



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2016 – 09:23 AM EDT

PDB ID : 4Y2L
Title : Structure of CFA/I pili major subunit CfaB trimer
Authors : Bao, R.; Xia, D.
Deposited on : 2015-02-10
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

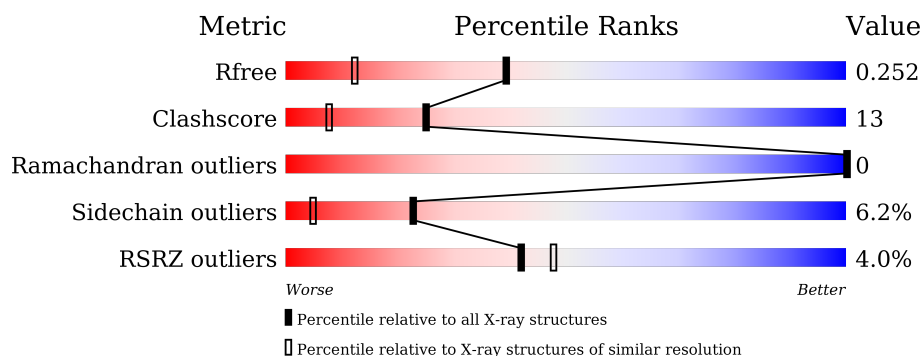
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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. 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 $\leq 5\%$. 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	153	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	153	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
1	C	153	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	153	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
1	E	153	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	F	153	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>

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	IPA	A	202	-	-	-	X
2	IPA	C	201	-	-	-	X
2	IPA	D	201	-	-	X	X
3	CA	F	202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13747 atoms, of which 6594 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 CFA/I fimbrial subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	147	Total	C	H	N	O	S	0	0	0
			2135	664	1075	175	218	3			
1	B	148	Total	C	H	N	O	S	0	0	0
			2153	670	1083	178	219	3			
1	C	147	Total	C	H	N	O	S	0	1	0
			2148	668	1080	177	220	3			
1	D	150	Total	C	H	N	O	S	0	4	0
			2242	698	1124	188	229	3			
1	E	150	Total	C	H	N	O	S	0	2	0
			2213	689	1109	187	225	3			
1	F	149	Total	C	H	N	O	S	0	0	0
			2171	676	1091	181	220	3			

There are 42 discrepancies between the modelled and reference sequences:

