



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:28 PM UTC

PDB ID : 7DMX / pdb_00007dmx
Title : Photocleavable Fluorescent Protein in green form
Authors : Wen, Y.; Lemieux, M.J.
Deposited on : 2020-12-08
Resolution : 2.10 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

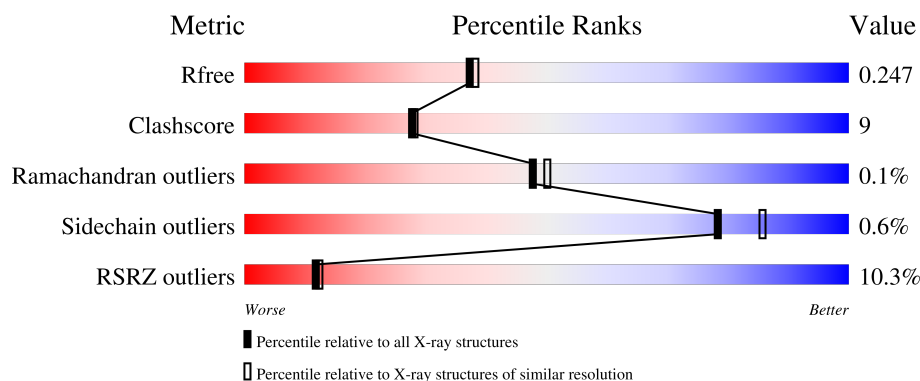
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	240	5% 72% 16% 12%
1	B	240	12% 70% 17% 12%
1	C	240	11% 70% 15% 13%
1	D	240	8% 79% 10% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7204 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 PhoCl green.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	4	3	0
			1705	1089	288	319	9			
1	B	210	Total	C	N	O	S	4	1	0
			1665	1066	276	314	9			
1	C	208	Total	C	N	O	S	4	2	0
			1680	1079	285	307	9			
1	D	216	Total	C	N	O	S	6	3	0
			1735	1111	295	320	9			

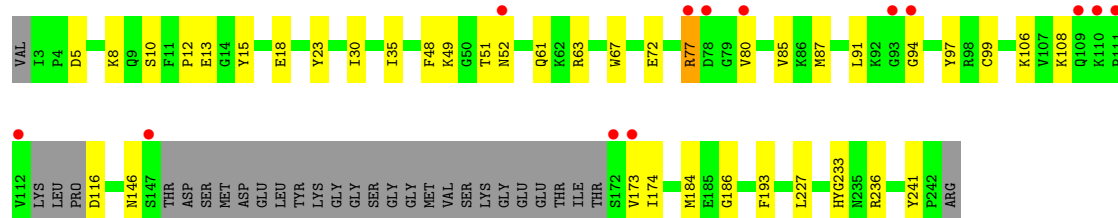
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	127	Total	O	0	0
			127	127		
2	B	103	Total	O	0	0
			103	103		
2	C	92	Total	O	0	0
			92	92		
2	D	97	Total	O	0	0
			97	97		

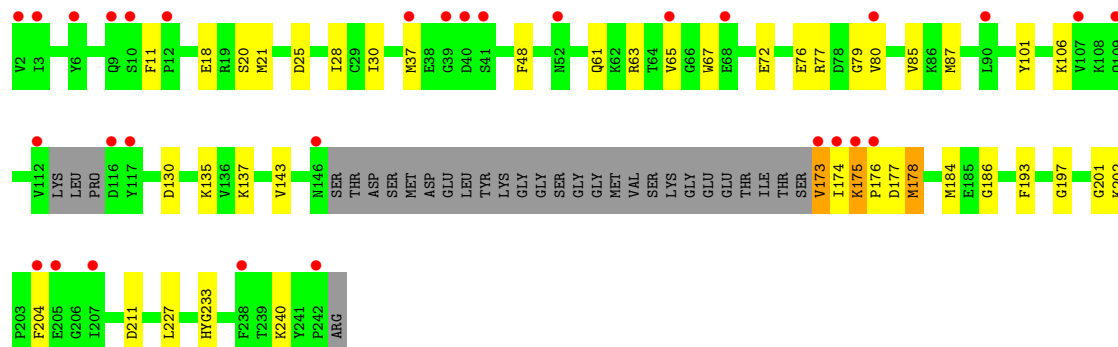
3 Residue-property plots [i](#)

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.

