



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:24 AM UTC

PDB ID : 5YVL / pdb_00005yvl
Title : Crystal structure of a cyclase Hpiu5 from Fischerella sp. ATCC 43239
Authors : Hu, X.Y.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2017-11-26
Resolution : 2.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

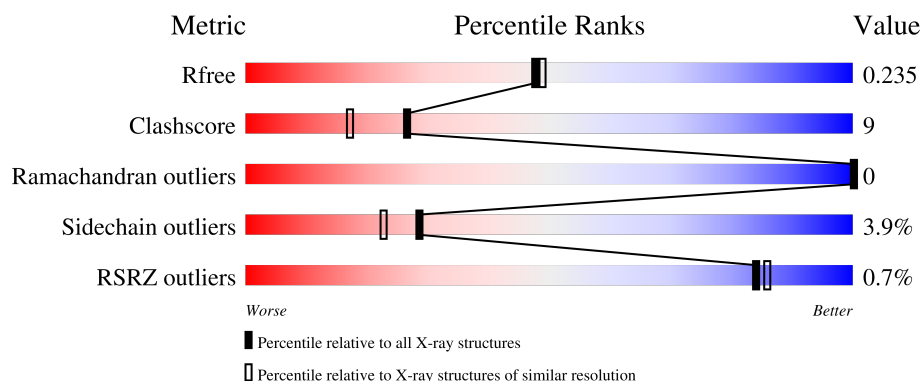
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. 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	225	
1	B	225	
1	C	225	
1	D	225	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6799 atoms, of which 36 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 cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O		0	0	0
			1548	991	250	307				
1	B	198	Total	C	N	O		0	0	0
			1533	983	247	303				
1	C	199	Total	C	N	O		0	0	0
			1539	986	248	305				
1	D	206	Total	C	N	O	S	0	0	0
			1585	1012	257	315	1			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP A0A076NBW8
A	4	GLY	-	expression tag	UNP A0A076NBW8
A	5	SER	-	expression tag	UNP A0A076NBW8
A	6	SER	-	expression tag	UNP A0A076NBW8
A	7	HIS	-	expression tag	UNP A0A076NBW8
A	8	HIS	-	expression tag	UNP A0A076NBW8
A	9	HIS	-	expression tag	UNP A0A076NBW8
A	10	HIS	-	expression tag	UNP A0A076NBW8
A	11	HIS	-	expression tag	UNP A0A076NBW8
A	12	HIS	-	expression tag	UNP A0A076NBW8
A	13	SER	-	expression tag	UNP A0A076NBW8
A	14	SER	-	expression tag	UNP A0A076NBW8
A	15	GLY	-	expression tag	UNP A0A076NBW8
A	16	LEU	-	expression tag	UNP A0A076NBW8
A	17	VAL	-	expression tag	UNP A0A076NBW8
A	18	PRO	-	expression tag	UNP A0A076NBW8
A	19	ARG	-	expression tag	UNP A0A076NBW8
A	20	GLY	-	expression tag	UNP A0A076NBW8
A	21	SER	-	expression tag	UNP A0A076NBW8
A	22	HIS	-	expression tag	UNP A0A076NBW8
A	23	MET	-	expression tag	UNP A0A076NBW8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	expression tag	UNP A0A076NBW8
A	25	SER	-	expression tag	UNP A0A076NBW8
B	3	MET	-	initiating methionine	UNP A0A076NBW8
B	4	GLY	-	expression tag	UNP A0A076NBW8
B	5	SER	-	expression tag	UNP A0A076NBW8
B	6	SER	-	expression tag	UNP A0A076NBW8
B	7	HIS	-	expression tag	UNP A0A076NBW8
B	8	HIS	-	expression tag	UNP A0A076NBW8
B	9	HIS	-	expression tag	UNP A0A076NBW8
B	10	HIS	-	expression tag	UNP A0A076NBW8
B	11	HIS	-	expression tag	UNP A0A076NBW8
B	12	HIS	-	expression tag	UNP A0A076NBW8
B	13	SER	-	expression tag	UNP A0A076NBW8
B	14	SER	-	expression tag	UNP A0A076NBW8
B	15	GLY	-	expression tag	UNP A0A076NBW8
B	16	LEU	-	expression tag	UNP A0A076NBW8
B	17	VAL	-	expression tag	UNP A0A076NBW8
B	18	PRO	-	expression tag	UNP A0A076NBW8
B	19	ARG	-	expression tag	UNP A0A076NBW8
B	20	GLY	-	expression tag	UNP A0A076NBW8
B	21	SER	-	expression tag	UNP A0A076NBW8
B	22	HIS	-	expression tag	UNP A0A076NBW8
B	23	MET	-	expression tag	UNP A0A076NBW8
B	24	ALA	-	expression tag	UNP A0A076NBW8
B	25	SER	-	expression tag	UNP A0A076NBW8
C	3	MET	-	initiating methionine	UNP A0A076NBW8
C	4	GLY	-	expression tag	UNP A0A076NBW8
C	5	SER	-	expression tag	UNP A0A076NBW8
C	6	SER	-	expression tag	UNP A0A076NBW8
C	7	HIS	-	expression tag	UNP A0A076NBW8
C	8	HIS	-	expression tag	UNP A0A076NBW8
C	9	HIS	-	expression tag	UNP A0A076NBW8
C	10	HIS	-	expression tag	UNP A0A076NBW8
C	11	HIS	-	expression tag	UNP A0A076NBW8
C	12	HIS	-	expression tag	UNP A0A076NBW8
C	13	SER	-	expression tag	UNP A0A076NBW8
C	14	SER	-	expression tag	UNP A0A076NBW8
C	15	GLY	-	expression tag	UNP A0A076NBW8
C	16	LEU	-	expression tag	UNP A0A076NBW8
C	17	VAL	-	expression tag	UNP A0A076NBW8
C	18	PRO	-	expression tag	UNP A0A076NBW8
C	19	ARG	-	expression tag	UNP A0A076NBW8