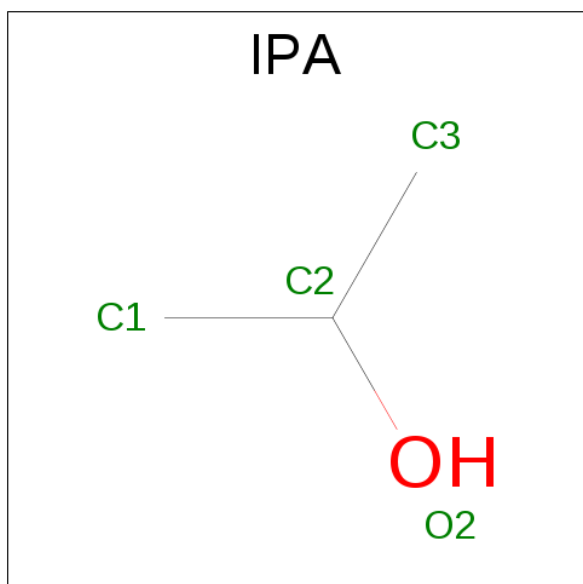
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP E3PPC4
A	-4	HIS	-	expression tag	UNP E3PPC4
A	-3	HIS	-	expression tag	UNP E3PPC4
A	-2	HIS	-	expression tag	UNP E3PPC4
A	-1	HIS	-	expression tag	UNP E3PPC4
A	0	HIS	-	expression tag	UNP E3PPC4
A	1	HIS	-	expression tag	UNP E3PPC4
B	-5	MET	-	initiating methionine	UNP E3PPC4
B	-4	HIS	-	expression tag	UNP E3PPC4
B	-3	HIS	-	expression tag	UNP E3PPC4
B	-2	HIS	-	expression tag	UNP E3PPC4
B	-1	HIS	-	expression tag	UNP E3PPC4
B	0	HIS	-	expression tag	UNP E3PPC4
B	1	HIS	-	expression tag	UNP E3PPC4
C	-5	MET	-	initiating methionine	UNP E3PPC4
C	-4	HIS	-	expression tag	UNP E3PPC4
C	-3	HIS	-	expression tag	UNP E3PPC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP E3PPC4
C	-1	HIS	-	expression tag	UNP E3PPC4
C	0	HIS	-	expression tag	UNP E3PPC4
C	1	HIS	-	expression tag	UNP E3PPC4
D	-5	MET	-	initiating methionine	UNP E3PPC4
D	-4	HIS	-	expression tag	UNP E3PPC4
D	-3	HIS	-	expression tag	UNP E3PPC4
D	-2	HIS	-	expression tag	UNP E3PPC4
D	-1	HIS	-	expression tag	UNP E3PPC4
D	0	HIS	-	expression tag	UNP E3PPC4
D	1	HIS	-	expression tag	UNP E3PPC4
E	-5	MET	-	initiating methionine	UNP E3PPC4
E	-4	HIS	-	expression tag	UNP E3PPC4
E	-3	HIS	-	expression tag	UNP E3PPC4
E	-2	HIS	-	expression tag	UNP E3PPC4
E	-1	HIS	-	expression tag	UNP E3PPC4
E	0	HIS	-	expression tag	UNP E3PPC4
E	1	HIS	-	expression tag	UNP E3PPC4
F	-5	MET	-	initiating methionine	UNP E3PPC4
F	-4	HIS	-	expression tag	UNP E3PPC4
F	-3	HIS	-	expression tag	UNP E3PPC4
F	-2	HIS	-	expression tag	UNP E3PPC4
F	-1	HIS	-	expression tag	UNP E3PPC4
F	0	HIS	-	expression tag	UNP E3PPC4
F	1	HIS	-	expression tag	UNP E3PPC4

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 12 3 8 1	0	0
2	A	1	Total C H O 12 3 8 1	0	0
2	C	1	Total C H O 12 3 8 1	0	0
2	D	1	Total C H O 12 3 8 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	2	Total Ca 2 2	0	0

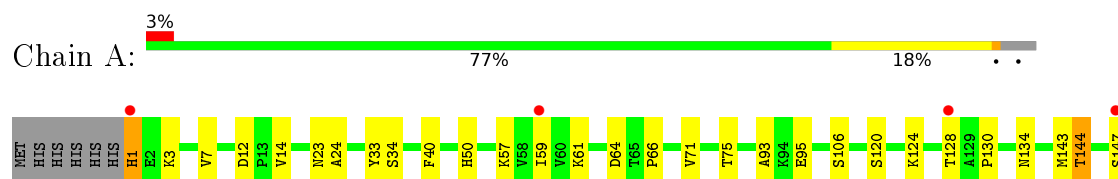
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	B	108	Total O 108 108	0	0
4	C	118	Total O 118 118	0	0
4	D	100	Total O 100 100	0	0
4	E	99	Total O 99 99	0	0
4	F	105	Total O 105 105	0	0

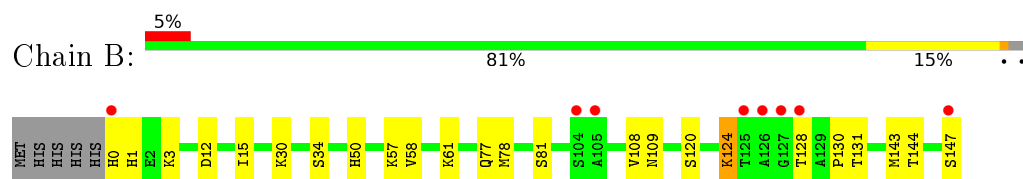
3 Residue-property plots [i](#)

