



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 1W7U / pdb_00001w7u
Title : Photoproduct of the Wild-Type Aequorea victoria Green Fluorescent Protein after structural annealing at 170K
Authors : Van Thor, J.J.; Georgiev, G.Y.; Towrie, M.; Sage, J.T.
Deposited on : 2004-09-09
Resolution : 1.85 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

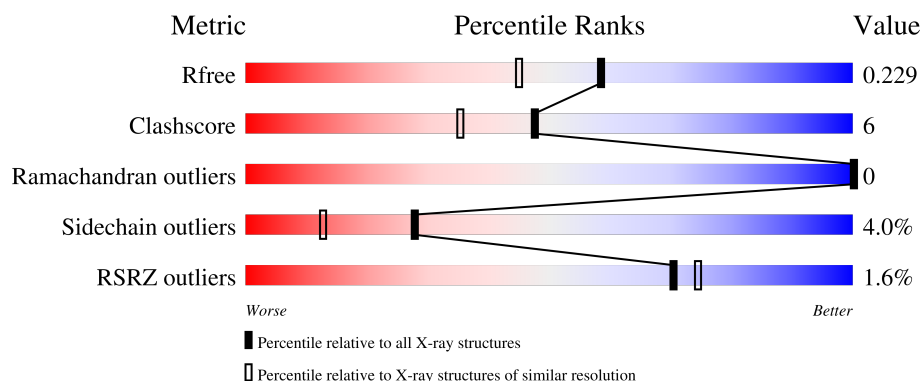
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	236	% 87% 8% . .
1	B	236	2% 85% 10% . .
1	C	236	2% 81% 14% . .
1	D	236	% 83% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8219 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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1827	1163	311	347	6			
1	B	227	Total	C	N	O	S	0	0	0
			1821	1160	310	345	6			
1	C	228	Total	C	N	O	S	0	0	0
			1827	1163	311	347	6			
1	D	228	Total	C	N	O	S	0	0	0
			1827	1163	311	347	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
B	66	GYS	SER	chromophore	UNP P42212
B	66	GYS	TYR	chromophore	UNP P42212
B	66	GYS	GLY	chromophore	UNP P42212
C	66	GYS	SER	chromophore	UNP P42212
C	66	GYS	TYR	chromophore	UNP P42212
C	66	GYS	GLY	chromophore	UNP P42212
D	66	GYS	SER	chromophore	UNP P42212
D	66	GYS	TYR	chromophore	UNP P42212
D	66	GYS	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212

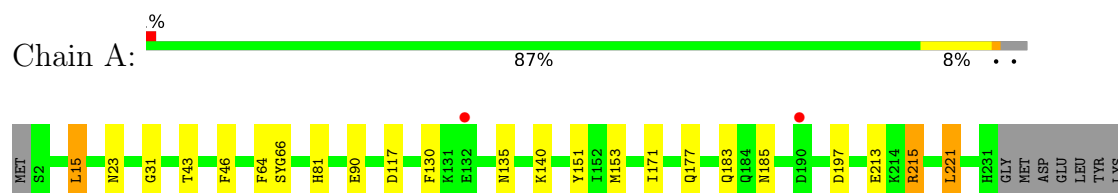
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	253	Total 253	O 253	0	0
2	B	192	Total 192	O 192	0	0
2	C	241	Total 241	O 241	0	0
2	D	231	Total 231	O 231	0	0