Continued on next page...

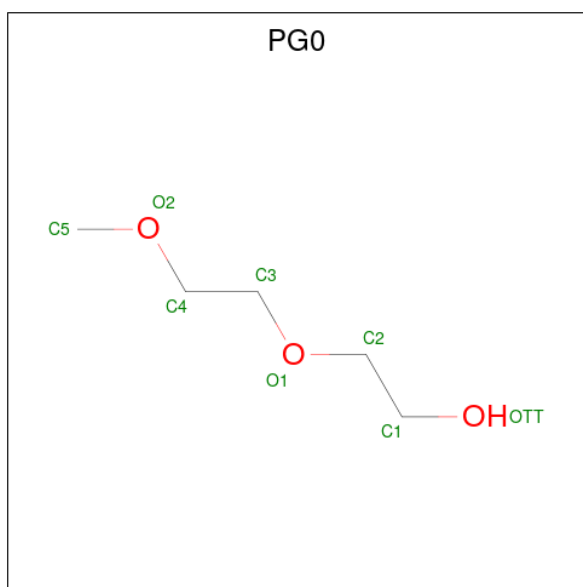
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	expression tag	UNP A0A076NBW8
C	21	SER	-	expression tag	UNP A0A076NBW8
C	22	HIS	-	expression tag	UNP A0A076NBW8
C	23	MET	-	expression tag	UNP A0A076NBW8
C	24	ALA	-	expression tag	UNP A0A076NBW8
C	25	SER	-	expression tag	UNP A0A076NBW8
D	3	MET	-	initiating methionine	UNP A0A076NBW8
D	4	GLY	-	expression tag	UNP A0A076NBW8
D	5	SER	-	expression tag	UNP A0A076NBW8
D	6	SER	-	expression tag	UNP A0A076NBW8
D	7	HIS	-	expression tag	UNP A0A076NBW8
D	8	HIS	-	expression tag	UNP A0A076NBW8
D	9	HIS	-	expression tag	UNP A0A076NBW8
D	10	HIS	-	expression tag	UNP A0A076NBW8
D	11	HIS	-	expression tag	UNP A0A076NBW8
D	12	HIS	-	expression tag	UNP A0A076NBW8
D	13	SER	-	expression tag	UNP A0A076NBW8
D	14	SER	-	expression tag	UNP A0A076NBW8
D	15	GLY	-	expression tag	UNP A0A076NBW8
D	16	LEU	-	expression tag	UNP A0A076NBW8
D	17	VAL	-	expression tag	UNP A0A076NBW8
D	18	PRO	-	expression tag	UNP A0A076NBW8
D	19	ARG	-	expression tag	UNP A0A076NBW8
D	20	GLY	-	expression tag	UNP A0A076NBW8
D	21	SER	-	expression tag	UNP A0A076NBW8
D	22	HIS	-	expression tag	UNP A0A076NBW8
D	23	MET	-	expression tag	UNP A0A076NBW8
D	24	ALA	-	expression tag	UNP A0A076NBW8
D	25	SER	-	expression tag	UNP A0A076NBW8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			20	5	12	3		
3	C	1	Total	C	H	O	0	0
			20	5	12	3		
3	D	1	Total	C	H	O	0	0
			20	5	12	3		