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

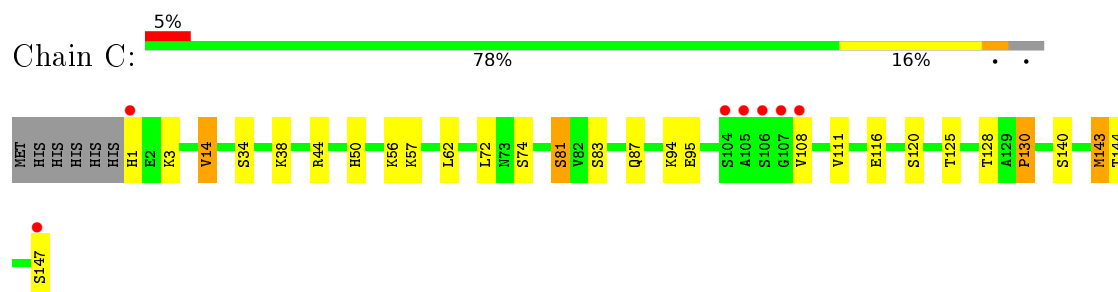
- Molecule 1: CFA/I fimbrial subunit B



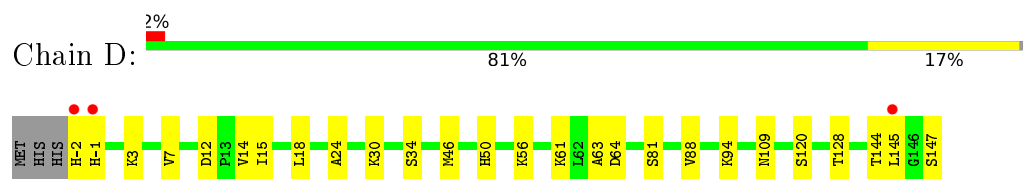
- Molecule 1: CFA/I fimbrial subunit B



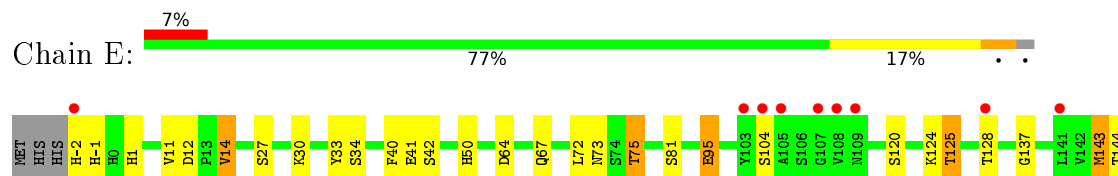
- Molecule 1: CFA/I fimbrial subunit B



- Molecule 1: CFA/I fimbrial subunit B

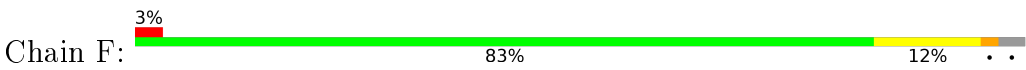


- Molecule 1: CFA/I fimbrial subunit B





● Molecule 1: CFA/I fimbrial subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.27Å 105.81Å 70.11Å 90.00° 114.05° 90.00°	Depositor
Resolution (Å)	40.78 – 1.75 40.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	84.8 (40.78-1.75) 86.6 (40.78-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1323)	Depositor
R, R_{free}	0.204 , 0.240 0.214 , 0.252	Depositor DCC
R_{free} test set	1987 reflections (2.35%)	DCC
Wilson B-factor (Å ²)	8.5	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13747	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/1076	0.74	1/1471 (0.1%)
1	B	0.67	0/1087	0.75	0/1486
1	C	0.79	2/1084 (0.2%)	0.76	1/1482 (0.1%)
1	D	0.70	0/1137	0.75	0/1554
1	E	0.62	0/1123	0.74	1/1535 (0.1%)
1	F	0.62	0/1098	0.79	0/1501
All	All	0.68	2/6605 (0.0%)	0.76	3/9029 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	SER	CB-OG	-5.91	1.34	1.42
1	C	130	PRO	N-CD	5.38	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	106	SER	C-N-CA	6.49	135.93	122.30
1	E	145	LEU	CA-CB-CG	6.25	129.67	115.30
1	C	72	LEU	CA-C-N	5.13	128.48	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	72	LEU	Mainchain

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	1060	1075	1075	39	0
1	B	1070	1083	1082	28	0
1	C	1068	1080	1080	33	0
1	D	1118	1124	1117	36	0
1	E	1104	1109	1105	49	0
1	F	1080	1091	1089	34	2
2	A	8	16	16	1	0
2	C	4	8	8	2	0
2	D	4	8	8	8	0
3	F	2	0	0	0	0
4	A	105	0	0	6	4
4	B	108	0	0	11	1
4	C	118	0	0	7	0
4	D	100	0	0	5	1
4	E	99	0	0	6	2
4	F	105	0	0	15	0
All	All	7153	6594	6580	166	5

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 13.

