Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 03:44 am GMT

PDB ID	:	7Z7O
Title	:	Structure of the fluorescent protein NeonCyan0.95 at pH 7.5
Authors	:	Clavel, D.; Dupuy, J.; Royant, A.
Deposited on	:	2022-03-16
Resolution	:	1.51 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 (i) 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 (1)) were used in the production of this report:

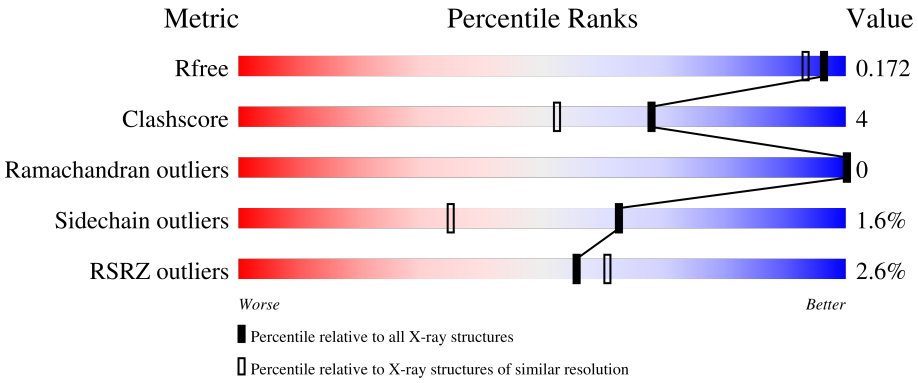
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 <=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	234	86% 12% ·
1	B	234	87% 10% ·
1	C	234	5% 86% 8% · 6%
1	D	234	4% 85% 6% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7596 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 NeonCyan0.95.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1829	1167	304	347	11			
1	B	227	Total	C	N	O	S	0	1	0
			1816	1161	302	343	10			
1	C	221	Total	C	N	O	S	0	0	0
			1756	1124	291	332	9			
1	D	215	Total	C	N	O	S	1	0	0
			1705	1092	286	320	7			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B1PNC0
A	2	VAL	-	expression tag	UNP B1PNC0
A	3	SER	-	expression tag	UNP B1PNC0
A	4	LYS	-	expression tag	UNP B1PNC0
A	5	GLY	-	expression tag	UNP B1PNC0
A	6	GLU	-	expression tag	UNP B1PNC0
A	7	GLU	-	expression tag	UNP B1PNC0
A	8	ASP	-	expression tag	UNP B1PNC0
A	9	ASN	-	expression tag	UNP B1PNC0
A	10	MET	-	expression tag	UNP B1PNC0
A	11	ALA	-	expression tag	UNP B1PNC0
A	25	ILE	PHE	engineered mutation	UNP B1PNC0
A	35	GLN	ARG	engineered mutation	UNP B1PNC0
A	42	GLU	ASP	engineered mutation	UNP B1PNC0
A	55	ASP	ALA	engineered mutation	UNP B1PNC0
A	66	HIS	GLN	engineered mutation	UNP B1PNC0
A	67	VAL	ILE	engineered mutation	UNP B1PNC0
A	69	IO8	GLY	chromophore	UNP B1PNC0
A	?	-	TYR	chromophore	UNP B1PNC0
A	?	-	GLY	chromophore	UNP B1PNC0
A	77	TYR	PHE	engineered mutation	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	89	VAL	LYS	engineered mutation	UNP B1PNC0
A	110	VAL	SER	engineered mutation	UNP B1PNC0
A	125	ALA	PHE	engineered mutation	UNP B1PNC0
A	128	LYS	ILE	engineered mutation	UNP B1PNC0
A	146	VAL	ALA	engineered mutation	UNP B1PNC0
A	148	SER	TRP	engineered mutation	UNP B1PNC0
A	150	TRP	VAL	engineered mutation	UNP B1PNC0
A	151	SER	THR	engineered mutation	UNP B1PNC0
A	153	LYS	MET	engineered mutation	UNP B1PNC0
A	154	THR	LEU	engineered mutation	UNP B1PNC0
A	166	LYS	ASP	engineered mutation	UNP B1PNC0
A	168	SER	THR	engineered mutation	UNP B1PNC0
A	173	ASN	SER	engineered mutation	UNP B1PNC0
A	175	GLU	LYS	engineered mutation	UNP B1PNC0
A	178	ARG	GLN	engineered mutation	UNP B1PNC0
A	181	ALA	VAL	engineered mutation	UNP B1PNC0
A	184	THR	ASN	engineered mutation	UNP B1PNC0
A	195	TYR	ILE	engineered mutation	UNP B1PNC0
A	201	VAL	MET	engineered mutation	UNP B1PNC0
A	202	TYR	PHE	engineered mutation	UNP B1PNC0
A	213	GLU	LYS	engineered mutation	UNP B1PNC0
A	230	GLY	-	expression tag	UNP B1PNC0
A	231	MET	-	expression tag	UNP B1PNC0
A	232	ASP	-	expression tag	UNP B1PNC0
A	233	GLU	-	expression tag	UNP B1PNC0
A	234	LEU	-	expression tag	UNP B1PNC0
A	235	TYR	-	expression tag	UNP B1PNC0
A	236	LYS	-	expression tag	UNP B1PNC0
