



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:52 am GMT

PDB ID : 4Y2O  
Title : Structure of CFA/I pili chaperone-major subunit complex (CfaA-CfaB)  
Authors : Bao, R.; Xia, D.  
Deposited on : 2015-02-10  
Resolution : 2.42 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

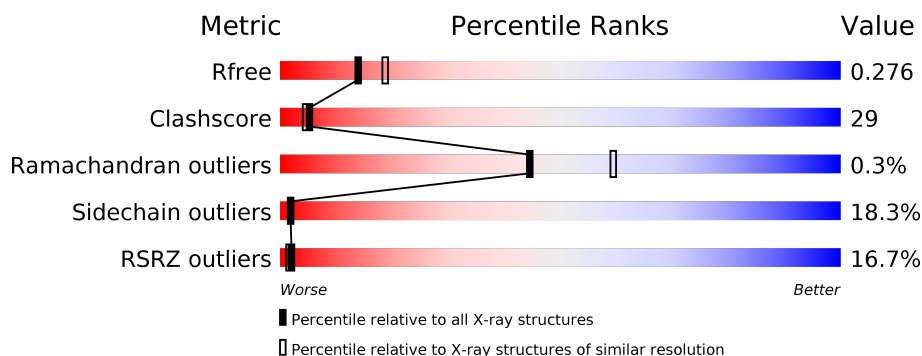
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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  $\geq 3$ , 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	231	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>8%</div> <div>9%</div> </div> </div>
2	B	142	<div> <div>33%</div> <div> <div></div> <div>36%</div> <div>51%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2894 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 CfA/I fimbrial subunit A (Colonization factor antigen subunit A putative chaperone).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	1	0	0
			1700	1095	284	318	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP E3PPC3
A	112	ILE	THR	engineered mutation	UNP E3PPC3
A	220	ALA	-	expression tag	UNP E3PPC3
A	221	ALA	-	expression tag	UNP E3PPC3
A	222	TRP	-	expression tag	UNP E3PPC3
A	223	SER	-	expression tag	UNP E3PPC3
A	224	HIS	-	expression tag	UNP E3PPC3
A	225	PRO	-	expression tag	UNP E3PPC3
A	226	GLN	-	expression tag	UNP E3PPC3
A	227	PHE	-	expression tag	UNP E3PPC3
A	228	GLU	-	expression tag	UNP E3PPC3
A	229	LYS	-	expression tag	UNP E3PPC3

- Molecule 2 is a protein called CFA/I fimbrial subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1033	646	178	205	4			

There are 12 discrepancies between the modelled and reference sequences:

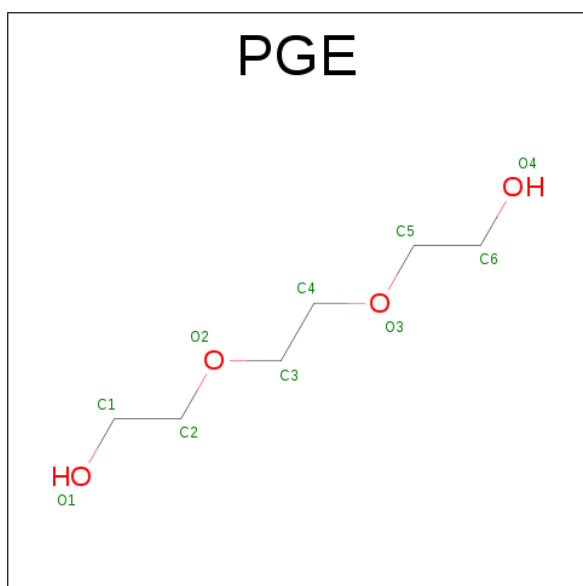
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP E3PPC4
B	-6	VAL	-	expression tag	UNP E3PPC4
B	-5	HIS	-	expression tag	UNP E3PPC4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	40	ALA	ASP	conflict	UNP E3PPC4
B	41	ASP	ALA	conflict	UNP E3PPC4
B	42	ALA	THR	conflict	UNP E3PPC4
B	55	ALA	LEU	conflict	UNP E3PPC4