All (166) 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:120:SER:HB2	4:A:385:HOH:O	1.37	1.24
1:E:41:GLU:HG3	4:E:272:HOH:O	1.46	1.13
1:A:14:VAL:HG11	1:E:-1:HIS:CD2	1.85	1.12
1:F:143:MET:SD	4:F:403:HOH:O	2.07	1.11
1:E:95:GLU:HG3	4:E:278:HOH:O	1.47	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:HIS:CD2	1:E:14:VAL:HG11	1.88	1.08
1:A:14:VAL:HG11	1:E:-1:HIS:CG	1.93	1.02
1:B:15:ILE:HD11	1:B:143:MET:CE	1.92	0.99
1:D:30:LYS:HZ1	2:D:201:IPA:H32	1.29	0.97
1:C:108:VAL:HG13	1:C:111:VAL:HB	1.45	0.96
1:A:144:THR:HG23	1:E:-1:HIS:O	1.65	0.95
1:D:30:LYS:NZ	2:D:201:IPA:H32	1.79	0.95
1:C:1:HIS:HA	4:C:326:HOH:O	1.68	0.94
1:D:-1:HIS:NE2	1:E:14:VAL:HG11	1.83	0.94
1:D:-1:HIS:NE2	1:E:14:VAL:CG1	2.31	0.93
1:E:143:MET:CE	4:E:259:HOH:O	2.19	0.91
1:D:-1:HIS:CE1	1:E:14:VAL:HG11	2.06	0.91
1:C:120:SER:HB2	4:C:401:HOH:O	1.70	0.90
1:E:143:MET:HE2	4:E:259:HOH:O	1.71	0.90
1:C:14:VAL:HG11	1:F:-1:HIS:CG	2.08	0.89
1:B:3:LYS:HE3	4:F:374:HOH:O	1.72	0.88
1:D:-1:HIS:CD2	1:E:14:VAL:CG1	2.57	0.88
1:B:15:ILE:HD11	1:B:143:MET:HE1	1.54	0.88
1:E:41:GLU:CG	4:E:272:HOH:O	2.09	0.86
1:B:120:SER:HB3	4:B:201:HOH:O	1.75	0.86
1:F:67:GLN:HG3	4:F:316:HOH:O	1.74	0.85
1:C:83:SER:OG	2:C:201:IPA:H32	1.76	0.84
1:F:75:THR:OG1	4:F:301:HOH:O	1.94	0.84
1:A:1:HIS:CE1	1:A:3:LYS:HG3	2.13	0.83
1:C:14:VAL:HG11	1:F:-1:HIS:CD2	2.13	0.83
1:D:-1:HIS:CG	1:E:14:VAL:HG11	2.13	0.82
1:A:144:THR:CG2	1:E:-1:HIS:O	2.27	0.82
1:D:46:MET:SD	4:D:323:HOH:O	2.37	0.81
1:A:24:ALA:HB1	2:D:201:IPA:H13	1.64	0.80
1:F:67:GLN:CG	4:F:316:HOH:O	2.31	0.79
1:D:-2:HIS:CD2	1:E:146:GLY:HA3	2.17	0.78
1:B:81:SER:OG	4:B:201:HOH:O	1.92	0.78
1:A:14:VAL:CG1	1:E:-1:HIS:CD2	2.67	0.77
4:A:369:HOH:O	2:D:201:IPA:H31	1.85	0.75
1:C:1:HIS:CA	4:C:326:HOH:O	2.29	0.75
1:A:14:VAL:CG1	1:E:-1:HIS:CE1	2.69	0.75
2:D:201:IPA:H11	4:D:387:HOH:O	1.87	0.73
1:F:67:GLN:CD	4:F:316:HOH:O	2.26	0.73
1:D:-1:HIS:CE1	1:E:14:VAL:CG1	2.71	0.73
1:B:15:ILE:HD11	1:B:143:MET:HE2	1.70	0.73
1:D:88:VAL:O	1:D:94:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LYS:HE2	2:D:201:IPA:H13	1.70	0.72
1:F:95:GLU:OE2	4:F:302:HOH:O	2.09	0.69
1:D:145:LEU:HD12	1:D:145:LEU:N	2.07	0.69
1:D:81:SER:HB2	4:D:339:HOH:O	1.92	0.69
1:B:15:ILE:CD1	1:B:143:MET:CE	2.70	0.68
1:B:15:ILE:CD1	1:B:143:MET:HE2	2.24	0.67
1:E:143:MET:SD	4:E:259:HOH:O	2.53	0.67
1:A:14:VAL:CG1	1:E:-1:HIS:NE2	2.59	0.65