B	1	MET	-	initiating methionine	UNP B1PNC0
B	2	VAL	-	expression tag	UNP B1PNC0
B	3	SER	-	expression tag	UNP B1PNC0
B	4	LYS	-	expression tag	UNP B1PNC0
B	5	GLY	-	expression tag	UNP B1PNC0
B	6	GLU	-	expression tag	UNP B1PNC0
B	7	GLU	-	expression tag	UNP B1PNC0
B	8	ASP	-	expression tag	UNP B1PNC0
B	9	ASN	-	expression tag	UNP B1PNC0
B	10	MET	-	expression tag	UNP B1PNC0
B	11	ALA	-	expression tag	UNP B1PNC0
B	25	ILE	PHE	engineered mutation	UNP B1PNC0
B	35	GLN	ARG	engineered mutation	UNP B1PNC0
B	42	GLU	ASP	engineered mutation	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	ASP	ALA	engineered mutation	UNP B1PNC0
B	66	HIS	GLN	engineered mutation	UNP B1PNC0
B	67	VAL	ILE	engineered mutation	UNP B1PNC0
B	69	IO8	GLY	chromophore	UNP B1PNC0
B	?	-	TYR	chromophore	UNP B1PNC0
B	?	-	GLY	chromophore	UNP B1PNC0
B	77	TYR	PHE	engineered mutation	UNP B1PNC0
B	89	VAL	LYS	engineered mutation	UNP B1PNC0
B	110	VAL	SER	engineered mutation	UNP B1PNC0
B	125	ALA	PHE	engineered mutation	UNP B1PNC0
B	128	LYS	ILE	engineered mutation	UNP B1PNC0
B	146	VAL	ALA	engineered mutation	UNP B1PNC0
B	148	SER	TRP	engineered mutation	UNP B1PNC0
B	150	TRP	VAL	engineered mutation	UNP B1PNC0
B	151	SER	THR	engineered mutation	UNP B1PNC0
B	153	LYS	MET	engineered mutation	UNP B1PNC0
B	154	THR	LEU	engineered mutation	UNP B1PNC0
B	166	LYS	ASP	engineered mutation	UNP B1PNC0
B	168	SER	THR	engineered mutation	UNP B1PNC0
B	173	ASN	SER	engineered mutation	UNP B1PNC0
B	175	GLU	LYS	engineered mutation	UNP B1PNC0
B	178	ARG	GLN	engineered mutation	UNP B1PNC0
B	181	ALA	VAL	engineered mutation	UNP B1PNC0
B	184	THR	ASN	engineered mutation	UNP B1PNC0
B	195	TYR	ILE	engineered mutation	UNP B1PNC0
B	201	VAL	MET	engineered mutation	UNP B1PNC0
B	202	TYR	PHE	engineered mutation	UNP B1PNC0
B	213	GLU	LYS	engineered mutation	UNP B1PNC0
B	230	GLY	-	expression tag	UNP B1PNC0
B	231	MET	-	expression tag	UNP B1PNC0
B	232	ASP	-	expression tag	UNP B1PNC0
B	233	GLU	-	expression tag	UNP B1PNC0
B	234	LEU	-	expression tag	UNP B1PNC0
B	235	TYR	-	expression tag	UNP B1PNC0
B	236	LYS	-	expression tag	UNP B1PNC0
C	1	MET	-	initiating methionine	UNP B1PNC0
C	2	VAL	-	expression tag	UNP B1PNC0
C	3	SER	-	expression tag	UNP B1PNC0
C	4	LYS	-	expression tag	UNP B1PNC0
C	5	GLY	-	expression tag	UNP B1PNC0
C	6	GLU	-	expression tag	UNP B1PNC0
C	7	GLU	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP B1PNC0
C	9	ASN	-	expression tag	UNP B1PNC0
C	10	MET	-	expression tag	UNP B1PNC0
C	11	ALA	-	expression tag	UNP B1PNC0
C	25	ILE	PHE	engineered mutation	UNP B1PNC0
C	35	GLN	ARG	engineered mutation	UNP B1PNC0
C	42	GLU	ASP	engineered mutation	UNP B1PNC0
C	55	ASP	ALA	engineered mutation	UNP B1PNC0
C	66	HIS	GLN	engineered mutation	UNP B1PNC0
C	67	VAL	ILE	engineered mutation	UNP B1PNC0
C	69	IO8	GLY	chromophore	UNP B1PNC0
C	?	-	TYR	chromophore	UNP B1PNC0
C	?	-	GLY	chromophore	UNP B1PNC0
C	77	TYR	PHE	engineered mutation	UNP B1PNC0
C	89	VAL	LYS	engineered mutation	UNP B1PNC0
C	110	VAL	SER	engineered mutation	UNP B1PNC0
C	125	ALA	PHE	engineered mutation	UNP B1PNC0
C	128	LYS	ILE	engineered mutation	UNP B1PNC0
C	146	VAL	ALA	engineered mutation	UNP B1PNC0