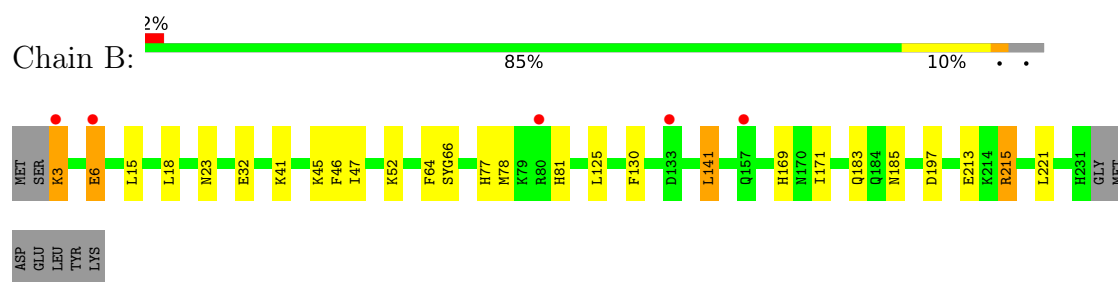
3 Residue-property plots [i](#)

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.

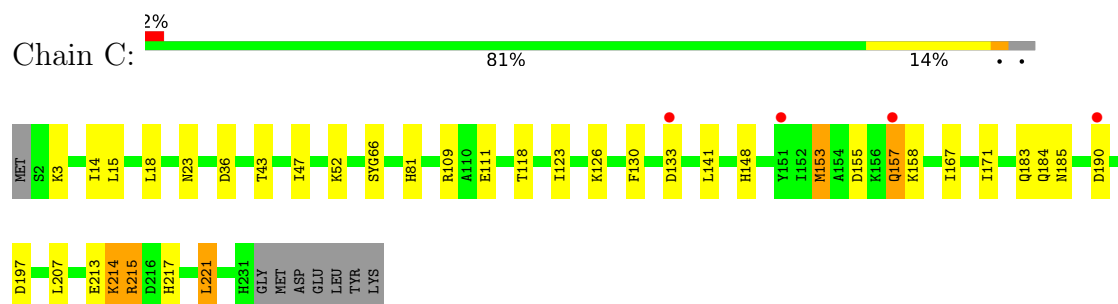
• Molecule 1: GREEN FLUORESCENT PROTEIN



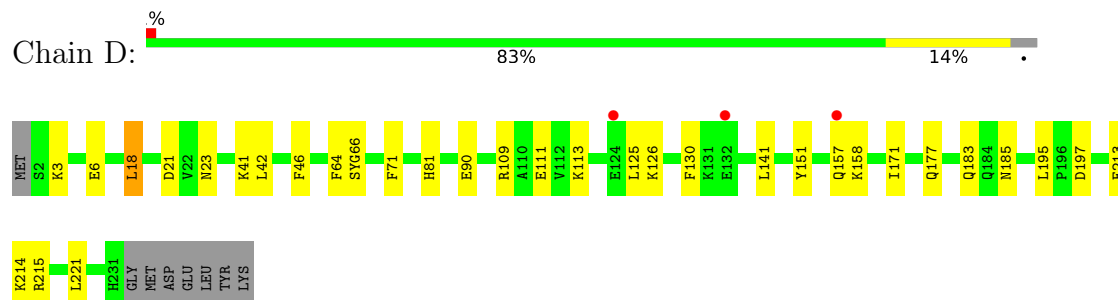
• Molecule 1: GREEN FLUORESCENT PROTEIN



• Molecule 1: GREEN FLUORESCENT PROTEIN



• Molecule 1: GREEN FLUORESCENT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.27Å 52.70Å 141.75Å 90.00° 119.91° 90.00°	Depositor
Resolution (Å)	119.52 – 1.85 119.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (119.52-1.85) 97.4 (119.52-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.226 0.186 , 0.229	Depositor DCC
R_{free} test set	4166 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.8	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	0.95	EDS
Total number of atoms	8219	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: ABA, GYS

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	0.77	0/1841	0.85	0/2485
1	B	0.73	0/1835	0.83	0/2477
1	C	0.76	0/1841	0.86	0/2485
1	D	0.75	0/1841	0.82	0/2485
All	All	0.75	0/7358	0.84	0/9932

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 [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	1827	0	1768	17	0
1	B	1821	0	1763	17	0
1	C	1827	0	1767	26	0
1	D	1827	0	1768	20	0
2	A	253	0	0	6	1
2	B	192	0	0	3	0
2	C	241	0	0	6	0
2	D	231	0	0	4	0
All	All	8219	0	7066	80	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 6.

