



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:04 AM UTC

PDB ID : 7SF9 / pdb_00007sf9
Title : Branchiostoma Floridae Violet Fluorescent Protein
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Deposited on : 2021-10-03
Resolution : 1.80 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

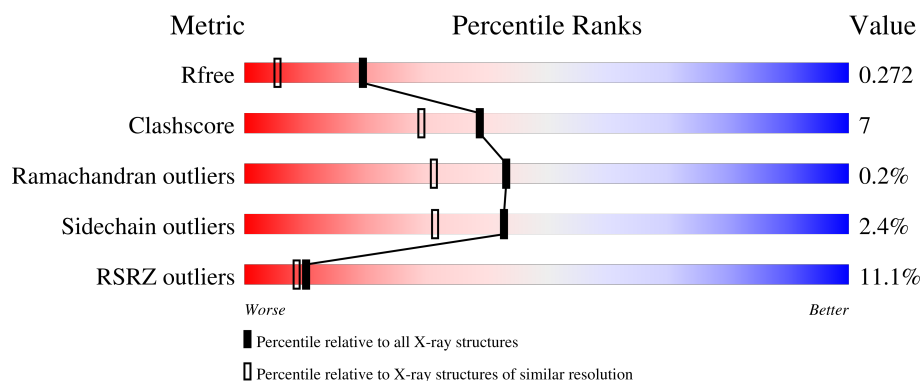
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	238	5% 83% 12% • •
1	B	238	5% 79% 11% • 8%
1	C	238	11% 74% 16% • 8%
1	D	238	21% 74% 15% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7559 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 Violet Fluorescent Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	6	0
			1857	1183	310	353	11			
1	B	218	Total	C	N	O	S	0	5	0
			1784	1142	300	332	10			
1	C	218	Total	C	N	O	S	0	3	0
			1765	1130	295	330	10			
1	D	219	Total	C	N	O	S	0	1	0
			1750	1122	290	328	10			

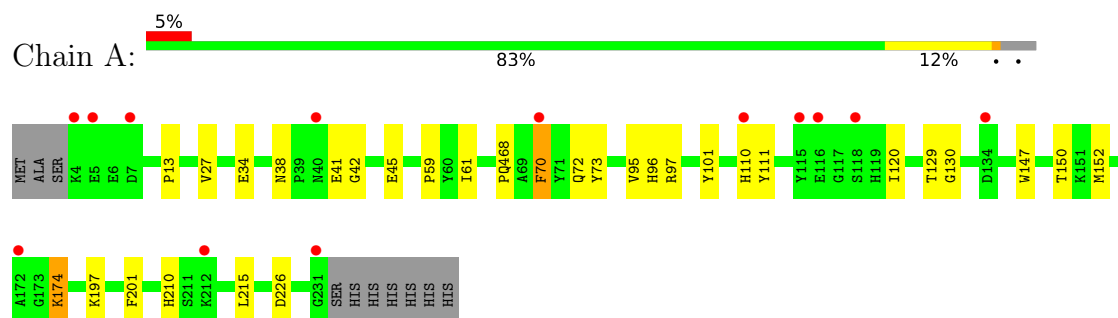
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	137	Total	O	0	0
			137	137		
2	C	93	Total	O	0	0
			93	93		
2	D	65	Total	O	0	0
			65	65		

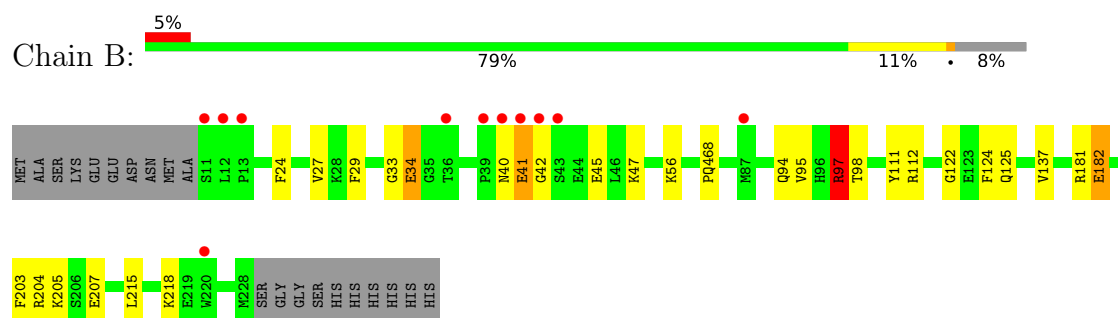
3 Residue-property plots [i](#)