C	148	SER	TRP	engineered mutation	UNP B1PNC0
C	150	TRP	VAL	engineered mutation	UNP B1PNC0
C	151	SER	THR	engineered mutation	UNP B1PNC0
C	153	LYS	MET	engineered mutation	UNP B1PNC0
C	154	THR	LEU	engineered mutation	UNP B1PNC0
C	166	LYS	ASP	engineered mutation	UNP B1PNC0
C	168	SER	THR	engineered mutation	UNP B1PNC0
C	173	ASN	SER	engineered mutation	UNP B1PNC0
C	175	GLU	LYS	engineered mutation	UNP B1PNC0
C	178	ARG	GLN	engineered mutation	UNP B1PNC0
C	181	ALA	VAL	engineered mutation	UNP B1PNC0
C	184	THR	ASN	engineered mutation	UNP B1PNC0
C	195	TYR	ILE	engineered mutation	UNP B1PNC0
C	201	VAL	MET	engineered mutation	UNP B1PNC0
C	202	TYR	PHE	engineered mutation	UNP B1PNC0
C	213	GLU	LYS	engineered mutation	UNP B1PNC0
C	230	GLY	-	expression tag	UNP B1PNC0
C	231	MET	-	expression tag	UNP B1PNC0
C	232	ASP	-	expression tag	UNP B1PNC0
C	233	GLU	-	expression tag	UNP B1PNC0
C	234	LEU	-	expression tag	UNP B1PNC0
C	235	TYR	-	expression tag	UNP B1PNC0
C	236	LYS	-	expression tag	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP B1PNC0
D	2	VAL	-	expression tag	UNP B1PNC0
D	3	SER	-	expression tag	UNP B1PNC0
D	4	LYS	-	expression tag	UNP B1PNC0
D	5	GLY	-	expression tag	UNP B1PNC0
D	6	GLU	-	expression tag	UNP B1PNC0
D	7	GLU	-	expression tag	UNP B1PNC0
D	8	ASP	-	expression tag	UNP B1PNC0
D	9	ASN	-	expression tag	UNP B1PNC0
D	10	MET	-	expression tag	UNP B1PNC0
D	11	ALA	-	expression tag	UNP B1PNC0
D	25	ILE	PHE	engineered mutation	UNP B1PNC0
D	35	GLN	ARG	engineered mutation	UNP B1PNC0
D	42	GLU	ASP	engineered mutation	UNP B1PNC0
D	55	ASP	ALA	engineered mutation	UNP B1PNC0
D	66	HIS	GLN	engineered mutation	UNP B1PNC0
D	67	VAL	ILE	engineered mutation	UNP B1PNC0
D	69	IO8	GLY	chromophore	UNP B1PNC0
D	?	-	TYR	chromophore	UNP B1PNC0
D	?	-	GLY	chromophore	UNP B1PNC0
D	77	TYR	PHE	engineered mutation	UNP B1PNC0
D	89	VAL	LYS	engineered mutation	UNP B1PNC0
D	110	VAL	SER	engineered mutation	UNP B1PNC0
D	125	ALA	PHE	engineered mutation	UNP B1PNC0
D	128	LYS	ILE	engineered mutation	UNP B1PNC0
D	146	VAL	ALA	engineered mutation	UNP B1PNC0
D	148	SER	TRP	engineered mutation	UNP B1PNC0
D	150	TRP	VAL	engineered mutation	UNP B1PNC0
D	151	SER	THR	engineered mutation	UNP B1PNC0
D	153	LYS	MET	engineered mutation	UNP B1PNC0
D	154	THR	LEU	engineered mutation	UNP B1PNC0
D	166	LYS	ASP	engineered mutation	UNP B1PNC0
D	168	SER	THR	engineered mutation	UNP B1PNC0
D	173	ASN	SER	engineered mutation	UNP B1PNC0
D	175	GLU	LYS	engineered mutation	UNP B1PNC0
D	178	ARG	GLN	engineered mutation	UNP B1PNC0
D	181	ALA	VAL	engineered mutation	UNP B1PNC0
D	184	THR	ASN	engineered mutation	UNP B1PNC0
D	195	TYR	ILE	engineered mutation	UNP B1PNC0
D	201	VAL	MET	engineered mutation	UNP B1PNC0
D	202	TYR	PHE	engineered mutation	UNP B1PNC0
D	213	GLU	LYS	engineered mutation	UNP B1PNC0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	230	GLY	-	expression tag	UNP B1PNC0
D	231	MET	-	expression tag	UNP B1PNC0
D	232	ASP	-	expression tag	UNP B1PNC0
D	233	GLU	-	expression tag	UNP B1PNC0
D	234	LEU	-	expression tag	UNP B1PNC0
D	235	TYR	-	expression tag	UNP B1PNC0
D	236	LYS	-	expression tag	UNP B1PNC0