All (80) 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:C:15:LEU:HD23	1:C:118:THR:HG21	1.45	0.96
1:D:183:GLN:HE21	1:D:185:ASN:HD21	1.16	0.92
1:A:183:GLN:HE21	1:A:185:ASN:HD21	1.17	0.89
1:C:183:GLN:HE21	1:C:185:ASN:HD21	1.16	0.88
1:D:3:LYS:O	1:D:6:GLU:HG3	1.81	0.80
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.27	0.80
1:A:90:GLU:HG2	2:A:2115:HOH:O	1.84	0.77
1:A:213:GLU:OE2	1:A:215:ARG:HD3	1.87	0.75
1:B:41:LYS:NZ	2:B:2039:HOH:O	2.21	0.74
1:C:15:LEU:HD23	1:C:118:THR:CG2	2.18	0.73
1:B:3:LYS:O	1:B:6:GLU:CG	2.37	0.72
1:B:213:GLU:OE2	1:B:215:ARG:HD3	1.90	0.71
1:A:153:MET:SD	2:C:2074:HOH:O	2.49	0.69
1:D:81:HIS:HD2	1:D:197:ASP:H	1.40	0.69
1:A:81:HIS:HD2	1:A:197:ASP:H	1.41	0.68
1:C:157:GLN:NE2	2:C:2172:HOH:O	2.27	0.67
1:C:81:HIS:HD2	1:C:197:ASP:H	1.43	0.67
1:B:3:LYS:O	1:B:6:GLU:HG3	1.96	0.66
1:C:213:GLU:OE2	1:C:215:ARG:HD3	1.95	0.66
1:B:81:HIS:HD2	1:B:197:ASP:H	1.46	0.63
1:B:45:LYS:HE2	1:B:47:ILE:HD11	1.79	0.63
1:B:3:LYS:O	1:B:6:GLU:HG2	1.98	0.62
1:D:151:TYR:CD2	2:D:2155:HOH:O	2.51	0.61
1:C:23:ASN:HD21	1:C:130:PHE:H	1.50	0.60
1:A:23:ASN:HD21	1:A:130:PHE:H	1.49	0.59
1:A:81:HIS:HE1	2:A:2252:HOH:O	1.84	0.59
1:A:117:ASP:HB3	2:A:2064:HOH:O	2.02	0.59
1:D:23:ASN:HD21	1:D:130:PHE:H	1.51	0.58
1:D:213:GLU:OE2	1:D:215:ARG:HD3	2.04	0.57
1:A:15:LEU:HD13	1:A:31:GLY:O	2.05	0.57
1:D:151:TYR:HD2	2:D:2155:HOH:O	1.86	0.57
1:D:81:HIS:HE1	2:D:2230:HOH:O	1.86	0.57
1:C:81:HIS:CD2	1:C:197:ASP:H	2.23	0.56
1:B:141:LEU:HD13	1:B:169:HIS:HB3	1.88	0.55
1:D:90:GLU:HG2	2:D:2018:HOH:O	2.06	0.55
1:A:81:HIS:CD2	1:A:197:ASP:H	2.24	0.53
1:B:81:HIS:CD2	1:B:197:ASP:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:HD22	1:B:171:ILE:CD1	2.39	0.53
1:D:81:HIS:CD2	1:D:197:ASP:H	2.25	0.52
1:B:23:ASN:HD21	1:B:130:PHE:H	1.56	0.52
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.92	0.52
1:C:141:LEU:HD22	1:C:171:ILE:CD1	2.39	0.51
1:C:81:HIS:HE1	2:C:2240:HOH:O	1.92	0.51
1:C:183:GLN:HE21	1:C:185:ASN:ND2	1.97	0.51
1:D:183:GLN:HE21	1:D:185:ASN:ND2	1.98	0.51
1:A:151:TYR:CE2	2:A:2173:HOH:O	2.64	0.50
1:B:46:PHE:CZ	1:B:64:PHE:HB3	2.46	0.50
1:C:47:ILE:HD13	1:C:217:HIS:HB3	1.92	0.50
1:C:155:ASP:OD2	1:C:184:GLN:NE2	2.37	0.50
1:D:18:LEU:C	1:D:18:LEU:HD13	2.37	0.49
1:A:43:THR:HG22	1:A:221:LEU:CD2	2.44	0.48
1:C:141:LEU:HD22	1:C:171:ILE:HD13	1.96	0.47
1:C:141:LEU:CD2	1:C:171:ILE:CD1	2.93	0.47
1:C:109:ARG:NH2	1:C:111:GLU:OE2	2.48	0.47
1:C:47:ILE:HD13	1:C:217:HIS:CB	2.45	0.46
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.51	0.46
1:C:14:ILE:C	1:C:15:LEU:HD22	2.39	0.46
1:B:32:GLU:OE2	2:B:2027:HOH:O	2.21	0.46
1:D:141:LEU:CD2	1:D:171:ILE:CD1	2.94	0.46
1:A:213:GLU:OE2	1:A:215:ARG:CD	2.62	0.46
1:C:43:THR:HG22	1:C:221:LEU:HD22	1.99	0.44
1:A:183:GLN:HE21	1:A:185:ASN:ND2	1.99	0.44
1:D:46:PHE:CZ	1:D:64:PHE:HB3	2.54	0.43
1:B:81:HIS:HE1	2:B:2192:HOH:O	2.01	0.43
1:C:153:MET:HE3	1:C:153:MET:HB3	1.92	0.43
2:A:2225:HOH:O	1:D:41:LYS:HE3	2.18	0.43
1:C:15:LEU:CD2	2:C:2010:HOH:O	2.67	0.43
1:C:214:LYS:HD3	2:C:2225:HOH:O	2.18	0.42
1:D:125:LEU:C	1:D:125:LEU:HD23	2.45	0.42
1:D:109:ARG:NH2	1:D:111:GLU:OE2	2.51	0.42
2:A:2077:HOH:O	1:C:153:MET:CE	2.68	0.42
1:A:135:ASN:HD22	1:A:140:LYS:HD2	1.85	0.42
1:C:36:ASP:OD1	2:C:2039:HOH:O	2.22	0.42
1:D:21:ASP:O	1:D:126:LYS:HD2	2.20	0.42
1:C:14:ILE:O	1:C:15:LEU:HD22	2.20	0.41
1:B:125:LEU:C	1:B:125:LEU:HD23	2.45	0.41
1:C:148:HIS:CD2	1:C:167:ILE:HD13	2.56	0.41
1:B:77:HIS:CD2	1:B:78:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LEU:HD21	1:D:71:PHE:CD2	2.56	0.40
1:A:171:ILE:HD11	1:A:177:GLN:HB2	2.03	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:A:2201:HOH:O	2:A:2201:HOH:O[2_657]	0.68	1.52