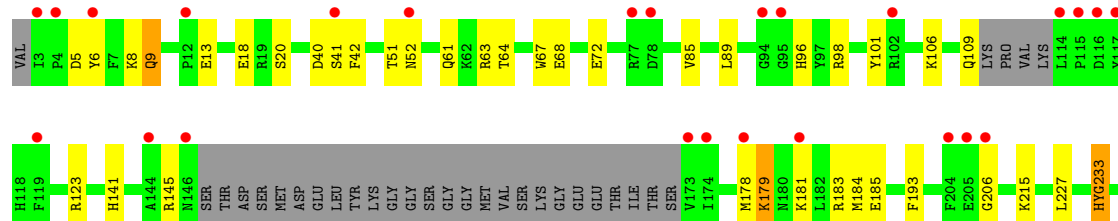
- Molecule 1: PhoCl green



- Molecule 1: PhoCl green

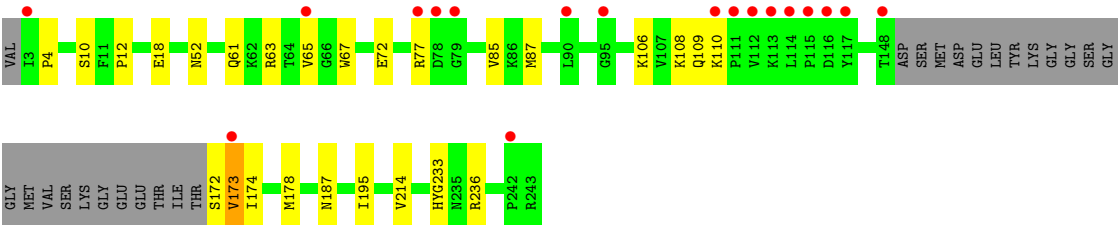
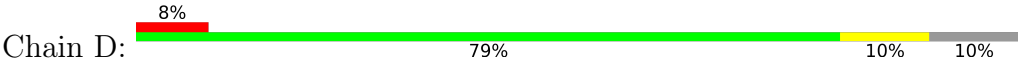


- Molecule 1: PhoCl green





● Molecule 1: PhoCl green



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.36Å 112.76Å 144.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 2.10 44.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	73.7 (44.39-2.10) 73.7 (44.39-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.44 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.205 , 0.249 0.205 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: CR8

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	0.43	0/1724	0.68	2/2325 (0.1%)
1	B	0.52	1/1681 (0.1%)	0.74	2/2274 (0.1%)
1	C	0.43	0/1696	0.69	2/2285 (0.1%)
1	D	0.49	2/1756 (0.1%)	0.68	3/2369 (0.1%)
All	All	0.47	3/6857 (0.0%)	0.70	9/9253 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	173	VAL	N-CA	-5.66	1.39	1.46
1	D	4	PRO	C-O	-5.55	1.17	1.23
1	B	175	LYS	C-O	-5.42	1.16	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	CB-CG-CD	-6.70	95.88	111.30
1	C	179	LYS	CB-CG-CD	6.19	125.54	111.30
1	C	9	GLN	CA-CB-CG	5.90	125.90	114.10
1	B	177	ASP	N-CA-C	-5.87	100.34	109.72
1	A	77	ARG	CA-CB-CG	5.69	125.49	114.10
1	D	173	VAL	CA-C-N	-5.56	115.89	123.12
1	D	173	VAL	C-N-CA	-5.56	115.89	123.12
1	D	65	VAL	CG1-CB-CG2	5.30	122.46	110.80
1	B	176	PRO	CA-N-CD	-5.06	104.92	112.00