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ni 2 2	0	0

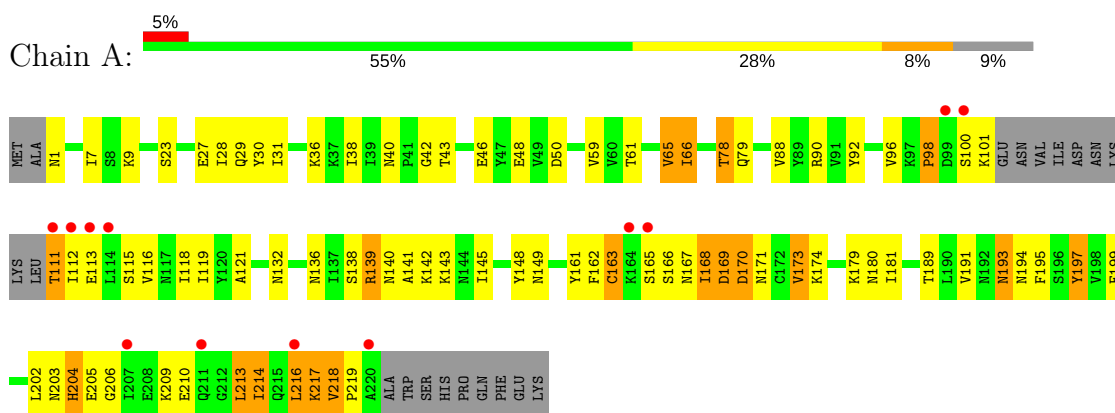
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total 94	O 94	0	0
5	B	45	Total 45	O 45	0	0

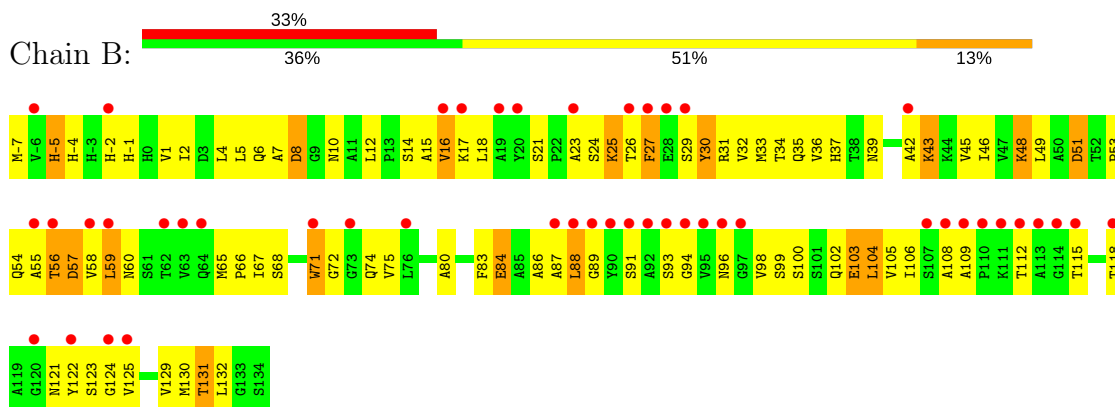
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CfA/I fimbrial subunit A (Colonization factor antigen subunit A putative chaper-one)



- Molecule 2: CFA/I fimbrial subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.19Å 129.19Å 73.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.46 – 2.42 44.46 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.46-2.42) 99.6 (44.46-2.42)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.236 , 0.262 0.245 , 0.276	Depositor DCC
$R_{free}$ test set	875 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 73.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI, PGE

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	0.88	0/1731	0.62	1/2337 (0.0%)
2	B	0.67	0/1053	0.73	1/1436 (0.1%)
All	All	0.80	0/2784	0.66	2/3773 (0.1%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	21	SER	C-N-CD	5.69	140.36	128.40
1	A	213	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	PRO	Peptide

### 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	1700	0	1752	93	0
2	B	1033	0	1031	82	0
3	A	20	0	28	0	0
4	B	2	0	0	0	0
5	A	94	0	0	5	0
5	B	45	0	0	3	0
All	All	2894	0	2811	163	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 29.