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	222/236 (94%)	218 (98%)	4 (2%)	0	100	100
1	B	221/236 (94%)	219 (99%)	2 (1%)	0	100	100
1	C	222/236 (94%)	220 (99%)	2 (1%)	0	100	100
1	D	222/236 (94%)	220 (99%)	2 (1%)	0	100	100
All	All	887/944 (94%)	877 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/205 (97%)	195 (98%)	3 (2%)	57	47
1	B	197/205 (96%)	189 (96%)	8 (4%)	27	12
1	C	198/205 (97%)	184 (93%)	14 (7%)	13	3
1	D	198/205 (97%)	191 (96%)	7 (4%)	32	16
All	All	791/820 (96%)	759 (96%)	32 (4%)	28	13

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	215	ARG
1	A	221	LEU
1	B	3	LYS
1	B	6	GLU
1	B	15	LEU
1	B	18	LEU
1	B	52	LYS
1	B	141	LEU
1	B	215	ARG
1	B	221	LEU
1	C	3	LYS
1	C	18	LEU
1	C	52	LYS
1	C	123	ILE
1	C	126	LYS
1	C	133	ASP
1	C	153	MET
1	C	157	GLN
1	C	158	LYS
1	C	190	ASP
1	C	207	LEU
1	C	214	LYS
1	C	215	ARG
1	C	221	LEU
1	D	18	LEU
1	D	113	LYS
1	D	157	GLN
1	D	158	LYS
1	D	195	LEU
1	D	214	LYS
1	D	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	81	HIS
1	A	105	ASN
1	A	135	ASN
1	A	146	ASN
1	A	149	ASN
1	A	159	ASN
1	A	170	ASN
1	A	177	GLN
1	A	185	ASN
1	A	198	ASN
1	B	23	ASN
1	B	81	HIS
1	B	105	ASN
1	B	121	ASN
1	B	146	ASN
1	B	149	ASN
1	B	170	ASN
1	B	185	ASN
1	B	204	GLN
1	C	23	ASN
1	C	81	HIS
1	C	149	ASN
1	C	185	ASN
1	D	23	ASN
1	D	81	HIS
1	D	146	ASN
1	D	170	ASN
1	D	184	GLN
1	D	185	ASN
1	D	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	ABA	B	222	1	4,5,6	0.69	0	1,5,7	0.05	0
1	GYS	A	66	1	20,22,23	4.00	14 (70%)	25,30,32	4.00	13 (52%)
1	GYS	D	66	1	20,22,23	3.52	11 (55%)	25,30,32	3.64	15 (60%)
1	ABA	C	222	1	4,5,6	0.47	0	1,5,7	0.20	0
1	GYS	C	66	1	20,22,23	5.63	9 (45%)	25,30,32	2.97	8 (32%)
1	ABA	D	222	1	4,5,6	0.60	0	1,5,7	0.25	0
1	GYS	B	66	1	20,22,23	3.01	10 (50%)	25,30,32	3.64	13 (52%)
1	ABA	A	222	1	4,5,6	0.43	0	1,5,7	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ABA	B	222	1	-	1/3/4/6	-
1	GYS	A	66	1	-	1/10/29/30	0/2/2/2
1	GYS	D	66	1	-	1/10/29/30	0/2/2/2
1	ABA	C	222	1	-	0/3/4/6	-
1	GYS	C	66	1	-	1/10/29/30	0/2/2/2