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	1705	0	1606	34	0
1	B	1665	0	1531	37	0
1	C	1680	0	1591	34	0
1	D	1735	0	1642	16	0
2	A	127	0	0	12	0
2	B	103	0	0	4	1
2	C	92	0	0	7	1
2	D	97	0	0	8	0
All	All	7204	0	6370	118	1

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 (118) 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:175:LYS:N	1:B:178:MET:HE1	1.58	1.16
1:B:175:LYS:H	1:B:178:MET:HE1	1.01	1.12
1:C:109:GLN:NE2	2:C:301:HOH:O	1.83	1.08
1:B:175:LYS:CB	1:B:178:MET:HE2	1.90	1.00
1:C:40:ASP:O	1:C:178:MET:HE3	1.66	0.95
1:B:175:LYS:H	1:B:178:MET:CE	1.79	0.95
1:C:40:ASP:C	1:C:178:MET:HE1	1.91	0.94
1:A:184:MET:HE3	1:A:193:PHE:HE1	1.35	0.90
1:B:175:LYS:N	1:B:178:MET:CE	2.36	0.89
1:A:13:GLU:OE2	1:A:108:LYS:NZ	2.05	0.88
1:A:116:ASP:N	2:A:302:HOH:O	2.08	0.86
1:C:40:ASP:O	1:C:178:MET:CE	2.23	0.86
1:B:25:ASP:O	2:B:301:HOH:O	1.94	0.84
1:C:40:ASP:C	1:C:178:MET:CE	2.51	0.83
1:B:61:GLN:OE1	1:B:63:ARG:NH1	2.12	0.82
1:C:68:GLU:OE2	1:C:96:HIS:NE2	2.14	0.80
1:D:178:MET:SD	2:D:339:HOH:O	2.38	0.80
1:D:12:PRO:O	2:D:301:HOH:O	2.01	0.79
1:A:184:MET:HE3	1:A:193:PHE:CE1	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:O	2:A:301:HOH:O	2.04	0.73
1:A:13:GLU:CD	1:A:108:LYS:HZ1	1.97	0.72
1:C:184:MET:HE1	1:C:227:LEU:HD22	1.72	0.72
1:C:215:LYS:NZ	2:C:303:HOH:O	2.20	0.72
1:C:9:GLN:HG2	2:C:301:HOH:O	1.89	0.72
1:D:109:GLN:NE2	2:D:304:HOH:O	2.23	0.72
1:A:173:VAL:HG13	1:A:174:ILE:HG13	1.72	0.71
1:C:123:ARG:NH1	2:C:306:HOH:O	2.24	0.71
1:B:175:LYS:CB	1:B:178:MET:CE	2.69	0.71
1:A:5:ASP:OD2	1:A:8:LYS:HD2	1.93	0.69
1:A:30:ILE:HD11	1:B:28:ILE:HG22	1.75	0.68
1:D:61:GLN:OE1	1:D:63:ARG:NH1	2.26	0.68
1:A:49:LYS:HD2	2:A:366:HOH:O	1.94	0.67
1:D:109:GLN:O	2:D:302:HOH:O	2.11	0.67
1:C:41:SER:OG	2:C:302:HOH:O	2.14	0.66
1:A:94:GLY:O	2:A:304:HOH:O	2.14	0.66
1:A:12:PRO:O	2:A:305:HOH:O	2.15	0.65
1:A:80:VAL:HA	2:A:321:HOH:O	1.97	0.65
1:A:146:ASN:ND2	2:A:306:HOH:O	2.18	0.64
1:A:80:VAL:HG23	2:A:321:HOH:O	1.97	0.63
1:B:174:ILE:O	1:B:204:PHE:CE2	2.53	0.62
1:A:10:SER:HA	1:A:108:LYS:HB2	1.82	0.61
1:B:137:LYS:NZ	2:B:302:HOH:O	1.95	0.61
1:B:175:LYS:CA	1:B:178:MET:CE	2.79	0.61
1:B:77:ARG:O	1:B:80:VAL:HG12	2.01	0.60
1:B:173:VAL:HG12	1:B:173:VAL:O	2.00	0.60
1:B:67:TRP:CE3	1:B:87:MET:HE3	2.37	0.59
1:C:41:SER:N	1:C:178:MET:HE1	2.17	0.59
1:B:65:VAL:O	2:B:303:HOH:O	2.16	0.58
1:B:184:MET:CE	1:B:193:PHE:HE1	2.18	0.57
1:C:41:SER:OG	1:C:179:LYS:HB2	2.05	0.57
1:C:184:MET:CE	1:C:193:PHE:HE1	2.17	0.56
1:D:77:ARG:HD2	2:D:314:HOH:O	2.05	0.56
1:B:130:ASP:OD2	1:B:135:LYS:HG2	2.06	0.56
1:A:18:GLU:OE2	1:A:106:LYS:NZ	2.34	0.56
1:D:187:ASN:OD1	2:D:303:HOH:O	2.18	0.55
1:A:77:ARG:O	1:A:80:VAL:HG12	2.07	0.55
1:B:184:MET:HE1	1:B:227:LEU:HD22	1.88	0.54