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.

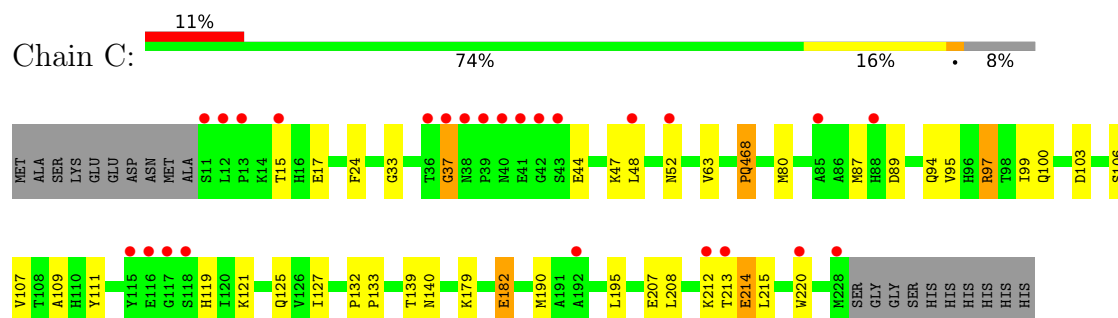
• Molecule 1: Violet Fluorescent Protein



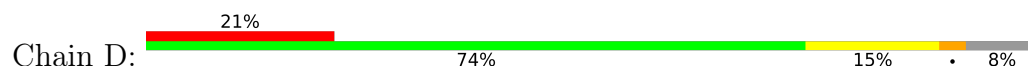
• Molecule 1: Violet Fluorescent Protein

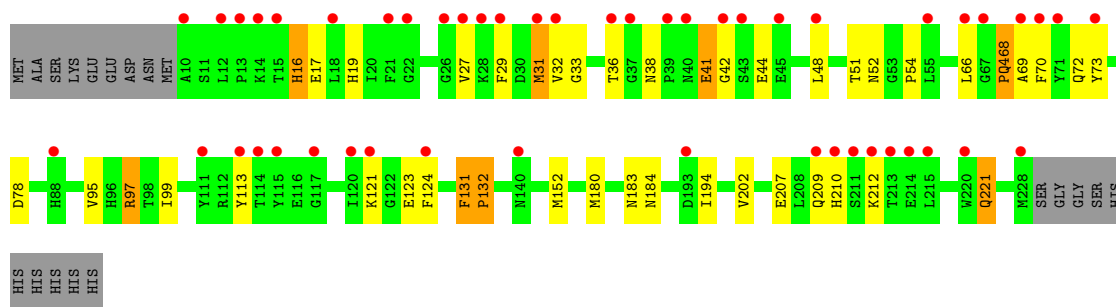


• Molecule 1: Violet Fluorescent Protein



• Molecule 1: Violet Fluorescent Protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	177.67Å 177.67Å 52.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.87 – 1.80 153.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (153.87-1.80) 95.7 (153.87-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.209 , 0.263 0.219 , 0.272	Depositor DCC
R_{free} test set	1647 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7559	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQ4

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	1.25	3/1895 (0.2%)	1.12	3/2557 (0.1%)
1	B	1.35	8/1822 (0.4%)	1.16	2/2461 (0.1%)
1	C	1.34	11/1803 (0.6%)	1.17	3/2436 (0.1%)
1	D	1.14	2/1788 (0.1%)	1.18	8/2417 (0.3%)
All	All	1.27	24/7308 (0.3%)	1.16	16/9871 (0.2%)