- Molecule 2 is water.

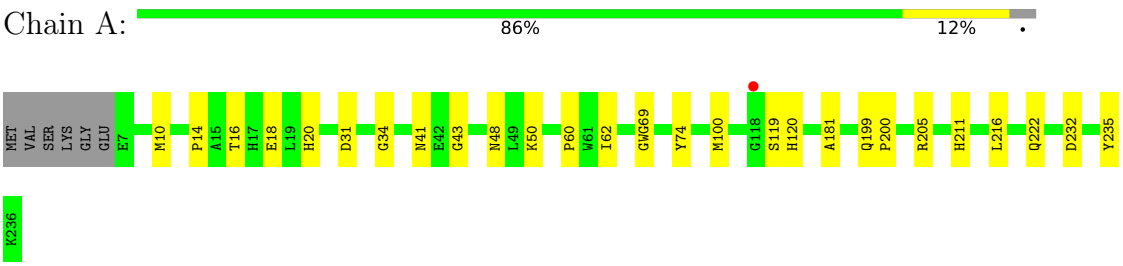
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	166	Total O 166 166	0	0
2	B	162	Total O 162 162	0	0
2	C	84	Total O 84 84	0	0
2	D	78	Total O 78 78	0	0

3 Residue-property plots (i)

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.

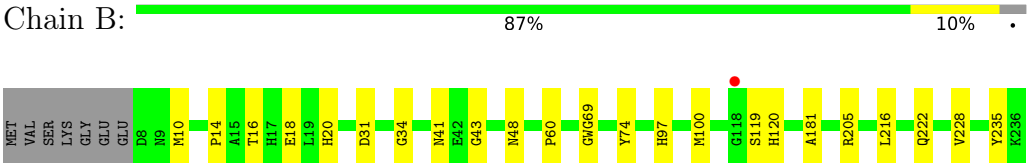
• Molecule 1: NeonCyan0.95

Chain A:



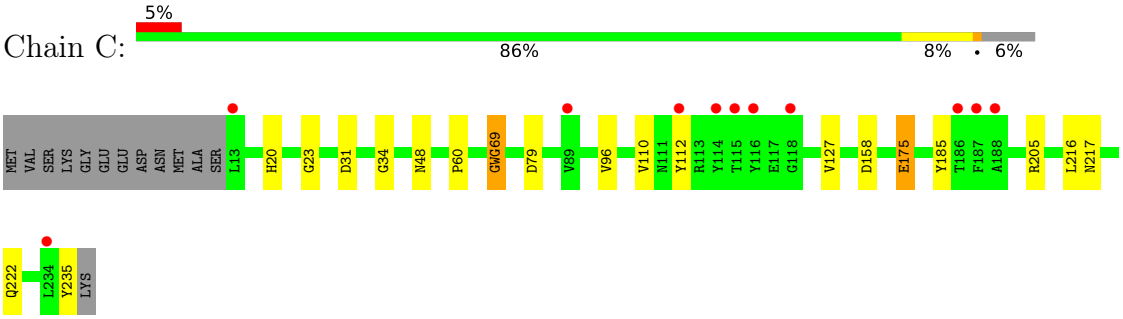
• Molecule 1: NeonCyan0.95

Chain B:



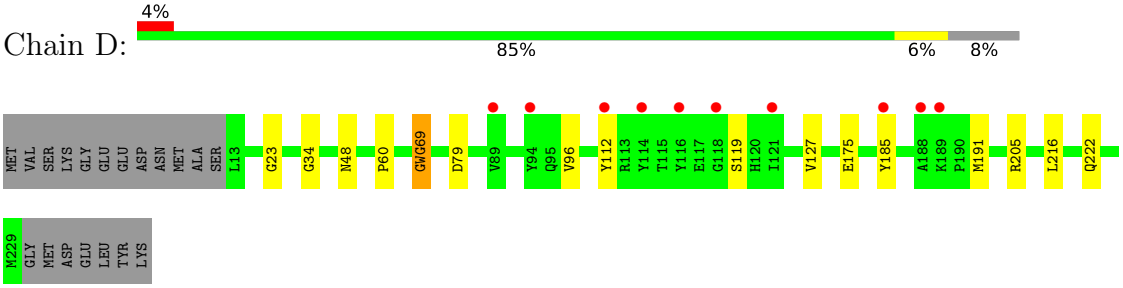
• Molecule 1: NeonCyan0.95

Chain C:



• Molecule 1: NeonCyan0.95

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.85Å 60.66Å 67.07Å 89.95° 71.79° 90.01°	Depositor
Resolution (Å)	63.71 – 1.51 63.71 – 1.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.71-1.51) 99.7 (63.71-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	50.06 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.163 , 0.186 0.154 , 0.172	Depositor DCC
R_{free} test set	3938 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.427 for -h,k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7596	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IO8

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	0.67	0/1859	0.92	0/2519
1	B	0.66	0/1849	0.92	0/2506
1	C	0.61	0/1786	0.77	0/2426
1	D	0.61	0/1734	0.78	0/2357
All	All	0.64	0/7228	0.85	0/9808

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1829	0	1712	17	0
1	B	1816	0	1704	15	0
1	C	1756	0	1628	13	0
1	D	1705	0	1583	8	0
2	A	166	0	0	1	0
2	B	162	0	0	1	0
2	C	84	0	0	0	0
2	D	78	0	0	0	0
All	All	7596	0	6627	52	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 4.