All (163) 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:197:TYR:CD1	1:A:216:LEU:HA	1.63	1.32
1:A:197:TYR:CE1	1:A:216:LEU:HB3	1.65	1.29
1:A:197:TYR:CE1	1:A:216:LEU:CB	2.18	1.26
1:A:197:TYR:HE1	1:A:216:LEU:CB	1.50	1.22
1:A:197:TYR:CE1	1:A:216:LEU:CA	2.27	1.16
1:A:197:TYR:CE1	1:A:216:LEU:HA	1.89	1.06
1:A:197:TYR:HE1	1:A:216:LEU:HB3	0.99	1.02
2:B:48:LYS:HB3	2:B:80:ALA:HA	1.43	0.99
1:A:197:TYR:HE1	1:A:216:LEU:CA	1.71	0.96
1:A:197:TYR:CD1	1:A:216:LEU:CA	2.47	0.96
1:A:197:TYR:HD1	1:A:216:LEU:HA	1.25	0.95
1:A:139:ARG:NE	1:A:218:VAL:O	2.03	0.90
1:A:204:HIS:HD2	1:A:210:GLU:HB3	1.37	0.88
1:A:36:LYS:NZ	1:A:50:ASP:OD1	2.10	0.84
1:A:27:GLU:HB3	1:A:101:LYS:HB3	1.57	0.84
2:B:-5:HIS:HA	2:B:-4:HIS:HB3	1.59	0.82
2:B:87:ALA:HB1	2:B:99:SER:O	1.82	0.80
1:A:204:HIS:CD2	1:A:210:GLU:HB3	2.18	0.79
1:A:216:LEU:HD23	1:A:216:LEU:O	1.84	0.78
2:B:48:LYS:O	2:B:129:VAL:HB	1.85	0.76
2:B:87:ALA:HA	2:B:100:SER:HA	1.66	0.76
1:A:205:GLU:HG3	1:A:206:GLY:N	2.01	0.75
2:B:8:ASP:N	2:B:8:ASP:OD1	2.17	0.75
1:A:1:ASN:N	1:A:29:GLN:OE1	2.20	0.74
2:B:57:ASP:HB2	2:B:60:ASN:O	1.87	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:O	5:A:401:HOH:O	2.07	0.73
2:B:29:SER:OG	2:B:31:ARG:NH1	2.20	0.73
1:A:139:ARG:CD	1:A:218:VAL:O	2.37	0.73
2:B:-4:HIS:O	2:B:-4:HIS:ND1	2.21	0.72
1:A:197:TYR:CZ	1:A:216:LEU:HB3	2.23	0.72
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.54	0.72
1:A:42:GLY:O	1:A:179:LYS:NZ	2.15	0.72
1:A:218:VAL:HG22	1:A:219:PRO:HD2	1.70	0.72
2:B:87:ALA:CA	2:B:100:SER:HA	2.19	0.71
1:A:205:GLU:HG3	1:A:206:GLY:H	1.53	0.71
1:A:31:ILE:HB	1:A:65:VAL:HG23	1.73	0.70
1:A:112:ILE:HG12	2:B:122:TYR:O	1.90	0.70
2:B:94:GLY:O	5:B:301:HOH:O	2.08	0.70
2:B:23:ALA:HB3	2:B:26:THR:CG2	2.22	0.70
2:B:35:GLN:OE1	2:B:37:HIS:NE2	2.25	0.70
2:B:88:LEU:N	2:B:89:GLY:HA3	2.06	0.69
2:B:67:ILE:HA	2:B:108:ALA:HA	1.75	0.69
2:B:16:VAL:HG21	2:B:30:TYR:CD2	2.28	0.69
2:B:10:ASN:OD1	5:B:302:HOH:O	2.11	0.68
2:B:54:GLN:N	2:B:54:GLN:OE1	2.27	0.68
2:B:87:ALA:HA	2:B:100:SER:CA	2.25	0.67
1:A:27:GLU:OE2	1:A:101:LYS:NZ	2.27	0.67
1:A:90:ARG:NH2	2:B:132:LEU:O	2.24	0.67
1:A:115:SER:HA	2:B:15:ALA:HA	1.75	0.67
1:A:90:ARG:HE	2:B:131:THR:HG21	1.59	0.66
2:B:87:ALA:CB	2:B:100:SER:HA	2.25	0.66
1:A:162:PHE:HB2	1:A:173:VAL:HG23	1.77	0.66
1:A:112:ILE:O	2:B:17:LYS:HG2	1.96	0.65
1:A:140:ASN:OD1	5:A:402:HOH:O	2.15	0.63
2:B:23:ALA:O	2:B:24:SER:OG	2.13	0.63
2:B:37:HIS:ND1	5:B:304:HOH:O	2.30	0.63