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	B	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	VAL	C-O	-7.48	1.16	1.24
1	B	122	GLY	CA-C	-7.22	1.47	1.52
1	B	207	GLU	CA-C	-6.91	1.44	1.52
1	C	94	GLN	C-O	-6.39	1.15	1.23
1	C	63	VAL	CA-CB	6.38	1.58	1.53
1	D	132	PRO	CA-C	6.31	1.58	1.52
1	B	137	VAL	C-O	-6.00	1.17	1.24
1	C	24	PHE	C-O	-5.92	1.17	1.24
1	C	179	LYS	N-CA	5.82	1.53	1.46
1	C	127	ILE	C-O	-5.82	1.17	1.24
1	C	15	THR	CA-C	5.79	1.59	1.52
1	B	34	GLU	C-O	-5.74	1.17	1.23
1	A	45	GLU	CA-C	-5.60	1.45	1.52
1	B	24	PHE	C-O	-5.58	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	ARG	C-O	-5.57	1.17	1.24
1	C	139	THR	N-CA	5.41	1.52	1.46
1	C	99	ILE	C-O	-5.35	1.18	1.24
1	B	29	PHE	CA-C	-5.32	1.46	1.52
1	D	183	ASN	C-O	-5.25	1.18	1.24
1	A	152	MET	C-O	-5.22	1.17	1.24
1	B	203	PHE	C-O	-5.21	1.17	1.24
1	A	147	TRP	C-O	-5.16	1.17	1.23
1	C	103	ASP	C-O	-5.13	1.17	1.24
1	C	208	LEU	C-O	-5.09	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	131	PHE	CA-C-N	-7.01	113.16	120.38
1	D	131	PHE	C-N-CA	-7.01	113.16	120.38
1	D	66	LEU	N-CA-C	-6.85	103.95	112.72
1	D	210	HIS	N-CA-C	6.49	118.80	109.14
1	D	97	ARG	CB-CG-CD	-6.43	96.51	111.30
1	C	37	GLY	N-CA-C	5.97	119.50	110.18
1	B	40	ASN	N-CA-C	5.86	118.38	110.88
1	C	87	MET	N-CA-C	-5.44	105.00	111.69
1	B	41	GLU	N-CA-C	5.40	122.31	110.80
1	A	130	GLY	N-CA-C	5.37	123.17	114.90
1	D	27	VAL	N-CA-C	5.22	116.21	108.23
1	D	16	HIS	O-C-N	5.16	129.13	123.25
1	A	70	PHE	CA-CB-CG	-5.06	108.74	113.80
1	C	52	ASN	CB-CA-C	-5.05	108.08	114.40
1	D	70	PHE	N-CA-C	5.05	115.67	108.54
1	A	27	VAL	N-CA-C	5.03	115.33	107.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	LEU	Mainchain
1	B	97	ARG	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1857	0	1777	16	0
1	B	1784	0	1718	16	0
1	C	1765	0	1693	26	0
1	D	1750	0	1679	40	0
2	A	108	0	0	1	0
2	B	137	0	0	0	0
2	C	93	0	0	5	0
2	D	65	0	0	1	0
All	All	7559	0	6867	96	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 7.