1:F:75:THR:CB	4:F:301:HOH:O	2.44	0.64
1:A:12:ASP:OD2	1:E:-1:HIS:HE1	1.79	0.64
1:F:146:GLY:O	4:F:303:HOH:O	2.15	0.64
1:A:59:ILE:HG12	1:A:95:GLU:HG2	1.78	0.64
1:E:73[A]:ASN:OD1	1:E:75:THR:OG1	2.17	0.62
1:B:124:LYS:HE3	4:B:250:HOH:O	1.99	0.61
1:C:14:VAL:CG1	1:F:-1:HIS:CD2	2.83	0.61
1:F:143:MET:CE	4:F:403:HOH:O	2.42	0.60
1:C:108:VAL:CG1	1:C:111:VAL:HB	2.24	0.60
1:C:130:PRO:HG2	1:F:11:VAL:HG11	1.82	0.59
1:A:1:HIS:O	1:A:1:HIS:ND1	2.35	0.59
1:B:128:THR:O	4:B:203:HOH:O	2.16	0.58
1:A:1:HIS:HE1	1:A:3:LYS:HG3	1.67	0.58
1:F:124:LYS:HE2	4:F:305:HOH:O	2.02	0.58
1:A:14:VAL:CG1	1:E:-1:HIS:CG	2.81	0.58
1:D:12:ASP:OD1	1:D:14:VAL:HG12	2.03	0.57
1:B:15:ILE:CD1	1:B:143:MET:HE1	2.33	0.57
1:D:63:ALA:O	1:D:64:ASP:OD1	2.23	0.57
1:A:130:PRO:HG2	1:E:11:VAL:HG11	1.88	0.56
1:B:50:HIS:HD2	1:F:34:SER:OG	1.89	0.55
1:C:108:VAL:HG13	1:C:111:VAL:CB	2.27	0.55
1:C:14:VAL:HG13	1:F:-1:HIS:CE1	2.42	0.55
1:B:0:HIS:HB2	1:F:144:THR:HG23	1.87	0.54
1:C:57:LYS:NZ	4:C:378:HOH:O	2.39	0.54
1:A:14:VAL:HG13	1:E:-1:HIS:CE1	2.40	0.54
1:D:-1:HIS:ND1	1:E:14:VAL:HG11	2.21	0.54
1:D:14:VAL:HG13	1:D:15:ILE:N	2.23	0.54
1:C:87:GLN:HB3	1:C:94:LYS:HD2	1.90	0.53
1:C:14:VAL:CG1	1:F:-1:HIS:CE1	2.92	0.53
1:A:66:PRO:HD2	2:A:201:IPA:C3	2.39	0.52
1:D:14:VAL:HG13	1:D:15:ILE:H	1.74	0.52
1:C:143:MET:HG3	1:F:1:HIS:HB3	1.90	0.52
1:D:128:THR:OG1	1:D:128:THR:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLN:O	1:B:124:LYS:HE2	2.09	0.52
1:A:34:SER:OG	1:E:50:HIS:HD2	1.94	0.51
1:B:143:MET:O	1:C:1:HIS:N	2.43	0.51
1:D:120[B]:SER:HB3	4:D:339:HOH:O	2.09	0.51
1:A:12:ASP:OD2	1:E:-1:HIS:CE1	2.63	0.51
1:C:1:HIS:N	4:C:326:HOH:O	2.34	0.51
1:D:15:ILE:CG2	1:D:145:LEU:HD11	2.41	0.51
1:D:145:LEU:CD1	1:D:145:LEU:N	2.73	0.51
1:D:50:HIS:HD2	1:E:34:SER:OG	1.94	0.51
1:F:75:THR:HG23	4:F:301:HOH:O	2.11	0.50
1:C:38:LYS:HE3	4:C:314:HOH:O	2.12	0.50
1:A:24:ALA:HB1	2:D:201:IPA:C1	2.39	0.50
1:E:146:GLY:O	1:E:147:SER:CB	2.60	0.50
1:D:-1:HIS:CD2	1:E:14:VAL:HG13	2.46	0.49
1:A:14:VAL:HG11	1:E:-1:HIS:CE1	2.43	0.49
1:B:30:LYS:CD	4:B:202:HOH:O	2.60	0.49
1:D:-2:HIS:HB3	1:E:144:THR:CG2	2.42	0.49
1:C:14:VAL:CG1	1:F:-1:HIS:CG	2.90	0.49
1:A:50:HIS:HD2	1:D:34:SER:OG	1.95	0.49
1:B:147:SER:C	4:B:238:HOH:O	2.51	0.49
1:C:44:ARG:NH1	1:C:116:GLU:OE2	2.46	0.49
4:B:227:HOH:O	1:F:38:LYS:HE2	2.13	0.49
1:E:12:ASP:OD1	1:E:14:VAL:HG13	2.13	0.48