All (52) 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:10:MET:HB3	1:B:41:ASN:HD22	1.50	0.77
1:A:10:MET:HB3	1:A:41:ASN:HD22	1.50	0.76
1:A:14:PRO:HB3	1:A:119:SER:O	1.87	0.74
1:B:10:MET:HB3	1:B:41:ASN:ND2	2.04	0.72
1:A:10:MET:HB3	1:A:41:ASN:ND2	2.07	0.69
1:A:10:MET:C	1:A:41:ASN:HD21	2.00	0.64
1:B:34:GLY:HA3	1:B:48:ASN:O	1.96	0.64
1:A:34:GLY:HA3	1:A:48:ASN:O	1.98	0.64
1:C:205:ARG:HG2	1:C:222:GLN:HB3	1.80	0.64
1:B:14:PRO:HB3	1:B:119:SER:O	1.97	0.63
1:B:10:MET:C	1:B:41:ASN:HD21	2.02	0.62
1:A:20:HIS:HE1	1:A:31:ASP:OD2	1.81	0.62
1:C:96:VAL:HB	1:C:112:TYR:HB2	1.83	0.60
1:D:205:ARG:HG2	1:D:222:GLN:HB3	1.82	0.60
1:D:96:VAL:HB	1:D:112:TYR:HB2	1.84	0.59
1:B:20:HIS:HE1	1:B:31:ASP:OD2	1.85	0.59
1:B:100:MET:HE2	2:B:310:HOH:O	2.02	0.58
1:D:34:GLY:HA3	1:D:48:ASN:O	2.04	0.58
1:A:18:GLU:OE1	1:A:120:HIS:HE1	1.87	0.57
1:C:34:GLY:HA3	1:C:48:ASN:O	2.06	0.55
1:B:18:GLU:OE1	1:B:120:HIS:HE1	1.90	0.54
1:C:48:ASN:HD22	1:C:217:ASN:ND2	2.06	0.53
1:C:60:PRO:HB3	1:C:216:LEU:HD21	1.90	0.53
1:C:48:ASN:HD22	1:C:217:ASN:HD21	1.57	0.52
1:B:97:HIS:HB2	1:C:175:GLU:OE2	2.12	0.50
1:D:60:PRO:HB3	1:D:216:LEU:HD21	1.94	0.49
1:A:205:ARG:HG2	1:A:222:GLN:HB3	1.96	0.47
1:B:100:MET:SD	1:B:181:ALA:HB2	2.54	0.47
1:A:16:THR:OG1	1:A:120:HIS:HD2	1.98	0.47
1:A:211:HIS:HE1	2:A:301:HOH:O	1.96	0.47
1:C:20:HIS:HE1	1:C:31:ASP:OD2	1.98	0.47
1:B:16:THR:OG1	1:B:120:HIS:HD2	1.98	0.46
1:D:23:GLY:HA3	1:D:127:VAL:O	2.15	0.46
1:B:10:MET:CB	1:B:41:ASN:ND2	2.78	0.45
1:D:96:VAL:HG22	1:D:185:TYR:CD1	2.52	0.44
1:B:43:GLY:HA2	1:B:74:TYR:O	2.17	0.43
1:C:69:IO8:CE2	1:C:205:ARG:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD12	1:A:62:ILE:HA	1.93	0.43
1:C:96:VAL:HG22	1:C:185:TYR:CD1	2.54	0.42
1:B:60:PRO:HB3	1:B:216:LEU:HD21	2.01	0.42
1:B:205:ARG:HG2	1:B:222:GLN:HB3	2.01	0.42
1:A:43:GLY:HA2	1:A:74:TYR:O	2.20	0.42
1:C:23:GLY:HA3	1:C:127:VAL:O	2.19	0.42
1:C:110:VAL:HG13	1:C:127:VAL:HG22	2.01	0.42
1:D:69:IO8:CE2	1:D:205:ARG:HD2	2.50	0.42
1:D:205:ARG:HG2	1:D:222:GLN:CB	2.48	0.42
1:A:60:PRO:HB3	1:A:216:LEU:HD21	2.02	0.41
1:A:100[A]:MET:SD	1:A:181:ALA:HB2	2.61	0.41
1:A:199:GLN:HB2	1:A:200:PRO:HA	2.02	0.41
1:A:10:MET:CB	1:A:41:ASN:ND2	2.82	0.40
1:A:48:ASN:HD21	1:A:50:LYS:NZ	2.19	0.40
1:C:20:HIS:CE1	1:C:31:ASP:OD2	2.73	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	224/234 (96%)	220 (98%)	4 (2%)	0	100	100
1	B	223/234 (95%)	220 (99%)	3 (1%)	0	100	100
1	C	216/234 (92%)	211 (98%)	5 (2%)	0	100	100
1	D	210/234 (90%)	205 (98%)	5 (2%)	0	100	100
All	All	873/936 (93%)	856 (98%)	17 (2%)	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	193/200 (96%)	191 (99%)	2 (1%)	76 56
1	B	191/200 (96%)	189 (99%)	2 (1%)	76 56
1	C	183/200 (92%)	179 (98%)	4 (2%)	52 21
1	D	177/200 (88%)	173 (98%)	4 (2%)	50 20
All	All	744/800 (93%)	732 (98%)	12 (2%)	62 35

