



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:13 PM UTC

PDB ID : 2OTE / pdb_00002ote
Title : Crystal structure of a monomeric cyan fluorescent protein in the photobleached state
Authors : Henderson, J.N.; Ai, H.; Campbell, R.E.; Remington, S.J.
Deposited on : 2007-02-07
Resolution : 1.47 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

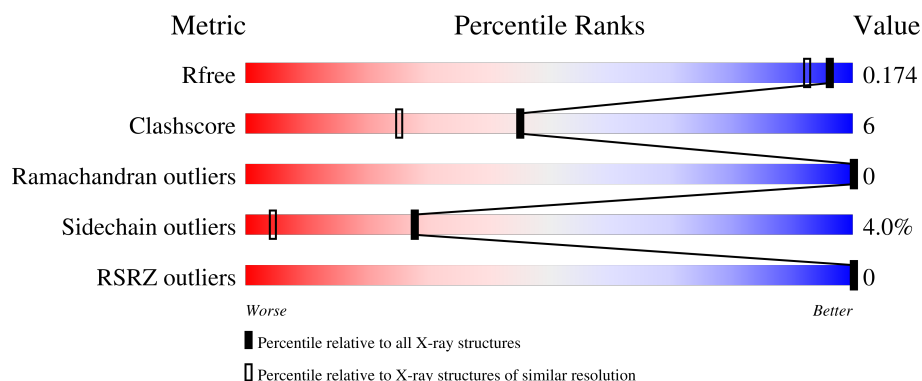
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	214	
1	B	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4007 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 GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	19	0
			1779	1164	282	328	5			
1	B	214	Total	C	N	O	S	0	14	0
			1774	1149	285	335	5			

There are 46 discrepancies between the modelled and reference sequences:

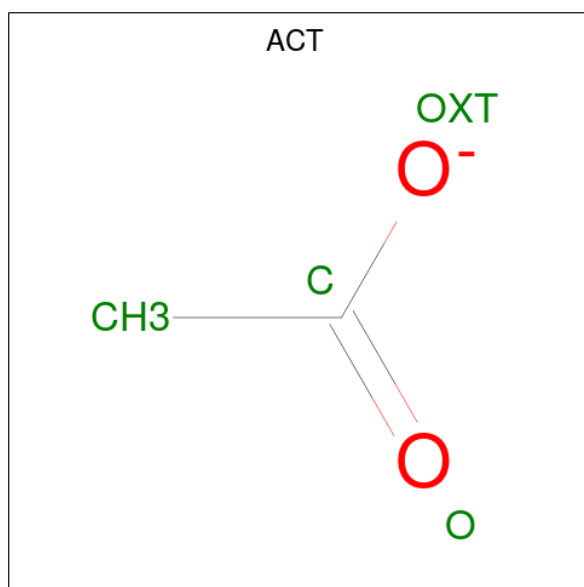
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASN	HIS	engineered mutation	UNP Q9U6Y3
A	44	ILE	LEU	engineered mutation	UNP Q9U6Y3
A	62	THR	SER	engineered mutation	UNP Q9U6Y3
A	66	PIA	GLN	chromophore	UNP Q9U6Y3
A	66	PIA	TYR	chromophore	UNP Q9U6Y3
A	66	PIA	GLY	chromophore	UNP Q9U6Y3
A	72	PHE	LEU	engineered mutation	UNP Q9U6Y3
A	80	PRO	ALA	engineered mutation	UNP Q9U6Y3
A	81	ASN	ASP	engineered mutation	UNP Q9U6Y3
A	123	HIS	ARG	engineered mutation	UNP Q9U6Y3
A	124	LEU	PHE	engineered mutation	UNP Q9U6Y3
A	125	LYS	ASP	engineered mutation	UNP Q9U6Y3
A	127	GLU	MET	engineered mutation	UNP Q9U6Y3
A	150	LEU	MET	engineered mutation	UNP Q9U6Y3
A	162	LYS	SER	engineered mutation	UNP Q9U6Y3
A	164	LYS	SER	engineered mutation	UNP Q9U6Y3
A	173	HIS	TYR	engineered mutation	UNP Q9U6Y3
A	175	VAL	CYS	engineered mutation	UNP Q9U6Y3
A	179	THR	SER	engineered mutation	UNP Q9U6Y3
A	182	ARG	LYS	engineered mutation	UNP Q9U6Y3
A	186	ALA	VAL	engineered mutation	UNP Q9U6Y3
A	213	VAL	LEU	engineered mutation	UNP Q9U6Y3
A	216	SER	ASN	engineered mutation	UNP Q9U6Y3
B	42	ASN	HIS	engineered mutation	UNP Q9U6Y3
B	44	ILE	LEU	engineered mutation	UNP Q9U6Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	THR	SER	engineered mutation	UNP Q9U6Y3
B	66	PIA	GLN	chromophore	UNP Q9U6Y3
B	66	PIA	TYR	chromophore	UNP Q9U6Y3
B	66	PIA	GLY	chromophore	UNP Q9U6Y3
B	72	PHE	LEU	engineered mutation	UNP Q9U6Y3
B	80	PRO	ALA	engineered mutation	UNP Q9U6Y3
B	81	ASN	ASP	engineered mutation	UNP Q9U6Y3
B	123	HIS	ARG	engineered mutation	UNP Q9U6Y3
B	124	LEU	PHE	engineered mutation	UNP Q9U6Y3
B	125	LYS	ASP	engineered mutation	UNP Q9U6Y3
B	127	GLU	MET	engineered mutation	UNP Q9U6Y3
B	150	LEU	MET	engineered mutation	UNP Q9U6Y3
B	162	LYS	SER	engineered mutation	UNP Q9U6Y3
B	164	LYS	SER	engineered mutation	UNP Q9U6Y3
B	173	HIS	TYR	engineered mutation	UNP Q9U6Y3
B	175	VAL	CYS	engineered mutation	UNP Q9U6Y3
B	179	THR	SER	engineered mutation	UNP Q9U6Y3
B	182	ARG	LYS	engineered mutation	UNP Q9U6Y3
B	186	ALA	VAL	engineered mutation	UNP Q9U6Y3
B	213	VAL	LEU	engineered mutation	UNP Q9U6Y3
B	216	SER	ASN	engineered mutation	UNP Q9U6Y3