1:A:57:LYS:NZ	4:A:303:HOH:O	2.46	0.48
1:A:12:ASP:OD2	1:E:1:HIS:HD2	1.97	0.48
1:F:75:THR:CA	4:F:301:HOH:O	2.61	0.48
1:B:3:LYS:NZ	1:F:16:ASP:OD1	2.45	0.48
1:B:78:MET:SD	1:B:130:PRO:HB3	2.54	0.48
1:D:-1:HIS:O	1:E:144:THR:HA	2.13	0.48
1:A:59:ILE:HG23	1:A:93:ALA:HB1	1.95	0.48
1:E:12:ASP:OD1	1:E:14:VAL:CG1	2.61	0.47
1:D:24:ALA:CB	1:E:30:LYS:HG2	2.44	0.47
1:A:23:ASN:ND2	4:A:397:HOH:O	2.48	0.46
1:A:1:HIS:HB2	1:D:12:ASP:OD2	2.15	0.46
1:A:71:VAL:HG22	1:A:134:ASN:O	2.16	0.46
1:C:34:SER:OG	1:F:50:HIS:HD2	1.99	0.46
1:E:67:GLN:O	1:E:137:GLY:HA3	2.16	0.46
1:F:56:LYS:HE2	1:F:147:SER:O	2.16	0.45
1:B:34:SER:OG	1:C:50:HIS:HD2	1.98	0.45
1:D:30:LYS:CE	2:D:201:IPA:H32	2.47	0.45
1:E:73[B]:ASN:N	1:E:73[B]:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:CG2	1:A:93:ALA:HB1	2.46	0.45
1:D:12:ASP:OD1	1:D:14:VAL:CG1	2.65	0.45
1:C:62:LEU:HA	1:C:140:SER:O	2.17	0.45
1:C:14:VAL:CG1	1:F:-1:HIS:NE2	2.80	0.44
1:A:14:VAL:HG11	1:E:-1:HIS:ND1	2.29	0.44
1:E:33:TYR:HB2	1:E:40:PHE:CE2	2.52	0.44
1:B:58:VAL:HG11	1:B:143:MET:HE3	1.98	0.44
1:C:56:LYS:HD2	1:C:147:SER:HA	1.99	0.44
1:A:14:VAL:CG1	1:E:-1:HIS:ND1	2.80	0.44
1:E:125:THR:O	1:E:128:THR:OG1	2.34	0.43
1:C:57:LYS:HD2	1:C:95:GLU:HB3	2.00	0.43
1:D:-1:HIS:NE2	1:E:14:VAL:HG13	2.26	0.43
1:C:81:SER:HB3	2:C:201:IPA:H2	2.01	0.43
1:C:50:HIS:HE1	4:C:304:HOH:O	2.02	0.43
1:C:108:VAL:CG1	1:C:111:VAL:CB	2.95	0.43
4:B:227:HOH:O	1:F:38:LYS:HD3	2.19	0.43
1:B:0:HIS:CD2	4:B:210:HOH:O	2.71	0.42
1:A:3:LYS:NZ	4:A:359:HOH:O	2.46	0.42
1:B:1:HIS:HD2	1:F:12:ASP:HB2	1.84	0.42
1:D:56:LYS:HA	1:D:147:SER:O	2.20	0.42
1:F:1:HIS:HE1	1:F:3:LYS:HE2	1.84	0.42
1:D:50:HIS:HE1	4:D:308:HOH:O	2.01	0.42
1:A:50:HIS:HE1	4:A:306:HOH:O	2.03	0.42
1:A:59:ILE:CG1	1:A:95:GLU:HG2	2.45	0.42
1:B:12:ASP:OD2	1:C:1:HIS:HB3	2.19	0.42
1:A:12:ASP:OD2	1:E:1:HIS:CD2	2.73	0.42
1:A:144:THR:HG22	1:E:-1:HIS:O	2.15	0.41
1:C:108:VAL:HG11	1:C:111:VAL:HG21	2.00	0.41
1:B:0:HIS:CB	1:F:144:THR:HG23	2.50	0.41
1:A:12:ASP:OD1	1:A:14:VAL:HG12	2.20	0.41
1:B:1:HIS:CD2	1:F:12:ASP:HB2	2.56	0.41
1:B:0:HIS:CE1	4:B:210:HOH:O	2.74	0.41
1:F:147:SER:C	4:F:303:HOH:O	2.59	0.41
1:B:61:LYS:NZ	4:B:215:HOH:O	2.48	0.41
1:E:42:SER:OG	1:E:120[B]:SER:HB2	2.21	0.41
1:C:125:THR:HG1	1:C:128:THR:HB	1.87	0.41
1:F:75:THR:CG2	4:F:301:HOH:O	2.66	0.40
1:A:33:TYR:HB2	1:A:40:PHE:CE2	2.57	0.40