1	ABA	D	222	1	-	0/3/4/6	-
1	GYS	B	66	1	-	1/10/29/30	0/2/2/2
1	ABA	A	222	1	-	0/3/4/6	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GYS	CB2-CA2	16.95	1.51	1.35
1	C	66	GYS	CA2-C2	-13.57	1.33	1.48
1	A	66	GYS	CA3-N3	-9.35	1.29	1.47
1	A	66	GYS	CD1-CG2	7.84	1.55	1.39
1	C	66	GYS	CE1-CD1	7.80	1.51	1.38
1	D	66	GYS	CA2-C2	-7.77	1.40	1.48
1	D	66	GYS	CD1-CG2	7.38	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CB2-CA2	7.14	1.42	1.35
1	B	66	GYS	C1-N3	-6.10	1.27	1.37
1	C	66	GYS	C1-N2	-5.86	1.23	1.32
1	B	66	GYS	CE1-CD1	5.23	1.47	1.38
1	B	66	GYS	CD2-CG2	5.01	1.49	1.39
1	B	66	GYS	CG2-CB2	-4.99	1.37	1.46
1	D	66	GYS	CE1-CD1	4.91	1.46	1.38
1	C	66	GYS	CA3-N3	-4.66	1.38	1.47
1	D	66	GYS	CE2-CD2	4.46	1.46	1.38
1	A	66	GYS	CE1-CD1	4.41	1.45	1.38
1	B	66	GYS	C1-N2	-4.36	1.25	1.32
1	D	66	GYS	OH-CZ	4.22	1.46	1.37
1	D	66	GYS	O3-C3	3.81	1.41	1.20
1	A	66	GYS	O3-C3	3.66	1.40	1.20
1	A	66	GYS	CA2-C2	-3.64	1.44	1.48
1	B	66	GYS	CA2-N2	3.61	1.46	1.38
1	D	66	GYS	CD2-CG2	3.52	1.46	1.39
1	A	66	GYS	CG2-CB2	3.32	1.53	1.46
1	A	66	GYS	OH-CZ	-3.25	1.29	1.37
1	C	66	GYS	C1-N3	-3.16	1.31	1.37
1	A	66	GYS	C2-N3	-3.12	1.32	1.40
1	A	66	GYS	CE2-CZ	-3.11	1.33	1.39
1	C	66	GYS	CG2-CB2	-3.09	1.41	1.46
1	D	66	GYS	CB2-CA2	-3.03	1.32	1.35
1	D	66	GYS	C1-N3	-2.92	1.32	1.37
1	A	66	GYS	CE1-CZ	2.84	1.44	1.39
1	C	66	GYS	C2-N3	-2.70	1.33	1.40
1	C	66	GYS	OG1-CB1	-2.54	1.31	1.42
1	A	66	GYS	C1-N3	2.35	1.41	1.37
1	B	66	GYS	OG1-CB1	-2.30	1.32	1.42
1	A	66	GYS	CA3-C3	-2.28	1.41	1.49
1	A	66	GYS	CA2-N2	2.24	1.43	1.38
1	B	66	GYS	C2-N3	-2.12	1.35	1.40
1	B	66	GYS	CA3-N3	-2.07	1.43	1.47
1	D	66	GYS	CA2-N2	2.05	1.43	1.38
1	B	66	GYS	O2-C2	2.03	1.27	1.23
1	D	66	GYS	O2-C2	2.01	1.27	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GYS	O2-C2-CA2	-11.02	123.99	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	C2-CA2-N2	-9.41	102.21	108.95
1	A	66	GYS	CA2-C2-N3	8.53	110.67	103.50
1	D	66	GYS	O2-C2-CA2	-8.46	125.62	131.02
1	B	66	GYS	C2-N3-C1	8.26	111.89	108.07
1	A	66	GYS	C2-CA2-N2	-7.62	103.49	108.95