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

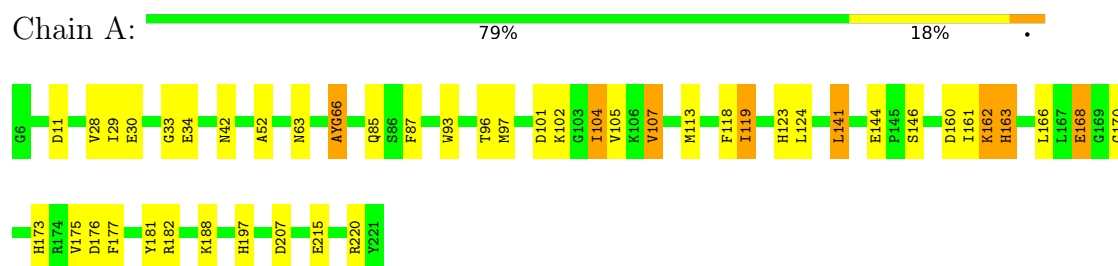
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	243	Total 243	O 243	0	13
3	B	207	Total 207	O 207	0	6

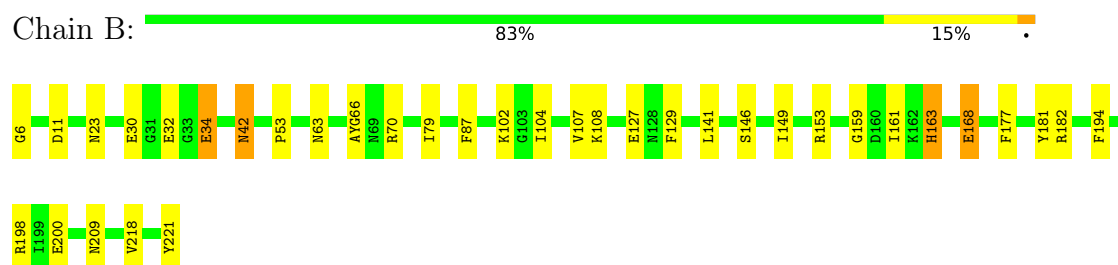
3 Residue-property plots

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: GFP-like fluorescent chromoprotein cFP484