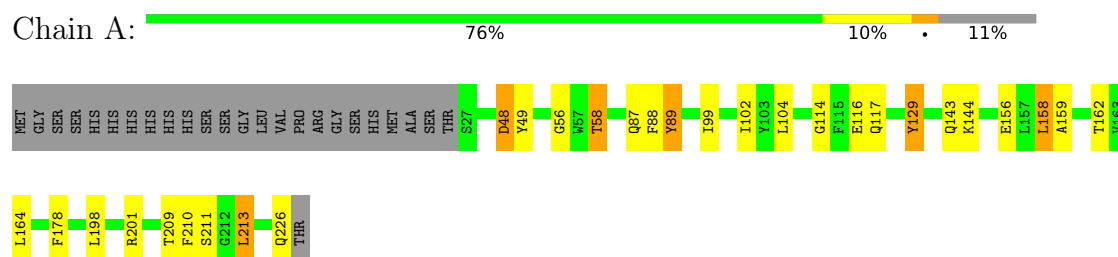
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	140	Total	O	0	0
			140	140		
4	C	130	Total	O	0	0
			130	130		
4	D	102	Total	O	0	0
			102	102		

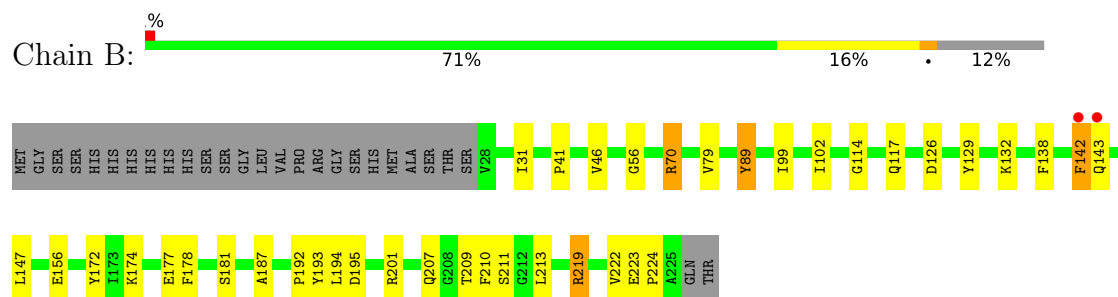
3 Residue-property plots

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.