1:C:61:GLN:OE1	1:C:63:ARG:NH1	2.39	0.54
1:D:174:ILE:HA	2:D:339:HOH:O	2.07	0.54
1:D:18:GLU:OE2	1:D:106:LYS:HE2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:CE	1:A:193:PHE:HE1	2.16	0.53
1:A:63:ARG:NH2	2:A:315:HOH:O	2.41	0.53
1:C:51:THR:OG1	1:C:52:ASN:N	2.42	0.53
1:C:184:MET:HE3	1:C:193:PHE:CE1	2.44	0.52
1:A:72:GLU:HA	1:A:85:VAL:HB	1.92	0.51
1:B:174:ILE:O	1:B:204:PHE:CZ	2.63	0.51
1:A:91:LEU:HD21	1:A:97:TYR:HB2	1.93	0.51
1:C:6:TYR:HE1	1:C:109:GLN:OE1	1.93	0.51
1:C:20:SER:HB3	1:D:52:ASN:ND2	2.26	0.51
1:B:85:VAL:HG13	1:B:101:TYR:HB2	1.93	0.50
1:C:141:HIS:HA	1:C:206:GLY:O	2.11	0.50
1:B:72:GLU:HA	1:B:85:VAL:HB	1.94	0.50
1:C:5:ASP:OD2	1:C:8:LYS:HD2	2.10	0.50
2:A:399:HOH:O	1:B:28:ILE:HD11	2.13	0.49
1:B:174:ILE:O	1:B:204:PHE:HE2	1.93	0.49
1:B:201:GLY:C	1:B:202:LYS:HD3	2.37	0.49
1:D:10:SER:HA	1:D:108:LYS:HB2	1.96	0.48
1:C:85:VAL:HG13	1:C:101:TYR:HB2	1.96	0.48
1:C:72:GLU:HA	1:C:85:VAL:HB	1.96	0.47
1:C:145:ARG:NH2	2:C:309:HOH:O	2.37	0.47
1:C:123:ARG:HG2	2:C:352:HOH:O	2.14	0.47
1:C:233:CR8:N2	1:C:233:CR8:H5	2.30	0.47
1:B:135:LYS:HE2	1:B:135:LYS:HB3	1.64	0.47
1:D:236:ARG:HA	1:D:236:ARG:NE	2.30	0.47
1:B:11:PHE:CD1	1:B:37:MET:HE2	2.50	0.46
1:A:51:THR:HG23	1:A:52:ASN:OD1	2.16	0.46
1:A:184:MET:HE1	1:A:227:LEU:HD13	1.97	0.46
1:C:183:ARG:NH1	1:C:185:GLU:OE2	2.35	0.46
1:B:143:VAL:HG13	1:B:240:LYS:HD3	1.99	0.45
1:B:184:MET:CE	1:B:193:PHE:CE1	3.00	0.45
1:C:18:GLU:OE2	1:C:106:LYS:NZ	2.33	0.45
1:B:197:GLY:HA2	1:B:211:ASP:O	2.17	0.45
1:B:48:PHE:O	1:B:186:GLY:HA2	2.17	0.45
1:C:42:PHE:O	1:C:181:LYS:HB2	2.17	0.44
1:A:15:TYR:CZ	1:A:35:ILE:HD13	2.52	0.44
1:A:236:ARG:NE	1:A:236:ARG:HA	2.33	0.44
1:A:52:ASN:OD1	1:B:20:SER:HB3	2.18	0.44
1:A:67:TRP:CE3	1:A:87:MET:HE3	2.52	0.44
1:C:64:THR:HB	1:C:89:LEU:HG	2.00	0.44
1:C:67:TRP:CD2	1:C:89:LEU:HD13	2.53	0.44
1:A:8:LYS:HG2	1:A:174:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:OE1	1:A:63:ARG:NH1	2.51	0.43
1:D:110:LYS:HA	2:D:302:HOH:O	2.18	0.43
1:B:76:GLU:OE2	1:B:79:GLY:N	2.45	0.43
1:B:80:VAL:HG23	2:B:306:HOH:O	2.17	0.43
1:C:98:ARG:HG2	1:C:98:ARG:HH11	1.85	0.42
1:A:48:PHE:O	1:A:186:GLY:HA2	2.21	0.41
1:A:63:ARG:NH1	2:A:308:HOH:O	2.42	0.41
1:B:18:GLU:OE2	1:B:106:LYS:NZ	2.25	0.41
1:B:21:MET:HG2	1:B:101:TYR:CE2	2.56	0.41
1:C:6:TYR:CE1	1:C:109:GLN:OE1	2.73	0.41
1:A:23:TYR:CD1	1:A:99:CYS:HB2	2.56	0.41
1:A:63:ARG:NH2	2:A:308:HOH:O	2.46	0.41
1:D:72:GLU:HA	1:D:85:VAL:HB	2.02	0.40
1:D:67:TRP:CE3	1:D:87:MET:HE3	2.57	0.40
1:B:30:ILE:HD13	1:B:30:ILE:HG21	1.85	0.40
1:C:41:SER:HG	1:C:179:LYS:HB2	1.86	0.40
1:D:195:ILE:HG12	1:D:214:VAL:HG22	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:HOH:O	2:C:383:HOH:O[3_554]	1.81	0.39