- Molecule 1: GFP-like fluorescent chromoprotein cFP484



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.49Å 66.31Å 97.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.47 10.00 – 1.47	Depositor EDS
% Data completeness (in resolution range)	94.7 (10.00-1.47) 85.4 (10.00-1.47)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 1.47Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, R_{free}	0.190 , 0.261 0.168 , 0.174	Depositor DCC
R_{free} test set	3442 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4007	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6779e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0/1847	1.48	19/2504 (0.8%)
1	B	0.62	0/1824	1.50	16/2468 (0.6%)
All	All	0.61	0/3671	1.49	35/4972 (0.7%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ARG	CD-NE-CZ	18.90	150.86	124.40
1	A	173	HIS	CA-CB-CG	12.83	126.63	113.80
1	B	177	PHE	CA-CB-CG	7.27	121.07	113.80
1	A	168	GLU	CA-C-N	-7.13	112.45	122.86
1	A	168	GLU	C-N-CA	-7.13	112.45	122.86
1	B	42	ASN	CA-CB-CG	6.75	119.35	112.60
1	B	34	GLU	CA-C-O	-6.41	113.58	120.75
1	A	207	ASP	CA-CB-CG	-6.40	106.20	112.60
1	A	52	ALA	N-CA-C	6.19	117.69	109.83
1	A	160	ASP	CA-C-O	-6.09	114.26	120.71
1	B	87	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	28	VAL	O-C-N	5.91	129.45	123.07
1	B	153	ARG	CD-NE-CZ	5.75	132.45	124.40
1	A	30	GLU	CA-C-N	-5.71	114.41	121.38
1	A	30	GLU	C-N-CA	-5.71	114.41	121.38
1	A	93	TRP	CA-CB-CG	5.64	124.32	113.60
1	B	102	LYS	CA-C-N	-5.61	114.77	120.10
1	B	102	LYS	C-N-CA	-5.61	114.77	120.10
1	B	30	GLU	CA-C-N	-5.56	116.18	121.46
1	B	30	GLU	C-N-CA	-5.56	116.18	121.46
1	B	127	GLU	O-C-N	5.52	129.54	123.25
1	B	168	GLU	CA-C-N	-5.49	113.48	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	GLU	C-N-CA	-5.49	113.48	122.20
1	A	123	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	42[A]	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	42[B]	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	194	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	175	VAL	CA-C-N	-5.22	115.51	122.72
1	A	175	VAL	C-N-CA	-5.22	115.51	122.72
1	B	70[A]	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	A	220	ARG	CD-NE-CZ	5.14	131.60	124.40
1	A	29	ILE	O-C-N	5.14	128.73	123.18
1	B	182	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	170	GLY	CA-C-N	-5.10	114.92	121.96
1	A	170	GLY	C-N-CA	-5.10	114.92	121.96

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	1779	0	1704	25	0
1	B	1774	0	1688	16	0
2	A	4	0	3	1	0
3	A	243	0	0	2	0
3	B	207	0	0	7	0
All	All	4007	0	3395	41	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 6.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66[A]:PIA:HE2	1:B:181:TYR:OH	1.89	0.71
1:B:209:ASN:HB3	3:B:368:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:HE22	1:A:188:LYS:H	1.36	0.70
1:A:96:THR:HG23	1:A:104[A]:ILE:HD11	1.78	0.65
1:A:33:GLY:HA2	2:A:1:ACT:H1	1.83	0.61
1:B:79:ILE:HG12	1:B:221:TYR:CZ	2.36	0.60
1:A:104[A]:ILE:HD12	1:A:105:VAL:N	2.19	0.58
1:B:23:ASN:HD21	1:B:129:PHE:H	1.51	0.57
1:A:146[B]:SER:HB3	1:A:163:HIS:CE1	2.40	0.57
1:B:63[B]:ASN:ND2	1:B:63[B]:ASN:H	2.04	0.56
1:A:66[A]:PIA:HE1	1:A:181:TYR:OH	2.07	0.54
1:A:146[A]:SER:HB2	3:A:327:HOH:O	2.07	0.54
1:A:104[A]:ILE:HD12	1:A:105:VAL:H	1.73	0.53
1:A:63[B]:ASN:ND2	1:A:63[B]:ASN:H	2.04	0.52
1:B:146[B]:SER:HB3	1:B:163:HIS:CE1	2.45	0.52
1:B:11:ASP:OD1	1:B:34:GLU:OE2	2.29	0.51
1:A:97:MET:HE3	1:A:177:PHE:CZ	2.47	0.49
1:A:105:VAL:HG12	1:A:107[B]:VAL:HG23	1.93	0.49
1:B:53:PRO:HD2	3:B:427:HOH:O	2.12	0.49
1:A:87:PHE:CD2	1:A:113:MET:HE3	2.48	0.48
1:A:182[A]:ARG:HD2	3:A:299:HOH:O	2.13	0.48
1:B:149:ILE:O	1:B:159:GLY:HA2	2.13	0.48
1:A:101:ASP:O	1:A:102:LYS:HB2	2.14	0.48
1:B:218[B]:VAL:HG13	3:B:362:HOH:O	2.12	0.48
1:A:85:GLN:NE2	1:A:188:LYS:H	2.08	0.47
1:A:96:THR:HG23	1:A:104[A]:ILE:CD1	2.44	0.47
1:A:107[B]:VAL:HG22	1:A:124:LEU:HG	1.96	0.46
1:A:118:PHE:C	1:A:119[A]:ILE:HD13	2.41	0.46
1:B:141:LEU:HD21	1:B:168:GLU:HG2	1.97	0.46
1:B:198:ARG:NE	3:B:384:HOH:O	2.49	0.46
1:B:6:GLY:N	3:B:390:HOH:O	2.50	0.45
1:A:141[B]:LEU:HD21	1:A:168:GLU:HG2	1.99	0.44
1:B:42:ASN:ND2	3:B:296:HOH:O	2.51	0.43
1:B:79:ILE:HG12	1:B:221:TYR:CE2	2.52	0.43
1:A:141[B]:LEU:HD12	1:A:166:LEU:HG	2.00	0.43
1:B:108:LYS:NZ	3:B:421:HOH:O	2.50	0.43
1:A:141[A]:LEU:HD12	1:A:141[A]:LEU:HA	1.90	0.41
1:A:11[A]:ASP:OD2	1:A:34[A]:GLU:OE2	2.38	0.41
1:A:162:LYS:HG2	1:A:176:ASP:OD1	2.21	0.41
1:A:144:GLU:O	1:A:163:HIS:HE1	2.04	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	224/214 (105%)	219 (98%)	5 (2%)	0	100	100
1	B	218/214 (102%)	212 (97%)	6 (3%)	0	100	100
All	All	442/428 (103%)	431 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	184/188 (98%)	172 (94%)	12 (6%)	15	1
1	B	187/188 (100%)	180 (96%)	7 (4%)	30	5
All	All	371/376 (99%)	352 (95%)	19 (5%)	28	2