1	D	66	GYS	C2-CA2-N2	-7.28	103.74	108.95
1	C	66	GYS	O2-C2-CA2	-6.95	126.58	131.02
1	B	66	GYS	CD1-CE1-CZ	-6.86	112.62	119.88
1	C	66	GYS	C2-N3-C1	-6.49	105.06	108.07
1	A	66	GYS	CG2-CB2-CA2	-5.94	122.81	129.87
1	C	66	GYS	CA2-C2-N3	5.43	108.06	103.50
1	D	66	GYS	CA2-N2-C1	5.36	109.99	105.80
1	D	66	GYS	CA2-C2-N3	5.31	107.96	103.50
1	C	66	GYS	N3-C1-N2	5.21	115.59	111.48
1	D	66	GYS	CD1-CE1-CZ	-4.98	114.61	119.88
1	B	66	GYS	CE2-CZ-CE1	4.50	126.93	119.77
1	B	66	GYS	CA3-N3-C2	-4.49	113.82	123.67
1	D	66	GYS	CD2-CE2-CZ	4.45	124.58	119.88
1	B	66	GYS	CB2-CA2-C2	4.33	127.61	122.36
1	D	66	GYS	CE2-CD2-CG2	-4.32	115.64	121.22
1	A	66	GYS	CB2-CA2-N2	4.28	134.58	128.76
1	A	66	GYS	CA3-N3-C2	-4.23	114.37	123.67
1	B	66	GYS	CE2-CD2-CG2	-3.87	116.22	121.22
1	D	66	GYS	CE2-CZ-CE1	3.83	125.87	119.77
1	C	66	GYS	CA3-N3-C2	-3.57	115.84	123.67
1	D	66	GYS	CG2-CB2-CA2	-3.48	125.73	129.87
1	A	66	GYS	CA2-N2-C1	3.40	108.46	105.80
1	C	66	GYS	CD1-CE1-CZ	-3.40	116.29	119.88
1	A	66	GYS	C2-N3-C1	-3.30	106.54	108.07
1	D	66	GYS	CA3-N3-C2	-3.17	116.71	123.67
1	A	66	GYS	CD1-CE1-CZ	-3.11	116.58	119.88
1	C	66	GYS	C2-CA2-N2	-3.05	106.76	108.95
1	D	66	GYS	N3-C1-N2	-2.92	109.18	111.48
1	A	66	GYS	OH-CZ-CE1	-2.84	112.10	120.00
1	A	66	GYS	CE2-CZ-CE1	2.81	124.25	119.77
1	D	66	GYS	O3-C3-CA3	-2.75	113.11	125.47
1	D	66	GYS	C3-CA3-N3	-2.72	106.24	112.43
1	B	66	GYS	C3-CA3-N3	-2.72	106.25	112.43
1	B	66	GYS	N3-C1-N2	2.71	113.62	111.48
1	A	66	GYS	O3-C3-CA3	-2.65	113.54	125.47
1	B	66	GYS	CA2-N2-C1	2.63	107.86	105.80
1	C	66	GYS	CB2-CA2-C2	2.62	125.53	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	O2-C2-CA2	-2.33	129.54	131.02
1	D	66	GYS	C2-N3-C1	2.30	109.13	108.07
1	D	66	GYS	CB2-CA2-C2	2.27	125.11	122.36
1	A	66	GYS	CE1-CD1-CG2	-2.27	118.29	121.22
1	B	66	GYS	CD2-CG2-CB2	-2.27	113.42	121.22
1	B	66	GYS	CD2-CE2-CZ	2.05	122.05	119.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	222	ABA	O-C-CA-CB
1	A	66	GYS	N1-CA1-CB1-OG1
1	B	66	GYS	N1-CA1-CB1-OG1
1	C	66	GYS	N1-CA1-CB1-OG1
1	D	66	GYS	N1-CA1-CB1-OG1