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	203/240 (85%)	198 (98%)	5 (2%)	0	100	100
1	B	201/240 (84%)	196 (98%)	5 (2%)	0	100	100
1	C	199/240 (83%)	194 (98%)	4 (2%)	1 (0%)	24	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
All	All	813/960 (85%)	795 (98%)	17 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	GLU

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	179/207 (86%)	179 (100%)	0	100	100
1	B	169/207 (82%)	167 (99%)	2 (1%)	63	72
1	C	173/207 (84%)	173 (100%)	0	100	100
1	D	180/207 (87%)	178 (99%)	2 (1%)	65	74
All	All	701/828 (85%)	697 (99%)	4 (1%)	78	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	173	VAL
1	B	178	MET
1	D	172	SER
1	D	173	VAL

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	56	ASN
1	A	208	GLN
1	B	96	HIS
1	C	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	52	ASN
1	D	109	GLN
1	D	187	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	CR8	C	233	1	25,27,28	2.43	8 (32%)	24,37,39	1.56	5 (20%)
1	CR8	A	233	1	25,27,28	2.32	7 (28%)	24,37,39	1.55	3 (12%)
1	CR8	B	233	1	25,27,28	2.46	9 (36%)	24,37,39	1.21	1 (4%)
1	CR8	D	233	1	25,27,28	2.42	8 (32%)	24,37,39	1.67	6 (25%)