All (96) 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:31:MET:HE3	1:D:48:LEU:HD11	1.27	1.12
1:D:31:MET:HE3	1:D:48:LEU:CD1	1.91	0.99
1:D:69:ALA:CB	1:D:124:PHE:HE2	1.79	0.95
1:D:31:MET:CE	1:D:48:LEU:HD11	2.01	0.91
1:B:125:GLN:HE22	1:C:125:GLN:HE22	1.22	0.88
1:D:17:GLU:HG2	1:D:121:LYS:HG2	1.57	0.85
1:D:69:ALA:CB	1:D:124:PHE:CE2	2.60	0.84
1:A:72:GLN:HE21	1:A:120:ILE:HD13	1.41	0.84
1:D:69:ALA:HB1	1:D:124:PHE:CE2	2.15	0.82
1:C:33:GLY:HA3	1:C:48:LEU:HD23	1.61	0.79
1:C:37:GLY:HA3	1:C:44:GLU:OE1	1.85	0.77
1:D:69:ALA:HB2	1:D:124:PHE:HE2	1.48	0.77
1:D:17:GLU:CG	1:D:121:LYS:HG2	2.16	0.75
1:C:37:GLY:CA	1:C:44:GLU:OE1	2.35	0.75
1:B:98[A]:THR:HG21	2:C:303:HOH:O	1.90	0.72
1:A:174:LYS:HE2	2:A:302:HOH:O	1.91	0.70
1:B:94:GLN:HG2	1:B:112[A]:ARG:HE	1.57	0.70
1:D:33:GLY:HA3	1:D:48:LEU:HB3	1.76	0.67
1:B:98[B]:THR:HG21	2:C:305:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:NE2	1:A:120:ILE:HD13	2.09	0.67
1:B:27:VAL:HG11	1:B:56:LYS:HE3	1.75	0.66
1:C:33:GLY:CA	1:C:48:LEU:HD23	2.28	0.63
1:D:17:GLU:CD	1:D:121:LYS:HG2	2.23	0.62
1:D:32:VAL:O	1:D:48:LEU:HB2	2.01	0.61
1:D:68:PQ4:CB	1:D:97:ARG:HH12	2.14	0.59
1:C:97:ARG:CB	1:C:182:GLU:HB2	2.34	0.57
1:C:207:GLU:HG3	1:C:220:TRP:HZ3	1.67	0.57
1:C:100[A]:GLN:HE22	1:C:106:SER:HB2	1.69	0.57
1:D:16:HIS:CE1	1:D:36:THR:N	2.73	0.56
1:D:19:HIS:ND1	1:D:123:GLU:OE1	2.38	0.56
1:C:37:GLY:HA2	1:C:44:GLU:OE1	2.06	0.55
1:C:97:ARG:HB3	1:C:182:GLU:HB2	1.88	0.55
1:D:152:MET:HE2	1:D:202:VAL:HG23	1.88	0.55
1:D:69:ALA:HB1	1:D:124:PHE:CZ	2.42	0.55
1:B:181[B]:ARG:HH11	1:B:181[B]:ARG:HG2	1.72	0.54
1:A:34:GLU:OE1	1:A:34:GLU:N	2.41	0.54
1:C:207:GLU:HG3	1:C:220:TRP:CZ3	2.41	0.54
1:D:31:MET:HA	1:D:51:THR:HG23	1.90	0.53
1:D:38:ASN:ND2	1:D:41:GLU:OE2	2.41	0.53
1:B:181[B]:ARG:HG2	1:B:181[B]:ARG:NH1	2.24	0.53
1:A:95:VAL:HB	1:A:111:TYR:HB3	1.91	0.52
1:A:96:HIS:CE1	1:A:110:HIS:CD2	2.98	0.52
1:C:17:GLU:OE2	1:C:119:HIS:NE2	2.30	0.51
1:D:31:MET:HB2	1:D:48:LEU:HD13	1.91	0.51
1:B:97:ARG:HB3	1:B:182:GLU:HB2	1.93	0.51
1:D:17:GLU:CD	1:D:121:LYS:HE2	2.36	0.51
1:D:16:HIS:HE1	1:D:36:THR:N	2.09	0.50
1:B:98[B]:THR:HG23	1:B:98[B]:THR:O	2.11	0.50
1:D:17:GLU:OE2	1:D:121:LYS:HE2	2.11	0.50
1:D:42:GLY:O	1:D:221:GLN:HG3	2.12	0.50
1:B:45:GLU:HG2	1:B:218:LYS:HG2	1.93	0.50