1:A:139:ARG:HD2	1:A:218:VAL:O	1.98	0.63
1:A:174:LYS:NZ	5:A:407:HOH:O	2.30	0.63
2:B:123:SER:OG	2:B:124:GLY:N	2.31	0.63
2:B:51:ASP:OD1	2:B:51:ASP:N	2.32	0.63
2:B:57:ASP:OD1	2:B:57:ASP:N	2.30	0.62
1:A:116:VAL:N	2:B:14:SER:O	2.24	0.61
1:A:161:TYR:HB2	1:A:199:PHE:HB2	1.81	0.61
2:B:23:ALA:O	2:B:26:THR:HG22	2.00	0.61
1:A:139:ARG:CG	1:A:139:ARG:HH11	2.14	0.61
2:B:6:GLN:NE2	2:B:8:ASP:OD2	2.33	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HD2	1:A:218:VAL:HG12	1.82	0.60
1:A:40:ASN:O	1:A:43:THR:OG1	2.17	0.60
2:B:7:ALA:HA	2:B:35:GLN:HG3	1.82	0.60
1:A:140:ASN:OD1	1:A:141:ALA:N	2.34	0.60
1:A:161:TYR:HE1	1:A:174:LYS:HB2	1.66	0.59
2:B:58:VAL:HG12	2:B:59:LEU:HD22	1.83	0.59
1:A:197:TYR:CE1	1:A:216:LEU:N	2.72	0.57
2:B:88:LEU:N	2:B:89:GLY:CA	2.67	0.57
2:B:33:MET:HA	2:B:103:GLU:HA	1.86	0.57
1:A:194:ASN:OD1	1:A:194:ASN:N	2.33	0.57
2:B:23:ALA:HB3	2:B:26:THR:HG23	1.86	0.57
2:B:49:LEU:HD11	2:B:53:PRO:HD3	1.86	0.56
1:A:143:LYS:NZ	1:A:143:LYS:HB2	2.21	0.56
2:B:87:ALA:HB1	2:B:100:SER:HA	1.86	0.56
1:A:163:CYS:SG	1:A:168:ILE:HA	2.47	0.55
1:A:165:SER:OG	1:A:166:SER:N	2.38	0.54
2:B:87:ALA:HB2	2:B:100:SER:HB2	1.89	0.54
2:B:18:LEU:HD21	2:B:30:TYR:HB2	1.88	0.54
2:B:24:SER:C	2:B:25:LYS:HG2	2.28	0.54
2:B:87:ALA:HA	2:B:100:SER:CB	2.39	0.53
1:A:170:ASP:N	1:A:170:ASP:OD1	2.25	0.53
1:A:216:LEU:H	1:A:216:LEU:HD22	1.73	0.53
1:A:90:ARG:NE	2:B:131:THR:HG21	2.25	0.52
1:A:46:GLU:OE2	5:A:403:HOH:O	2.18	0.52
2:B:6:GLN:HG3	2:B:12:LEU:CD2	2.39	0.52
2:B:23:ALA:HB3	2:B:26:THR:HG22	1.90	0.52
1:A:38:ILE:HB	1:A:88:VAL:HG13	1.91	0.51
2:B:34:THR:OG1	2:B:102:GLN:O	2.14	0.51
1:A:216:LEU:CD2	1:A:216:LEU:N	2.73	0.51
2:B:23:ALA:CB	2:B:26:THR:CG2	2.89	0.51
1:A:197:TYR:HE1	1:A:216:LEU:N	2.05	0.51
1:A:169:ASP:HB2	1:A:171:ASN:OD1	2.12	0.50
1:A:139:ARG:HD2	1:A:218:VAL:CG1	2.42	0.50
2:B:71:TRP:CD1	2:B:104:LEU:HB2	2.46	0.50
2:B:57:ASP:CB	2:B:60:ASN:O	2.56	0.50
1:A:96:VAL:HG13	1:A:98:PRO:HD3	1.93	0.50
2:B:6:GLN:HB3	2:B:8:ASP:OD1	2.13	0.48
1:A:216:LEU:CD2	1:A:216:LEU:H	2.26	0.48
1:A:59:VAL:HB	1:A:78:THR:HG23	1.95	0.48
2:B:118:THR:OG1	2:B:122:TYR:OH	2.30	0.48
1:A:136:ASN:HB2	1:A:148:TYR:HB3	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLN:HG2	2:B:99:SER:HB2	1.96	0.48
2:B:56:THR:N	2:B:123:SER:O	2.32	0.47
1:A:7:ILE:HD13	2:B:2:ILE:HD12	1.97	0.47
2:B:43:LYS:HD3	2:B:84:GLU:HG3	1.96	0.47
1:A:204:HIS:HD1	1:A:204:HIS:C	2.18	0.47
2:B:30:TYR:HB3	2:B:106:ILE:HG23	1.97	0.47