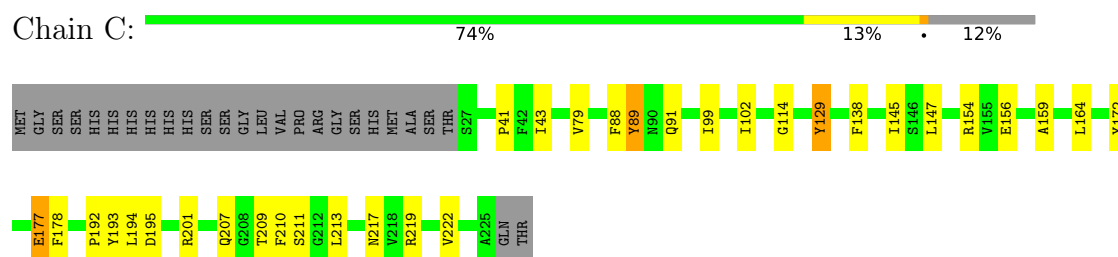
- Molecule 1: cyclase



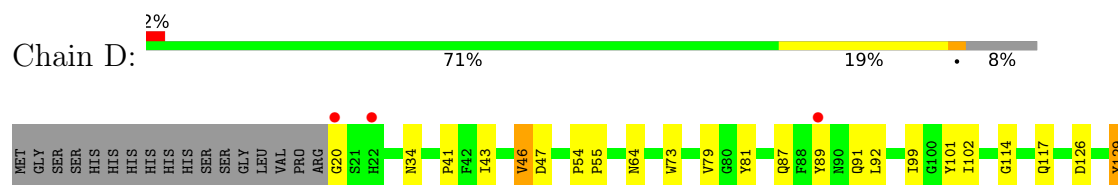
- Molecule 1: cyclase

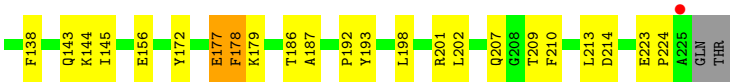


- Molecule 1: cyclase



- Molecule 1: cyclase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.39Å 114.31Å 132.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.06 24.99 – 2.06	Depositor EDS
% Data completeness (in resolution range)	94.9 (24.99-2.06) 94.8 (24.99-2.06)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.179 , 0.236 0.179 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: PG0, CA

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	0.61	0/1587	0.83	0/2171
1	B	0.61	0/1572	0.84	2/2151 (0.1%)
1	C	0.59	0/1578	0.83	0/2159
1	D	0.54	0/1625	0.83	0/2222
All	All	0.59	0/6362	0.83	2/8703 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	PHE	CA-C-N	-5.16	115.51	123.04
1	B	142	PHE	C-N-CA	-5.16	115.51	123.04

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	1548	0	1490	26	0
1	B	1533	0	1477	28	0
1	C	1539	0	1482	27	0
1	D	1585	0	1523	35	0
2	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	8	12	12	0	0
3	C	8	12	12	2	0
3	D	8	12	12	1	0
4	A	154	0	0	3	0
4	B	140	0	0	1	0
4	C	130	0	0	0	0
4	D	102	0	0	1	0
All	All	6763	36	6008	114	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 9.