1:C:33:GLY:HA3	1:C:47:LYS:O	2.12	0.50
1:C:95:VAL:HB	1:C:111:TYR:HB3	1.94	0.49
1:A:70:PHE:HB3	1:A:73:TYR:HD2	1.78	0.49
1:D:68:PQ4:CG	1:D:97:ARG:HH12	2.25	0.49
1:C:190:MET:HE3	1:C:195:LEU:HD21	1.95	0.49
1:D:29:PHE:HA	1:D:52:ASN:HD21	1.77	0.48
1:D:31:MET:CE	1:D:48:LEU:CD1	2.76	0.48
1:D:31:MET:HG3	1:D:48:LEU:HD13	1.96	0.48
1:B:27:VAL:HG11	1:B:56:LYS:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.30	0.47
1:C:100[A]:GLN:NE2	2:C:303:HOH:O	2.47	0.47
1:A:61:ILE:HD11	1:A:101:TYR:CZ	2.50	0.47
1:A:150:THR:O	1:A:201:PHE:HA	2.16	0.46
1:D:54:PRO:HB3	1:D:212:LYS:HG3	1.98	0.46
1:D:123:GLU:C	1:D:124:PHE:HD1	2.24	0.46
1:B:47:LYS:O	1:B:47:LYS:HG3	2.14	0.46
1:D:78:ASP:HB2	2:D:315:HOH:O	2.16	0.46
1:B:95:VAL:HB	1:B:111:TYR:HB3	1.97	0.46
1:B:33:GLY:HA3	1:B:47:LYS:O	2.14	0.45
1:A:215:LEU:C	1:A:215:LEU:HD12	2.41	0.45
1:A:13:PRO:CG	1:A:120:ILE:HD11	2.47	0.44
1:D:95:VAL:HG22	1:D:184:ASN:OD1	2.17	0.44
1:C:48:LEU:HB2	1:C:215:LEU:HG	1.99	0.44
1:D:42:GLY:HA2	1:D:73:TYR:O	2.17	0.44
1:D:207:GLU:HG2	1:D:209:GLN:HE22	1.83	0.43
1:C:100[A]:GLN:NE2	2:C:305:HOH:O	2.50	0.43
1:C:33:GLY:N	1:C:48:LEU:HD23	2.33	0.43
1:A:42:GLY:HA2	1:A:73:TYR:O	2.19	0.43
1:B:94:GLN:HG2	1:B:112[A]:ARG:NE	2.30	0.43
1:D:99:ILE:HG12	1:D:180:MET:HG3	2.01	0.42
1:C:89:ASP:C	1:C:89:ASP:OD1	2.62	0.42
1:C:132:PRO:HA	1:C:133:PRO:HD3	1.91	0.42
1:C:212:LYS:HA	2:C:311:HOH:O	2.20	0.42
1:D:31:MET:CG	1:D:48:LEU:HD13	2.50	0.42
1:C:17:GLU:CG	1:C:121:LYS:HG2	2.49	0.42
1:D:72:GLN:OE1	1:D:72:GLN:N	2.46	0.42
1:D:16:HIS:HE1	1:D:36:THR:C	2.27	0.42
1:A:226:ASP:OD2	1:B:205:LYS:NZ	2.47	0.41
1:C:68:PQ4:CG	1:C:97:ARG:HH12	2.32	0.41
1:C:213:THR:O	1:C:214:GLU:HB3	2.20	0.41
1:C:109:ALA:HA	1:C:125:GLN:O	2.19	0.41
1:A:13:PRO:HG2	1:A:120:ILE:HD11	2.02	0.41
1:D:131:PHE:O	1:D:132:PRO:C	2.60	0.40
1:A:59:PRO:HG2	1:A:210:HIS:CD2	2.57	0.40
1:D:69:ALA:O	1:D:113:TYR:OH	2.37	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	231/238 (97%)	226 (98%)	5 (2%)	0	100	100
1	B	220/238 (92%)	217 (99%)	2 (1%)	1 (0%)	24	14
1	C	218/238 (92%)	213 (98%)	4 (2%)	1 (0%)	24	14
1	D	217/238 (91%)	215 (99%)	2 (1%)	0	100	100
All	All	886/952 (93%)	871 (98%)	13 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	GLY
1	C	214	GLU