All (5) 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:73:ASN:HB2	4:A:305:HOH:O[1_656]	1.15	0.45
4:A:331:HOH:O	4:B:292:HOH:O[1_554]	1.98	0.22
4:D:320:HOH:O	4:E:217:HOH:O[2_454]	1.98	0.22
4:A:329:HOH:O	4:E:217:HOH:O[2_454]	2.03	0.17
1:F:73:ASN:CB	4:A:305:HOH:O[1_656]	2.07	0.13

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	145/153 (95%)	145 (100%)	0	0	100	100
1	B	146/153 (95%)	146 (100%)	0	0	100	100
1	C	146/153 (95%)	145 (99%)	1 (1%)	0	100	100
1	D	152/153 (99%)	151 (99%)	1 (1%)	0	100	100
1	E	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	F	147/153 (96%)	147 (100%)	0	0	100	100
All	All	886/918 (96%)	883 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	119/125 (95%)	109 (92%)	10 (8%)	14	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	120/125 (96%)	114 (95%)	6 (5%)	30	8
1	C	120/125 (96%)	115 (96%)	5 (4%)	36	12
1	D	126/125 (101%)	120 (95%)	6 (5%)	31	8
1	E	124/125 (99%)	112 (90%)	12 (10%)	10	1
1	F	121/125 (97%)	115 (95%)	6 (5%)	30	8
All	All	730/750 (97%)	685 (94%)	45 (6%)	23	5