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	CR8	C	233	1	-	3/12/25/26	0/3/3/3
1	CR8	A	233	1	-	5/12/25/26	0/3/3/3
1	CR8	B	233	1	-	3/12/25/26	0/3/3/3
1	CR8	D	233	1	-	4/12/25/26	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	CR8	C8-CA2	6.40	1.55	1.40
1	C	233	CR8	C8-CA2	6.16	1.54	1.40
1	A	233	CR8	C8-CA2	6.15	1.54	1.40
1	B	233	CR8	C20-C21	5.81	1.58	1.49
1	C	233	CR8	C20-C21	5.70	1.58	1.49
1	D	233	CR8	C8-CA2	5.54	1.53	1.40
1	D	233	CR8	C20-C21	5.29	1.57	1.49
1	A	233	CR8	C20-C21	5.25	1.57	1.49
1	D	233	CR8	C1-N2	4.66	1.39	1.32
1	C	233	CR8	C1-N2	3.99	1.38	1.32
1	D	233	CR8	C21-N22	-3.84	1.31	1.37
1	C	233	CR8	C21-N22	-3.74	1.31	1.37
1	B	233	CR8	C1-N2	3.63	1.37	1.32
1	C	233	CR8	O2-C2	3.62	1.41	1.31
1	A	233	CR8	C21-N22	-3.56	1.31	1.37
1	B	233	CR8	O2-C2	3.54	1.41	1.31
1	B	233	CR8	C21-N22	-3.49	1.31	1.37
1	A	233	CR8	O2-C2	3.39	1.41	1.31
1	D	233	CR8	O2-C2	3.31	1.41	1.31
1	A	233	CR8	C1-N2	3.12	1.36	1.32
1	B	233	CR8	C5-C4	2.89	1.42	1.35
1	A	233	CR8	C12-C11	-2.79	1.39	1.46
1	D	233	CR8	C12-C11	-2.41	1.40	1.46
1	B	233	CR8	C6-C12	2.31	1.40	1.35
1	B	233	CR8	CA2-N2	-2.29	1.33	1.38
1	D	233	CR8	C5-C4	2.22	1.40	1.35
1	A	233	CR8	C5-C4	2.15	1.40	1.35
1	C	233	CR8	C12-C11	-2.12	1.40	1.46
1	C	233	CR8	C8-C7	-2.12	1.33	1.39
1	B	233	CR8	C12-C11	-2.11	1.40	1.46
1	D	233	CR8	C6-C12	2.07	1.40	1.35
1	C	233	CR8	C5-C4	2.07	1.40	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	CR8	N3-C1-N2	-3.64	108.62	111.48
1	B	233	CR8	N3-C1-N2	-3.61	108.64	111.48
1	C	233	CR8	C8-CA2-C2	-3.59	121.99	129.19
1	D	233	CR8	CA2-N2-C1	-3.49	103.07	105.80
1	C	233	CR8	N3-C1-N2	-3.44	108.77	111.48
1	D	233	CR8	C8-CA2-C2	-3.43	122.32	129.19
1	A	233	CR8	C8-CA2-C2	-3.41	122.35	129.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	CR8	C4-C5-C7	-2.78	119.47	122.10
1	D	233	CR8	N3-C1-N2	-2.64	109.40	111.48
1	A	233	CR8	CA2-N2-C1	-2.60	103.77	105.80
1	D	233	CR8	C3-CA3-N3	2.58	118.31	112.43
1	C	233	CR8	C3-CA3-N3	2.32	117.70	112.43
1	C	233	CR8	CA1-C20-C21	-2.08	109.78	113.23
1	D	233	CR8	CA1-C20-C21	-2.04	109.84	113.23
1	C	233	CR8	CA2-N2-C1	-2.00	104.24	105.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	233	CR8	CA1-C20-C21-N22
1	A	233	CR8	CA1-C20-C21-C23
1	B	233	CR8	CA1-C20-C21-N22
1	B	233	CR8	CA1-C20-C21-C23
1	C	233	CR8	CA1-C20-C21-N22
1	C	233	CR8	CA1-C20-C21-C23
1	D	233	CR8	CA1-C20-C21-N22
1	D	233	CR8	CA1-C20-C21-C23
1	A	233	CR8	C21-C20-CA1-N1