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	226/236 (95%)	-0.10	2 (0%) 81 84	12, 18, 29, 36	0
1	B	225/236 (95%)	0.05	5 (2%) 62 66	14, 21, 33, 40	0
1	C	226/236 (95%)	-0.03	4 (1%) 67 71	13, 19, 30, 39	0
1	D	226/236 (95%)	0.04	3 (1%) 75 79	14, 20, 32, 40	0
All	All	903/944 (95%)	-0.01	14 (1%) 70 74	12, 20, 31, 40	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	GLN	3.1
1	A	190	ASP	3.1
1	B	6	GLU	2.8
1	B	133	ASP	2.7
1	A	132	GLU	2.6
1	C	151	TYR	2.6
1	B	3	LYS	2.5
1	B	80	ARG	2.5
1	B	157	GLN	2.5
1	C	190	ASP	2.3
1	D	132	GLU	2.2
1	C	157	GLN	2.2
1	D	124	GLU	2.2
1	C	133	ASP	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, 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	ABA	B	222	6/7	0.93	0.10	16,17,19,22	0
1	ABA	D	222	6/7	0.93	0.09	18,19,22,23	0
1	GYS	A	66	21/22	0.94	0.09	12,19,24,32	0
1	ABA	A	222	6/7	0.94	0.08	15,15,16,18	0
1	GYS	C	66	21/22	0.95	0.07	16,20,25,30	0
1	ABA	C	222	6/7	0.95	0.08	17,17,18,22	0
1	GYS	D	66	21/22	0.95	0.07	18,22,28,29	0
1	GYS	B	66	21/22	0.95	0.07	18,21,29,37	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.