2:B:48:LYS:HB3	2:B:80:ALA:CA	2.30	0.47
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.73	0.47
1:A:23:SER:OG	5:A:404:HOH:O	2.21	0.46
1:A:193:ASN:HB2	1:A:195:PHE:CE2	2.50	0.46
2:B:36:VAL:HB	2:B:100:SER:HB3	1.96	0.46
2:B:45:VAL:O	2:B:83:PHE:HB2	2.15	0.46
1:A:121:ALA:O	2:B:131:THR:HG23	2.16	0.46
1:A:38:ILE:HD11	1:A:90:ARG:HG3	1.97	0.46
1:A:161:TYR:CE1	1:A:174:LYS:HB2	2.49	0.45
1:A:48:GLU:OE2	1:A:90:ARG:HD2	2.15	0.45
1:A:9:LYS:HA	1:A:9:LYS:HD3	1.75	0.45
1:A:145:ILE:N	1:A:191:VAL:O	2.46	0.45
1:A:115:SER:OG	2:B:125:VAL:HG12	2.17	0.45
1:A:179:LYS:HG2	1:A:180:ASN:N	2.32	0.45
2:B:4:LEU:HD13	2:B:130:MET:HE3	1.99	0.45
2:B:65:MET:HA	2:B:66:PRO:HD3	1.76	0.44
2:B:66:PRO:HB2	2:B:109:ALA:HB3	1.99	0.44
1:A:217:LYS:HG2	1:A:218:VAL:N	2.31	0.44
1:A:121:ALA:HB3	2:B:131:THR:HG23	1.99	0.44
1:A:141:ALA:C	1:A:142:LYS:HG3	2.38	0.44
2:B:55:ALA:HB1	2:B:122:TYR:HB3	1.99	0.44
1:A:141:ALA:O	1:A:142:LYS:HG3	2.18	0.43
1:A:30:TYR:CE2	1:A:66:ILE:HG23	2.53	0.43
1:A:28:ILE:HD11	1:A:66:ILE:HG22	1.99	0.43
1:A:199:PHE:CZ	1:A:214:ILE:HD12	2.53	0.43
1:A:139:ARG:NH1	1:A:143:LYS:O	2.52	0.43
1:A:38:ILE:HD12	1:A:88:VAL:HG22	2.01	0.43
2:B:24:SER:O	2:B:25:LYS:HG2	2.19	0.43
1:A:142:LYS:HE3	1:A:142:LYS:HB3	1.83	0.42
2:B:72:GLY:O	2:B:74:GLN:NE2	2.44	0.42
1:A:145:ILE:HB	1:A:189:THR:OG1	2.20	0.42
1:A:143:LYS:HB2	1:A:143:LYS:HZ3	1.85	0.42
2:B:57:ASP:HB3	2:B:121:ASN:HD21	1.85	0.42
1:A:149:ASN:ND2	1:A:181:ILE:O	2.50	0.41
2:B:131:THR:HG22	2:B:132:LEU:H	1.86	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:SER:HB2	2:B:96:ASN:O	2.20	0.41
2:B:24:SER:O	2:B:25:LYS:CB	2.68	0.41
2:B:112:THR:O	2:B:115:THR:OG1	2.23	0.41
1:A:111:THR:HB	1:A:112:ILE:H	1.73	0.41
1:A:119:ILE:HB	2:B:129:VAL:HG22	2.01	0.41
2:B:86:ALA:O	2:B:100:SER:OG	2.39	0.41
2:B:26:THR:OG1	2:B:27:PHE:N	2.54	0.41
1:A:195:PHE:O	1:A:217:LYS:HE2	2.21	0.41
1:A:48:GLU:OE1	1:A:92:TYR:OH	2.35	0.41
1:A:168:ILE:HG13	1:A:168:ILE:H	1.56	0.40
2:B:31:ARG:HG3	2:B:105:VAL:HG13	2.02	0.40
1:A:111:THR:HG22	1:A:112:ILE:HG13	2.02	0.40
2:B:30:TYR:CG	2:B:30:TYR:O	2.71	0.40
2:B:39:ASN:O	2:B:42:ALA:HB2	2.22	0.40
2:B:58:VAL:HG12	2:B:59:LEU:CD2	2.50	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	A	207/231 (90%)	200 (97%)	7 (3%)	0	100	100
2	B	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	25	35
All	All	347/373 (93%)	328 (94%)	18 (5%)	1 (0%)	44	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	LYS