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	7	VAL
1	A	61	LYS
1	A	64	ASP
1	A	75	THR
1	A	124	LYS
1	A	128	THR
1	A	143	MET
1	A	144	THR
1	A	147	SER
1	B	57	LYS
1	B	108	VAL
1	B	109	ASN
1	B	124	LYS
1	B	131	THR
1	B	144	THR
1	C	3	LYS
1	C	14	VAL
1	C	81	SER
1	C	143	MET
1	C	144	THR
1	D	3	LYS
1	D	7	VAL
1	D	18	LEU
1	D	61	LYS
1	D	109	ASN
1	D	144	THR
1	E	-2	HIS
1	E	14	VAL
1	E	27	SER

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Mol	Chain	Res	Type
1	E	64	ASP
1	E	75	THR
1	E	81	SER
1	E	95	GLU
1	E	104	SER
1	E	124	LYS
1	E	125	THR
1	E	143	MET
1	E	145	LEU
1	F	61	LYS
1	F	75	THR
1	F	94	LYS
1	F	128	THR
1	F	144	THR
1	F	147	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	B	1	HIS
1	B	50	HIS
1	C	50	HIS
1	D	-2	HIS
1	D	1	HIS
1	D	50	HIS
1	E	-1	HIS
1	E	0	HIS
1	E	1	HIS
1	E	50	HIS
1	F	1	HIS
1	F	50	HIS

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	IPA	A	201	-	3,3,3	0.53	0	3,3,3	0.22	0
2	IPA	A	202	-	3,3,3	0.53	0	3,3,3	0.20	0
2	IPA	C	201	-	3,3,3	0.54	0	3,3,3	0.04	0
2	IPA	D	201	-	3,3,3	0.53	0	3,3,3	0.21	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	IPA	A	201	-	-	0/0/0/0	0/0/0/0
2	IPA	A	202	-	-	0/0/0/0	0/0/0/0
2	IPA	C	201	-	-	0/0/0/0	0/0/0/0
2	IPA	D	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	IPA	1	0
2	C	201	IPA	2	0
2	D	201	IPA	8	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, 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	A	147/153 (96%)	0.24	4 (2%)	58	64	9, 18, 34, 60	1 (0%)
1	B	148/153 (96%)	0.22	8 (5%)	29	34	8, 15, 34, 51	2 (1%)
1	C	147/153 (96%)	0.30	7 (4%)	34	39	7, 15, 42, 58	1 (0%)
1	D	150/153 (98%)	0.33	3 (2%)	68	75	8, 18, 35, 49	2 (1%)
1	E	150/153 (98%)	0.54	10 (6%)	21	25	11, 20, 44, 65	1 (0%)
1	F	149/153 (97%)	0.34	4 (2%)	58	64	7, 17, 37, 63	2 (1%)
All	All	891/918 (97%)	0.33	36 (4%)	42	48	7, 17, 38, 65	9 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	147	SER	7.6
1	B	127	GLY	5.4
1	E	104	SER	5.4
1	C	147	SER	5.2
1	E	147	SER	4.8
1	A	147	SER	4.4
1	F	128	THR	4.1
1	E	-2	HIS	3.9
1	C	108	VAL	3.8
1	A	1	HIS	3.6
1	C	107	GLY	3.4
1	E	108	VAL	3.4
1	E	109	ASN	3.0
1	E	105	ALA	3.0
1	B	105	ALA	3.0
1	C	105	ALA	2.9
1	F	125	THR	2.9
1	E	128	THR	2.8
1	B	147	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	104	SER	2.7
1	D	-1	HIS	2.7
1	D	145	LEU	2.6
1	B	104	SER	2.6
1	E	107	GLY	2.5
1	B	126	ALA	2.4
1	D	-2	HIS	2.4
1	A	128	THR	2.4
1	C	106	SER	2.3
1	F	126	ALA	2.3
1	A	59	ILE	2.3
1	B	128	THR	2.2
1	E	141	LEU	2.1
1	B	125	THR	2.1
1	B	0	HIS	2.1
1	C	1	HIS	2.1
1	E	103	TYR	2.1

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	IPA	D	201	4/4	0.93	0.17	5.21	19,26,43,43	0
3	CA	F	202	1/1	0.94	0.22	4.36	58,58,58,58	0
2	IPA	A	202	4/4	0.83	0.17	3.58	15,33,39,43	0
2	IPA	C	201	4/4	0.80	0.18	2.66	13,28,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	IPA	A	201	4/4	0.86	0.13	1.13	21,38,44,44	0
3	CA	F	201	1/1	0.84	0.17	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.