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104[A]	ILE
1	A	104[B]	ILE
1	A	107[A]	VAL
1	A	107[B]	VAL
1	A	119[A]	ILE
1	A	119[C]	ILE
1	A	141[A]	LEU
1	A	141[B]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	161	ILE
1	A	162	LYS
1	A	163	HIS
1	A	197[A]	HIS
1	B	32[A]	GLU
1	B	32[B]	GLU
1	B	104	ILE
1	B	107	VAL
1	B	161	ILE
1	B	163	HIS
1	B	200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	85	GLN
1	A	132	ASN
1	B	23	ASN
1	B	42	ASN
1	B	163	HIS
1	B	197[A]	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PIA	A	66[A]	1	20,21,22	2.33	7 (35%)	28,29,31	2.59	10 (35%)

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
1	PIA	A	66[A]	1	-	6/8/27/28	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[A]	PIA	OH-CZ	-4.94	1.25	1.37
1	A	66[A]	PIA	CG2-CB2	-4.93	1.37	1.46
1	A	66[A]	PIA	C1-N3	3.93	1.43	1.37
1	A	66[A]	PIA	CE1-CZ	3.47	1.45	1.39
1	A	66[A]	PIA	CE2-CZ	3.16	1.44	1.39
1	A	66[A]	PIA	CE2-CD2	-3.04	1.33	1.38
1	A	66[A]	PIA	CD2-CG2	2.26	1.44	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66[A]	PIA	O2-C2-CA2	9.32	136.97	131.02
1	A	66[A]	PIA	CB1-CA1-C1	-3.87	106.00	111.43
1	A	66[A]	PIA	CD2-CE2-CZ	3.18	123.24	119.88
1	A	66[A]	PIA	C2-N3-C1	-3.07	106.65	108.07
1	A	66[A]	PIA	CA3-N3-C2	3.02	130.30	123.67
1	A	66[A]	PIA	O2-C2-N3	-2.81	118.45	124.31
1	A	66[A]	PIA	CG2-CB2-CA2	2.77	133.16	129.87
1	A	66[A]	PIA	O3-C3-CA3	-2.37	114.80	125.47
1	A	66[A]	PIA	CE2-CZ-CE1	-2.36	116.00	119.77
1	A	66[A]	PIA	OH-CZ-CE1	2.31	126.44	120.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66[A]	PIA	N2-CA2-CB2-CG2
1	A	66[A]	PIA	C2-CA2-CB2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	66[A]	PIA	C3-CA3-N3-C2
1	A	66[A]	PIA	CA2-CB2-CG2-CD2
1	A	66[A]	PIA	CA2-CB2-CG2-CD1
1	A	66[A]	PIA	N2-C1-CA1-CB1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66[A]	PIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	1	-	3,3,3	1.90	1 (33%)	3,3,3	1.49	1 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ACT	O-C	3.04	1.35	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ACT	OXT-C-CH3	2.03	123.58	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ACT	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	213/214 (99%)	-0.46	0 100 100	9, 17, 25, 35	24 (11%)
1	B	213/214 (99%)	-0.48	0 100 100	8, 17, 25, 31	18 (8%)
All	All	426/428 (99%)	-0.47	0 100 100	8, 17, 25, 35	42 (9%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PIA	B	66[A]	20/21	0.95	0.07	13,18,30,38	8
1	PIA	A	66[A]	20/21	0.96	0.07	13,18,30,38	8

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($\text{\AA}^2$)	Q<0.9
2	ACT	A	1	4/4	0.93	0.08	29,34,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.