### 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	A	193/211 (92%)	165 (86%)	28 (14%)	4	4
2	B	113/113 (100%)	85 (75%)	28 (25%)	1	0
All	All	306/324 (94%)	250 (82%)	56 (18%)	2	2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	65	VAL
1	A	66	ILE
1	A	78	THR
1	A	79	GLN
1	A	100	SER
1	A	111	THR
1	A	113	GLU
1	A	132	ASN
1	A	138	SER
1	A	139	ARG
1	A	163	CYS
1	A	167	ASN
1	A	168	ILE
1	A	169	ASP
1	A	170	ASP
1	A	173	VAL
1	A	193	ASN
1	A	197	TYR
1	A	202	LEU
1	A	203	ASN
1	A	204	HIS
1	A	209	LYS
1	A	213	LEU
1	A	214	ILE
1	A	216	LEU
1	A	217	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	218	VAL
2	B	-7	MET
2	B	-5	HIS
2	B	-2	HIS
2	B	-1	HIS
2	B	1	VAL
2	B	5	LEU
2	B	8	ASP
2	B	16	VAL
2	B	27	PHE
2	B	30	TYR
2	B	32	VAL
2	B	43	LYS
2	B	46	ILE
2	B	48	LYS
2	B	51	ASP
2	B	56	THR
2	B	57	ASP
2	B	59	LEU
2	B	68	SER
2	B	71	TRP
2	B	75	VAL
2	B	84	GLU
2	B	88	LEU
2	B	91	SER
2	B	98	VAL
2	B	103	GLU
2	B	104	LEU
2	B	131	THR