All (114) 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:D:138:PHE:CE1	1:D:214:ASP:OD1	2.20	0.95
1:C:156:GLU:HG3	1:C:201:ARG:HB2	1.56	0.88
1:D:89:TYR:CE2	1:D:178:PHE:CE1	2.69	0.81
1:D:89:TYR:CD2	1:D:178:PHE:HE1	1.99	0.81
1:D:89:TYR:CD2	1:D:178:PHE:CE1	2.70	0.79
1:A:102:ILE:HD13	1:A:114:GLY:HA2	1.65	0.78
1:A:88:PHE:HB2	1:A:89:TYR:CE1	2.20	0.77
1:B:142:PHE:CD2	1:B:143:GLN:HG3	2.22	0.75
1:B:142:PHE:O	1:B:143:GLN:HB2	1.85	0.75
1:B:142:PHE:CE2	1:B:143:GLN:HG3	2.23	0.74
1:D:102:ILE:HD13	1:D:114:GLY:HA2	1.70	0.74
1:A:87:GLN:HG2	4:A:533:HOH:O	1.89	0.73
1:D:177:GLU:HA	1:D:177:GLU:OE1	1.88	0.73
1:D:138:PHE:HE1	1:D:214:ASP:OD1	1.73	0.69
1:D:64:ASN:HB2	3:D:301:PG0:H21	1.75	0.69
1:B:102:ILE:HD13	1:B:114:GLY:HA2	1.77	0.66
1:D:47:ASP:OD2	1:D:87:GLN:HG2	1.97	0.65
1:A:156:GLU:OE1	1:A:201:ARG:HD2	1.99	0.62
1:C:43:ILE:HD11	1:C:79:VAL:HG23	1.82	0.61
1:B:209:THR:HG22	1:B:211:SER:OG	2.00	0.61
1:C:156:GLU:OE2	1:C:201:ARG:HD2	2.00	0.61
1:C:192:PRO:HG2	1:C:193:TYR:CE2	2.36	0.60
1:D:73:TRP:CH2	1:D:145:ILE:HD12	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:TYR:CD2	1:C:222:VAL:HG12	2.37	0.59
1:D:99:ILE:C	1:D:99:ILE:HD12	2.28	0.58
1:B:70:ARG:N	1:B:70:ARG:HD2	2.17	0.58
1:C:102:ILE:HD13	1:C:114:GLY:HA2	1.84	0.58
1:D:43:ILE:HD11	1:D:79:VAL:HG23	1.86	0.56
1:A:209:THR:HA	1:A:210:PHE:C	2.30	0.56
1:B:192:PRO:HG2	1:B:193:TYR:CE2	2.41	0.56
1:B:223:GLU:HB2	1:B:224:PRO:HD2	1.88	0.56
1:A:143:GLN:O	1:A:144:LYS:HB2	2.06	0.55
1:A:226:GLN:NE2	1:B:172:TYR:OH	2.40	0.55
1:C:41:PRO:HD2	1:C:79:VAL:HG21	1.88	0.55
1:A:48:ASP:C	1:A:49:TYR:HD1	2.15	0.55
1:B:142:PHE:CE2	1:B:143:GLN:CG	2.89	0.55
1:B:31:ILE:HD11	1:B:222:VAL:CG1	2.38	0.54
1:C:213:LEU:HD12	1:C:213:LEU:C	2.34	0.53
1:B:209:THR:HA	1:B:210:PHE:C	2.34	0.53
1:B:129:TYR:CD2	1:B:222:VAL:HG12	2.43	0.53
1:A:89:TYR:CD1	1:A:89:TYR:N	2.76	0.53
1:D:209:THR:HA	1:D:210:PHE:C	2.33	0.53
1:D:143:GLN:O	1:D:144:LYS:HB2	2.09	0.52
1:C:91:GLN:OE1	1:C:177:GLU:OE1	2.28	0.52
1:A:88:PHE:HB2	1:A:89:TYR:CD1	2.44	0.52
1:D:89:TYR:OH	1:D:214:ASP:CG	2.53	0.52
1:A:56:GLY:O	1:A:117:GLN:HG3	2.09	0.52
1:C:172:TYR:CD1	1:D:186:THR:HB	2.44	0.51
1:C:209:THR:HA	1:C:210:PHE:C	2.35	0.51
1:B:174:LYS:HB2	1:B:177:GLU:HG3	1.93	0.50
1:A:159:ALA:HB2	1:A:164:LEU:HD11	1.94	0.50
1:A:213:LEU:HD12	1:A:213:LEU:O	2.12	0.50
1:C:156:GLU:CG	1:C:201:ARG:HB2	2.37	0.50
1:A:158:LEU:HB3	1:A:162:THR:O	2.11	0.49
1:A:102:ILE:CD1	1:A:114:GLY:HA2	2.39	0.49
1:B:156:GLU:OE2	1:B:201:ARG:HD2	2.13	0.49
1:C:43:ILE:CD1	1:C:79:VAL:HG23	2.43	0.48
1:D:223:GLU:HB2	1:D:224:PRO:HD2	1.93	0.48
1:D:101:TYR:C	1:D:101:TYR:CD1	2.91	0.48
1:A:213:LEU:HD12	1:A:213:LEU:C	2.38	0.48
1:D:41:PRO:HD2	1:D:79:VAL:HG21	1.94	0.48
1:B:31:ILE:HD11	1:B:222:VAL:HG11	1.96	0.48
1:C:217:ASN:OD1	1:C:219:ARG:HD2	2.14	0.48