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	ASP
1	A	235	TYR
1	B	228	VAL
1	B	235	TYR
1	C	79	ASP
1	C	158	ASP
1	C	175	GLU
1	C	235	TYR
1	D	79	ASP
1	D	119	SER
1	D	175	GLU
1	D	191	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	41	ASN
1	A	48	ASN
1	A	120	HIS
1	A	198	ASN
1	A	211	HIS
1	A	217	ASN

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Mol	Chain	Res	Type
1	B	20	HIS
1	B	41	ASN
1	B	48	ASN
1	B	120	HIS
1	B	198	ASN
1	B	217	ASN
1	C	20	HIS
1	C	120	HIS
1	C	198	ASN
1	C	217	ASN
1	D	20	HIS
1	D	48	ASN
1	D	95	GLN
1	D	120	HIS
1	D	173	ASN
1	D	217	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	IO8	A	69	1	22,23,24	1.86	4 (18%)	27,32,34	4.13	14 (51%)
1	IO8	C	69	1	22,23,24	1.80	3 (13%)	27,32,34	3.03	9 (33%)
1	IO8	D	69	1	22,23,24	1.62	2 (9%)	27,32,34	3.06	9 (33%)
1	IO8	B	69	1	22,23,24	1.74	3 (13%)	27,32,34	4.36	14 (51%)