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

Mol	Chain	Res	Type
1	A	79	GLN
1	A	167	ASN
1	A	211	GLN
2	B	-3	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	PGE	A	301	-	9,9,9	0.30	0	8,8,8	0.26	0
3	PGE	A	302	-	9,9,9	0.29	0	8,8,8	0.19	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
3	PGE	A	301	-	-	0/7/7/7	0/0/0/0
3	PGE	A	302	-	-	0/7/7/7	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.

No monomer is involved in short contacts.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9	
1	A	211/231 (91%)	0.07	12 (5%)	24	22	28, 58, 121, 174	3 (1%)
2	B	142/142 (100%)	2.28	47 (33%)	0	0	44, 100, 154, 168	22 (15%)
All	All	353/373 (94%)	0.96	59 (16%)	2	1	28, 74, 144, 174	25 (7%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	TYR	36.1
2	B	89	GLY	29.5
2	B	88	LEU	17.7
2	B	110	PRO	11.7
2	B	94	GLY	11.4
2	B	120	GLY	8.9
2	B	93	SER	8.0
2	B	96	ASN	7.4
2	B	95	VAL	7.2
2	B	87	ALA	6.6
2	B	109	ALA	6.4
2	B	111	LYS	6.3
2	B	92	ALA	5.6
2	B	122	TYR	5.6
2	B	58	VAL	5.6
2	B	29	SER	5.5
2	B	28	GLU	5.5
2	B	62	THR	5.5
2	B	91	SER	5.4
2	B	20	TYR	4.9
2	B	19	ALA	4.8
2	B	59	LEU	4.7
1	A	112	ILE	4.7
2	B	26	THR	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	108	ALA	4.2
2	B	27	PHE	4.1
2	B	76	LEU	4.0
1	A	211	GLN	3.8
2	B	16	VAL	3.7
2	B	114	GLY	3.6
1	A	100	SER	3.5
1	A	114	LEU	3.5
2	B	113	ALA	3.5
2	B	97	GLY	3.4
1	A	113	GLU	3.4
2	B	63	VAL	3.3
2	B	71	TRP	3.2
2	B	55	ALA	3.1
2	B	64	GLN	3.1
2	B	112	THR	3.0
2	B	118	THR	3.0
2	B	-6	VAL	3.0
2	B	115	THR	3.0
2	B	23	ALA	2.8
1	A	99	ASP	2.8
2	B	17	LYS	2.6
2	B	107	SER	2.5
2	B	-2	HIS	2.5
2	B	125	VAL	2.4
2	B	124	GLY	2.4
1	A	216	LEU	2.4
1	A	207	ILE	2.3
2	B	56	THR	2.3
1	A	164	LYS	2.3
1	A	165	SER	2.2
1	A	111	THR	2.2
2	B	73	GLY	2.2
1	A	220	ALA	2.1
2	B	42	ALA	2.1

## 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 [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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PGE	A	302	10/10	0.60	0.27	0.83	69,81,96,102	0
3	PGE	A	301	10/10	0.79	0.20	-	68,82,90,104	0
4	NI	B	202	1/1	0.87	0.12	-	89,89,89,89	0
4	NI	B	201	1/1	0.92	0.31	-	68,68,68,68	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.