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	200/203 (98%)	196 (98%)	4 (2%)	48	38
1	B	192/203 (95%)	187 (97%)	5 (3%)	40	28
1	C	190/203 (94%)	186 (98%)	4 (2%)	47	36
1	D	188/203 (93%)	183 (97%)	5 (3%)	39	27
All	All	770/812 (95%)	752 (98%)	18 (2%)	43	33

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	129	THR
1	A	174	LYS
1	A	197	LYS
1	B	34	GLU
1	B	41	GLU
1	B	97	ARG
1	B	124	PHE
1	B	182	GLU
1	C	80	MET
1	C	97	ARG
1	C	140	ASN
1	C	182	GLU
1	D	31	MET
1	D	41	GLU
1	D	44	GLU
1	D	194	ILE
1	D	221	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	96	HIS
1	A	110	HIS
1	B	88	HIS
1	B	94	GLN
1	B	100	GLN
1	B	110	HIS
1	B	210	HIS
1	C	38	ASN
1	C	40	ASN
1	C	125	GLN
1	C	140	ASN
1	D	52	ASN
1	D	88	HIS
1	D	110	HIS
1	D	140	ASN
1	D	209	GLN

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	PQ4	B	68	1	11,12,13	1.05	0	13,15,17	1.72	3 (23%)
1	PQ4	D	68	1	11,12,13	1.39	1 (9%)	13,15,17	1.85	4 (30%)
1	PQ4	A	68	1	11,12,13	1.88	4 (36%)	13,15,17	1.15	0
1	PQ4	C	68	1	11,12,13	1.04	1 (9%)	13,15,17	1.34	2 (15%)