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	IO8	A	69	1	-	1/4/25/26	0/3/3/3
1	IO8	C	69	1	-	1/4/25/26	0/3/3/3
1	IO8	D	69	1	-	1/4/25/26	0/3/3/3
1	IO8	B	69	1	-	1/4/25/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	IO8	CB-CA2	6.61	1.40	1.35
1	B	69	IO8	CB-CA2	6.32	1.40	1.35
1	C	69	IO8	CB-CA2	-6.25	1.29	1.35
1	D	69	IO8	CB-CA2	-5.10	1.30	1.35
1	C	69	IO8	C2-N3	-3.42	1.31	1.39
1	D	69	IO8	C2-N3	-3.22	1.32	1.39
1	A	69	IO8	CA2-C2	-2.78	1.45	1.48
1	A	69	IO8	C2-N3	-2.69	1.33	1.39
1	B	69	IO8	C2-N3	-2.53	1.33	1.39
1	A	69	IO8	C1-N3	-2.50	1.33	1.37
1	B	69	IO8	C1-N3	-2.24	1.33	1.37
1	C	69	IO8	C1-N3	-2.00	1.34	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	IO8	O2-C2-CA2	-14.34	122.91	130.96
1	A	69	IO8	O2-C2-CA2	-13.79	123.22	130.96
1	B	69	IO8	CA2-C2-N3	11.01	108.58	103.37
1	A	69	IO8	CA2-C2-N3	9.80	108.00	103.37
1	D	69	IO8	O2-C2-CA2	-9.29	125.74	130.96
1	C	69	IO8	O2-C2-CA2	-8.55	126.16	130.96
1	D	69	IO8	CA2-C2-N3	7.95	107.13	103.37
1	C	69	IO8	CA2-C2-N3	7.50	106.92	103.37
1	B	69	IO8	C1-CA1-N1	-6.79	97.84	112.85
1	A	69	IO8	C1-CA1-N1	-6.70	98.04	112.85
1	C	69	IO8	C1-CA1-N1	-5.82	99.99	112.85
1	A	69	IO8	CB-CA2-C2	5.74	129.13	122.28
1	B	69	IO8	C2-CA2-N2	-5.67	104.96	108.93
1	D	69	IO8	C1-CA1-N1	-5.58	100.50	112.85
1	A	69	IO8	C2-CA2-N2	-5.14	105.33	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	69	IO8	C2-CA2-N2	-4.93	105.48	108.93
1	B	69	IO8	CB-CA2-C2	4.85	128.07	122.28
1	D	69	IO8	C2-CA2-N2	-4.75	105.61	108.93
1	B	69	IO8	C2-N3-C1	-4.10	105.98	107.99
1	C	69	IO8	O3-C3-CA3	-3.87	114.69	126.39
1	D	69	IO8	O3-C3-CA3	-3.46	115.96	126.39
1	B	69	IO8	CG-CB-CA2	-3.33	124.34	130.81
1	C	69	IO8	CB-CA2-C2	3.27	126.18	122.28
1	C	69	IO8	CA3-N3-C1	-3.19	123.45	127.86
1	D	69	IO8	CA3-N3-C1	-3.05	123.64	127.86
1	B	69	IO8	CA1-C1-N2	-2.97	120.30	124.28
1	A	69	IO8	CG-CB-CA2	-2.91	125.16	130.81
1	B	69	IO8	N3-C1-N2	2.88	115.21	111.76
1	A	69	IO8	CA1-C1-N2	-2.86	120.44	124.28
1	A	69	IO8	CA3-N3-C1	-2.66	124.19	127.86
1	B	69	IO8	O3-C3-CA3	-2.54	118.71	126.39