1	A	233	CR8	C5-C7-C8-CA2
1	A	233	CR8	C6-C7-C8-CA2
1	B	233	CR8	C5-C7-C8-CA2
1	C	233	CR8	C5-C7-C8-CA2
1	D	233	CR8	C5-C7-C8-CA2
1	D	233	CR8	C6-C7-C8-CA2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	233	CR8	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	210/240 (87%)	0.14	13 (6%) 26 28	13, 25, 54, 82	4 (1%)
1	B	209/240 (87%)	0.70	30 (14%) 6 6	16, 32, 65, 105	3 (1%)
1	C	207/240 (86%)	0.61	26 (12%) 8 8	17, 32, 61, 83	3 (1%)
1	D	215/240 (89%)	0.22	18 (8%) 17 18	11, 28, 59, 84	5 (2%)
All	All	841/960 (87%)	0.41	87 (10%) 12 12	11, 29, 62, 105	15 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ILE	6.1
1	C	114	LEU	5.1
1	A	112	VAL	5.1
1	B	173	VAL	4.9
1	A	78	ASP	4.7
1	B	40	ASP	4.5
1	C	174	ILE	4.1
1	D	114	LEU	3.9
1	C	119	PHE	3.8
1	B	176	PRO	3.7
1	A	173	VAL	3.7
1	D	116	ASP	3.6
1	B	9	GLN	3.6
1	B	2	VAL	3.4
1	B	3	ILE	3.4
1	D	113	LYS	3.3
1	C	206	GLY	3.3
1	C	77	ARG	3.3
1	A	110	LYS	3.3
1	B	68	GLU	3.2
1	B	207	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	242	PRO	3.2
1	B	117	TYR	3.1
1	B	109	GLN	3.1
1	C	116	ASP	3.1
1	A	111	PRO	3.1
1	A	80	VAL	3.1
1	C	117	TYR	3.0
1	B	116	ASP	3.0
1	C	144	ALA	3.0
1	A	93	GLY	3.0
1	C	4	PRO	3.0
1	D	78	ASP	3.0
1	C	78	ASP	3.0
1	C	242	PRO	3.0
1	C	204	PHE	3.0
1	C	173	VAL	2.9
1	A	94	GLY	2.9
1	C	205	GLU	2.9
1	B	112	VAL	2.9
1	C	41	SER	2.9
1	B	107	VAL	2.8
1	D	65	VAL	2.8
1	B	41	SER	2.7
1	B	6	TYR	2.7
1	D	111	PRO	2.7
1	C	178	MET	2.7
1	B	65	VAL	2.7
1	B	205	GLU	2.6
1	D	148	THR	2.6
1	C	115	PRO	2.6
1	A	77	ARG	2.6
1	C	3	ILE	2.5
1	C	6	TYR	2.5
1	B	37	MET	2.5
1	C	94	GLY	2.5
1	A	172	SER	2.5
1	D	115	PRO	2.5
1	A	147	SER	2.5
1	C	12	PRO	2.5
1	A	52	ASN	2.5
1	C	181	LYS	2.4
1	D	110	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	3	ILE	2.4
1	B	175	LYS	2.4
1	B	39	GLY	2.4
1	C	146	ASN	2.4
1	C	52	ASN	2.3
1	B	80	VAL	2.3
1	B	90	LEU	2.3
1	B	10	SER	2.2
1	B	204	PHE	2.2
1	D	77	ARG	2.2
1	B	146	ASN	2.2
1	A	109	GLN	2.2
1	C	102	ARG	2.2
1	D	90	LEU	2.1
1	B	12	PRO	2.1
1	B	238	PHE	2.1
1	D	242	PRO	2.1
1	D	79	GLY	2.1
1	D	173	VAL	2.1
1	D	95	GLY	2.0
1	D	117	TYR	2.0
1	D	112	VAL	2.0
1	B	52	ASN	2.0
1	C	95	GLY	2.0

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($\text{\AA}^2$)	Q<0.9
1	CR8	B	233	25/26	0.92	0.08	20,24,31,35	0
1	CR8	C	233	25/26	0.94	0.07	21,25,30,31	0
1	CR8	D	233	25/26	0.95	0.07	13,17,23,23	0
1	CR8	A	233	25/26	0.97	0.05	11,16,19,21	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.