1:C:89:TYR:CD1	1:C:89:TYR:N	2.81	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLY:HA3	1:D:202:LEU:O	2.14	0.47
1:C:194:LEU:O	1:C:195:ASP:HB2	2.14	0.47
1:D:101:TYR:C	1:D:102:ILE:HG13	2.39	0.47
1:A:48:ASP:C	1:A:49:TYR:CD1	2.92	0.47
1:A:99:ILE:C	1:A:99:ILE:HD12	2.40	0.46
1:B:132:LYS:HA	1:B:181:SER:O	2.15	0.46
1:D:34:ASN:O	1:D:117:GLN:NE2	2.42	0.46
1:B:70:ARG:HD2	1:B:70:ARG:H	1.78	0.46
1:C:159:ALA:HB2	1:C:164:LEU:HD11	1.96	0.46
1:D:20:GLY:N	4:D:402:HOH:O	2.48	0.46
1:C:138:PHE:HE2	3:C:301:PG0:H41	1.80	0.45
1:D:156:GLU:OE2	1:D:201:ARG:HD2	2.16	0.45
1:B:194:LEU:O	1:B:195:ASP:HB2	2.18	0.44
1:C:177:GLU:OE1	1:C:177:GLU:HA	2.16	0.44
1:D:73:TRP:CH2	1:D:145:ILE:CD1	3.00	0.44
1:C:209:THR:HG22	1:C:211:SER:OG	2.17	0.44
1:A:213:LEU:C	1:A:213:LEU:CD1	2.90	0.44
1:A:58:THR:HG21	4:A:431:HOH:O	2.18	0.44
1:D:102:ILE:CD1	1:D:114:GLY:HA2	2.45	0.44
1:D:129:TYR:HE2	1:D:198:LEU:HD11	1.83	0.44
1:C:88:PHE:HB2	1:C:89:TYR:CE1	2.53	0.43
1:B:138:PHE:CD2	1:B:147:LEU:HD23	2.52	0.43
1:B:126:ASP:N	1:B:187:ALA:O	2.51	0.43
1:A:58:THR:HG22	1:A:116:GLU:HB3	2.01	0.43
1:B:46:VAL:HG23	4:B:471:HOH:O	2.19	0.43
1:D:91:GLN:HG3	1:D:92:LEU:O	2.19	0.42
1:B:56:GLY:O	1:B:117:GLN:HG3	2.18	0.42
1:B:41:PRO:HD2	1:B:79:VAL:HG21	2.01	0.42
1:B:99:ILE:C	1:B:99:ILE:HD12	2.44	0.42
1:C:213:LEU:C	1:C:213:LEU:CD1	2.93	0.42
1:A:144:LYS:N	4:A:401:HOH:O	2.27	0.42
1:D:172:TYR:O	1:D:179:LYS:CE	2.68	0.42
1:D:192:PRO:HG2	1:D:193:TYR:CE2	2.55	0.42
1:A:102:ILE:HD13	1:A:114:GLY:CA	2.43	0.42
1:B:102:ILE:CD1	1:B:114:GLY:HA2	2.48	0.41
1:B:132:LYS:HB2	1:B:219:ARG:HG3	2.02	0.41
1:B:89:TYR:CD1	1:B:89:TYR:N	2.87	0.41
1:C:154:ARG:HH11	1:C:154:ARG:HD3	1.75	0.41
1:D:99:ILE:HD12	1:D:99:ILE:O	2.19	0.41
1:A:104:LEU:O	1:A:211:SER:OG	2.34	0.41
1:A:88:PHE:C	1:A:89:TYR:CD1	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HD12	1:C:99:ILE:C	2.45	0.41
1:C:217:ASN:O	1:C:219:ARG:HD3	2.20	0.41
1:A:129:TYR:HE2	1:A:198:LEU:HD11	1.86	0.40
1:D:54:PRO:HA	1:D:55:PRO:HD3	2.01	0.40
1:C:88:PHE:C	1:C:89:TYR:CD1	2.99	0.40
1:D:129:TYR:CE2	1:D:198:LEU:HD11	2.56	0.40
1:C:138:PHE:CE2	3:C:301:PG0:H41	2.55	0.40
1:D:46:VAL:HA	1:D:81:TYR:CD2	2.57	0.40
1:D:126:ASP:N	1:D:187:ALA:O	2.54	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	198/225 (88%)	197 (100%)	1 (0%)	0	100	100
1	B	196/225 (87%)	194 (99%)	2 (1%)	0	100	100
1	C	197/225 (88%)	196 (100%)	1 (0%)	0	100	100
1	D	204/225 (91%)	202 (99%)	2 (1%)	0	100	100
All	All	795/900 (88%)	789 (99%)	6 (1%)	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	168/189 (89%)	161 (96%)	7 (4%)	26	20
1	B	166/189 (88%)	160 (96%)	6 (4%)	31	25
1	C	167/189 (88%)	160 (96%)	7 (4%)	26	20
1	D	172/189 (91%)	166 (96%)	6 (4%)	32	26
All	All	673/756 (89%)	647 (96%)	26 (4%)	28	23