1	A	69	IO8	CD1-CG-CB	2.54	138.24	126.29
1	D	69	IO8	CB-CA2-C2	2.50	125.25	122.28
1	B	69	IO8	CD1-CG-CB	2.47	137.93	126.29
1	B	69	IO8	CA3-N3-C2	2.47	129.46	123.80
1	B	69	IO8	CA3-N3-C1	-2.39	124.56	127.86
1	D	69	IO8	N3-C1-N2	2.39	114.62	111.76
1	A	69	IO8	CB-CA2-N2	-2.37	125.54	128.83
1	A	69	IO8	O3-C3-CA3	-2.26	119.57	126.39
1	A	69	IO8	O2-C2-N3	2.23	128.78	124.35
1	A	69	IO8	CA1-C1-N3	2.17	125.43	122.52
1	A	69	IO8	CA3-N3-C2	2.17	128.78	123.80
1	C	69	IO8	N3-C1-N2	2.17	114.36	111.76
1	D	69	IO8	CA3-N3-C2	2.14	128.70	123.80
1	B	69	IO8	O2-C2-N3	2.10	128.51	124.35
1	C	69	IO8	CA3-N3-C2	2.08	128.57	123.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	69	IO8	N2-CA2-CB-CG
1	A	69	IO8	N2-CA2-CB-CG
1	B	69	IO8	N2-CA2-CB-CG
1	C	69	IO8	N2-CA2-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	69	IO8	1	0
1	D	69	IO8	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} 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	227/234 (97%)	-0.52	1 (0%)	92	94	14, 21, 38, 48	0
1	B	226/234 (96%)	-0.51	1 (0%)	92	94	13, 21, 38, 48	0
1	C	220/234 (94%)	0.28	11 (5%)	28	31	20, 39, 58, 78	0
1	D	214/234 (91%)	0.33	10 (4%)	31	34	20, 38, 56, 75	1 (0%)
All	All	887/936 (94%)	-0.12	23 (2%)	56	61	13, 29, 52, 78	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	VAL	6.5
1	D	118	GLY	4.8
1	D	121	ILE	3.9
1	C	188	ALA	3.8
1	C	187	PHE	3.5
1	D	114	TYR	3.4
1	B	118	GLY	3.3
1	C	114	TYR	3.1
1	C	13	LEU	3.0
1	C	186	THR	3.0
1	D	112	TYR	2.8
1	A	118	GLY	2.6
1	D	185	TYR	2.5
1	C	118	GLY	2.4
1	C	115	THR	2.4
1	C	116	TYR	2.3
1	C	112	TYR	2.3
1	D	188	ALA	2.2
1	C	234	LEU	2.2
1	D	116	TYR	2.2
1	D	189	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	VAL	2.1
1	D	94	TYR	2.1

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, 95^{th} 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	IO8	C	69	21/22	0.91	0.11	27,36,39,40	0
1	IO8	D	69	21/22	0.91	0.08	28,36,38,39	0
1	IO8	A	69	21/22	0.98	0.06	13,15,21,21	0
1	IO8	B	69	21/22	0.98	0.07	13,15,19,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.