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	PQ4	B	68	1	-	0/4/6/8	0/1/1/1
1	PQ4	D	68	1	-	1/4/6/8	0/1/1/1
1	PQ4	A	68	1	-	1/4/6/8	0/1/1/1
1	PQ4	C	68	1	-	1/4/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PQ4	CE1-CD1	3.27	1.44	1.38
1	A	68	PQ4	C-CA	2.98	1.50	1.45
1	A	68	PQ4	CD2-CG	2.48	1.44	1.39
1	D	68	PQ4	OH-CZ	-2.46	1.31	1.37
1	C	68	PQ4	C-CA	2.32	1.49	1.45
1	A	68	PQ4	CG-CB	2.27	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	PQ4	CD1-CE1-CZ	3.74	123.84	119.88
1	D	68	PQ4	CB-CA-N	3.39	129.40	123.25
1	D	68	PQ4	CD2-CE2-CZ	-3.36	116.33	119.88
1	C	68	PQ4	O-C-CA	-3.12	121.48	125.39
1	D	68	PQ4	CE1-CD1-CG	-2.88	117.50	121.22
1	D	68	PQ4	CD2-CG-CD1	2.47	121.32	117.65
1	B	68	PQ4	CE2-CD2-CG	2.31	124.20	121.22
1	B	68	PQ4	CD1-CG-CB	2.18	128.70	121.22
1	C	68	PQ4	CE1-CD1-CG	-2.15	118.45	121.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	PQ4	O-C-CA-CB
1	C	68	PQ4	O-C-CA-CB
1	D	68	PQ4	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	68	PQ4	2	0
1	C	68	PQ4	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/238 (95%)	0.28	13 (5%) 29 28	8, 23, 43, 63	6 (2%)
1	B	217/238 (91%)	0.12	11 (5%) 33 32	6, 17, 42, 79	5 (2%)
1	C	217/238 (91%)	0.73	25 (11%) 9 8	7, 25, 62, 95	3 (1%)
1	D	218/238 (91%)	1.19	49 (22%) 2 2	11, 32, 60, 111	1 (0%)
All	All	879/952 (92%)	0.58	98 (11%) 10 8	6, 24, 54, 111	15 (1%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	PRO	9.3
1	D	27	VAL	7.5
1	D	210	HIS	6.5
1	C	40	ASN	6.2
1	C	36	THR	5.6
1	C	37	GLY	5.6
1	C	42	GLY	5.4
1	D	213	THR	5.3
1	D	124	PHE	5.1
1	D	115	TYR	5.0
1	D	212	LYS	5.0
1	B	12	LEU	5.0
1	D	215	LEU	4.8
1	D	211	SER	4.4
1	B	40	ASN	4.4
1	C	220	TRP	4.3
1	D	48	LEU	4.2
1	D	36	THR	4.2
1	D	13	PRO	4.2
1	C	212	LYS	4.1
1	D	69	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	70	PHE	4.0
1	B	42	GLY	4.0
1	C	41	GLU	4.0
1	B	41	GLU	4.0
1	C	213	THR	3.9
1	C	43	SER	3.8
1	B	11	SER	3.8
1	D	214	GLU	3.6
1	D	113	TYR	3.6
1	B	39	PRO	3.6
1	D	42	GLY	3.5
1	C	38	ASN	3.5
1	C	228	MET	3.5
1	A	4	LYS	3.5
1	C	11	SER	3.4
1	D	12	LEU	3.4
1	C	115	TYR	3.3
1	C	12	LEU	3.3
1	D	21	PHE	3.2
1	C	52	ASN	3.1
1	D	22	GLY	3.1
1	A	212	LYS	3.1
1	D	43	SER	3.1
1	D	55	LEU	3.0
1	D	117	GLY	3.0
1	D	37	GLY	3.0
1	D	67	GLY	3.0
1	D	209	GLN	3.0
1	D	228	MET	2.9
1	D	45	GLU	2.9
1	D	220	TRP	2.9
1	D	40	ASN	2.9
1	A	110	HIS	2.9
1	D	31	MET	2.9
1	A	134	ASP	2.8
1	D	29	PHE	2.7
1	C	15	THR	2.7
1	C	88	HIS	2.7
1	D	14	LYS	2.7
1	C	192	ALA	2.7
1	A	7	ASP	2.7
1	D	28	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	13	PRO	2.6
1	C	116	GLU	2.5
1	D	10	ALA	2.5
1	D	39	PRO	2.5
1	D	111	TYR	2.5
1	D	32	VAL	2.5
1	D	193	ASP	2.5
1	D	15	THR	2.5
1	D	121	LYS	2.5
1	B	220	TRP	2.4
1	A	116	GLU	2.4
1	B	43	SER	2.4
1	D	71	TYR	2.4
1	C	117	GLY	2.4
1	D	26	GLY	2.4
1	A	118	SER	2.3
1	D	18	LEU	2.3
1	D	66	LEU	2.3
1	A	172	ALA	2.3
1	A	231	GLY	2.3
1	B	36	THR	2.3
1	D	114	THR	2.2
1	C	13	PRO	2.2
1	D	120	ILE	2.2
1	D	140	ASN	2.1
1	A	5	GLU	2.1
1	A	70	PHE	2.1
1	D	73	TYR	2.1
1	D	88	HIS	2.1
1	A	40	ASN	2.1
1	C	48	LEU	2.1
1	A	115	TYR	2.0
1	B	87	MET	2.0
1	C	85	ALA	2.0
1	C	118	SER	2.0

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

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
1	PQ4	D	68	12/13	0.79	0.16	28,34,45,55	0
1	PQ4	A	68	12/13	0.95	0.06	11,14,18,19	0
1	PQ4	C	68	12/13	0.96	0.05	16,20,21,24	0
1	PQ4	B	68	12/13	0.97	0.05	7,10,13,14	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.