LEU	6.9
5	D	28	LEU	6.6
5	D	27	GLU	5.7
5	D	63	CYS	5.5
4	F	25	PHE	5.2
4	F	154	GLN	5.2
3	C	135	ARG	4.9
5	D	303	ILE	4.9
5	D	44	MET	4.5
3	C	8	ARG	4.5
5	D	37	ILE	4.4
5	D	45	ALA	4.2
5	D	476	LEU	4.2
3	C	105	LEU	4.1
5	D	30	PRO	4.1
5	D	29	PRO	4.1
5	D	82	MET	4.1

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Mol	Chain	Res	Type	RSRZ
5	D	101	THR	3.8
4	F	36	GLN	3.6
5	D	111	LEU	3.3
4	F	39	ASN	3.2
5	D	91	VAL	3.2
5	D	43	TYR	3.2
4	F	91	LEU	3.1
3	C	112	LYS	3.1
5	D	39	LEU	3.1
5	D	84	LEU	3.1
5	D	113	LEU	3.0
5	D	47	ARG	3.0
2	H	240	LEU	3.0
5	D	254	PRO	3.0
3	C	10	ILE	2.9
5	D	51	PHE	2.8
3	C	67	ILE	2.8
5	D	110	ARG	2.8
4	F	137	PRO	2.8
4	F	95	LEU	2.8
5	D	312	ILE	2.7
5	D	657	LEU	2.7
5	D	745	PHE	2.6
5	D	61	VAL	2.5
5	D	57	GLU	2.5
1	G	86	LEU	2.5
5	D	256	ILE	2.5
3	C	93	MET	2.5
5	D	117	GLN	2.4
4	F	37	PHE	2.4
2	H	131	LEU	2.4
5	D	42	GLY	2.4
3	C	142	LEU	2.4
2	H	276	PHE	2.4
4	F	143	ILE	2.4
5	D	60	ILE	2.4
5	D	133	TRP	2.4
3	C	181	ALA	2.3
5	D	313	PHE	2.3
5	D	742	ARG	2.3
4	F	23	THR	2.3
5	D	287	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
5	D	81	GLY	2.3
5	D	244	MET	2.3
5	D	103	HIS	2.3
5	D	58	GLN	2.3
2	H	146	TRP	2.2
5	D	743	ALA	2.2
5	D	444	PHE	2.2
4	F	40	ILE	2.2
5	D	49	VAL	2.2
4	F	67	PHE	2.2
4	F	65	VAL	2.1
5	D	93	LEU	2.1
4	F	51	ILE	2.1
5	D	311	GLN	2.1
5	D	755	MET	2.1
5	D	90	CYS	2.1
2	H	10	ALA	2.1
3	C	163	GLU	2.1
4	F	93	ILE	2.0
4	F	79	LEU	2.0
2	H	22	VAL	2.0
3	C	131	LEU	2.0
5	D	115	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.