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	58	THR
1	A	89	TYR
1	A	129	TYR
1	A	158	LEU
1	A	178	PHE
1	A	213	LEU
1	B	70	ARG
1	B	89	TYR
1	B	178	PHE
1	B	207	GLN
1	B	213	LEU
1	B	219	ARG
1	C	89	TYR
1	C	129	TYR
1	C	145	ILE
1	C	147	LEU
1	C	177	GLU
1	C	178	PHE
1	C	207	GLN
1	D	46	VAL
1	D	129	TYR
1	D	177	GLU
1	D	178	PHE
1	D	207	GLN
1	D	213	LEU

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

Mol	Chain	Res	Type
1	A	170	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	ASN
1	C	170	ASN
1	D	196	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	PG0	C	301	-	7,7,7	0.53	0	6,6,6	0.58	0
3	PG0	D	301	-	7,7,7	0.67	0	6,6,6	0.93	0
3	PG0	B	301	-	7,7,7	0.62	0	6,6,6	0.77	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	PG0	C	301	-	-	2/5/5/5	-
3	PG0	D	301	-	-	2/5/5/5	-
3	PG0	B	301	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	PG0	OTT-C1-C2-O1
3	D	301	PG0	OTT-C1-C2-O1
3	D	301	PG0	C4-C3-O1-C2
3	B	301	PG0	OTT-C1-C2-O1
3	B	301	PG0	O1-C3-C4-O2
3	C	301	PG0	O1-C3-C4-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	PG0	2	0
3	D	301	PG0	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	200/225 (88%)	-0.30	0 100 100	24, 34, 50, 71	0
1	B	198/225 (88%)	-0.34	2 (1%) 79 82	23, 33, 54, 82	0
1	C	199/225 (88%)	-0.25	0 100 100	24, 33, 56, 75	0
1	D	206/225 (91%)	0.03	4 (1%) 66 68	26, 42, 60, 70	0
All	All	803/900 (89%)	-0.21	6 (0%) 84 86	23, 35, 57, 82	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	PHE	2.8
1	D	89	TYR	2.7
1	D	20	GLY	2.4
1	D	22	HIS	2.2
1	D	225	ALA	2.1
1	B	143	GLN	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	CA	C	303	1/1	0.50	0.20	63,63,63,63	0
2	CA	B	303	1/1	0.55	0.22	59,59,59,59	0
2	CA	A	302	1/1	0.61	0.17	52,52,52,52	0
2	CA	D	303	1/1	0.65	0.16	66,66,66,66	0
3	PG0	B	301	8/8	0.79	0.12	46,56,66,66	0
3	PG0	C	301	8/8	0.80	0.13	47,56,62,62	0
3	PG0	D	301	8/8	0.82	0.12	34,49,59,59	0
2	CA	C	302	1/1	0.87	0.08	32,32,32,32	0
2	CA	A	301	1/1	0.99	0.01	31,31,31,31	0
2	CA	D	302	1/1	0.99	0.03	42,42,42,42	0
2	CA	B	302	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.