



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:01 PM UTC

PDB ID : 4JFG / pdb_00004jfg
Title : Crystal structure of sfGFP-66-HqAla
Authors : Wang, J.; Liu, X.; Li, J.; Zhang, W.; Hu, M.; Zhou, J.
Deposited on : 2013-02-28
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

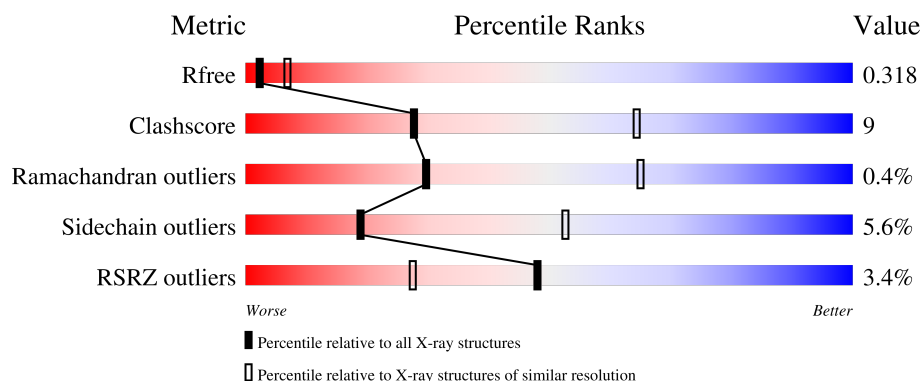
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	244	 3% 79% 11% • 7%
1	B	244	 4% 67% 21% • 9%
1	C	244	 2% 72% 18% • 7%
1	D	244	 2% 74% 14% • 11%
1	E	244	 3% 69% 22% • 7%

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Mol	Chain	Length	Quality of chain
1	F	244	4% 67% 20% • 11%
1	G	244	5% 61% 25% 5% 9%
1	H	244	2% 71% 19% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14241 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	226	Total	C	N	O	S	0	0	0
			1775	1122	306	342	5			
1	B	223	Total	C	N	O	S	0	0	0
			1746	1100	300	341	5			
1	C	226	Total	C	N	O	S	0	0	0
			1778	1123	307	343	5			
1	D	218	Total	C	N	O	S	0	0	0
			1698	1073	295	325	5			
1	E	226	Total	C	N	O	S	0	0	0
			1775	1120	306	344	5			
1	F	218	Total	C	N	O	S	0	0	0
			1710	1079	294	332	5			
1	G	222	Total	C	N	O	S	0	0	0
			1739	1097	300	337	5			
1	H	226	Total	C	N	O	S	0	0	0
			1771	1118	306	342	5			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P42212
A	-6	SER	-	expression tag	UNP P42212
A	-5	HIS	-	expression tag	UNP P42212
A	-4	HIS	-	expression tag	UNP P42212
A	-3	HIS	-	expression tag	UNP P42212
A	-2	HIS	-	expression tag	UNP P42212
A	-1	HIS	-	expression tag	UNP P42212
A	0	HIS	-	expression tag	UNP P42212
A	30	ARG	SER	engineered mutation	UNP P42212
A	39	ASN	TYR	engineered mutation	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	105	THR	ASN	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	145	PHE	TYR	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	206	VAL	ALA	engineered mutation	UNP P42212
B	-7	GLY	-	expression tag	UNP P42212
B	-6	SER	-	expression tag	UNP P42212
B	-5	HIS	-	expression tag	UNP P42212
B	-4	HIS	-	expression tag	UNP P42212
B	-3	HIS	-	expression tag	UNP P42212
B	-2	HIS	-	expression tag	UNP P42212
B	-1	HIS	-	expression tag	UNP P42212
B	0	HIS	-	expression tag	UNP P42212
B	30	ARG	SER	engineered mutation	UNP P42212
B	39	ASN	TYR	engineered mutation	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	105	THR	ASN	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	206	VAL	ALA	engineered mutation	UNP P42212
C	-7	GLY	-	expression tag	UNP P42212
C	-6	SER	-	expression tag	UNP P42212
C	-5	HIS	-	expression tag	UNP P42212
C	-4	HIS	-	expression tag	UNP P42212
C	-3	HIS	-	expression tag	UNP P42212
C	-2	HIS	-	expression tag	UNP P42212
C	-1	HIS	-	expression tag	UNP P42212
C	0	HIS	-	expression tag	UNP P42212
C	30	ARG	SER	engineered mutation	UNP P42212
C	39	ASN	TYR	engineered mutation	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	99	SER	PHE	engineered mutation	UNP P42212
C	105	THR	ASN	engineered mutation	UNP P42212
C	145	PHE	TYR	engineered mutation	UNP P42212
C	153	THR	MET	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	171	VAL	ILE	engineered mutation	UNP P42212
C	206	VAL	ALA	engineered mutation	UNP P42212
D	-7	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP P42212
D	-5	HIS	-	expression tag	UNP P42212
D	-4	HIS	-	expression tag	UNP P42212
D	-3	HIS	-	expression tag	UNP P42212
D	-2	HIS	-	expression tag	UNP P42212
D	-1	HIS	-	expression tag	UNP P42212
D	0	HIS	-	expression tag	UNP P42212
D	30	ARG	SER	engineered mutation	UNP P42212
D	39	ASN	TYR	engineered mutation	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212
D	99	SER	PHE	engineered mutation	UNP P42212
D	105	THR	ASN	engineered mutation	UNP P42212
D	145	PHE	TYR	engineered mutation	UNP P42212
D	153	THR	MET	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	171	VAL	ILE	engineered mutation	UNP P42212
D	206	VAL	ALA	engineered mutation	UNP P42212
E	-7	GLY	-	expression tag	UNP P42212
E	-6	SER	-	expression tag	UNP P42212
E	-5	HIS	-	expression tag	UNP P42212
E	-4	HIS	-	expression tag	UNP P42212
E	-3	HIS	-	expression tag	UNP P42212
E	-2	HIS	-	expression tag	UNP P42212
E	-1	HIS	-	expression tag	UNP P42212
E	0	HIS	-	expression tag	UNP P42212
E	30	ARG	SER	engineered mutation	UNP P42212
E	39	ASN	TYR	engineered mutation	UNP P42212
E	80	ARG	GLN	engineered mutation	UNP P42212
E	99	SER	PHE	engineered mutation	UNP P42212
E	105	THR	ASN	engineered mutation	UNP P42212
E	145	PHE	TYR	engineered mutation	UNP P42212
E	153	THR	MET	engineered mutation	UNP P42212
E	163	ALA	VAL	engineered mutation	UNP P42212
E	171	VAL	ILE	engineered mutation	UNP P42212
E	206	VAL	ALA	engineered mutation	UNP P42212
F	-7	GLY	-	expression tag	UNP P42212
F	-6	SER	-	expression tag	UNP P42212
F	-5	HIS	-	expression tag	UNP P42212
F	-4	HIS	-	expression tag	UNP P42212
F	-3	HIS	-	expression tag	UNP P42212
F	-2	HIS	-	expression tag	UNP P42212
F	-1	HIS	-	expression tag	UNP P42212

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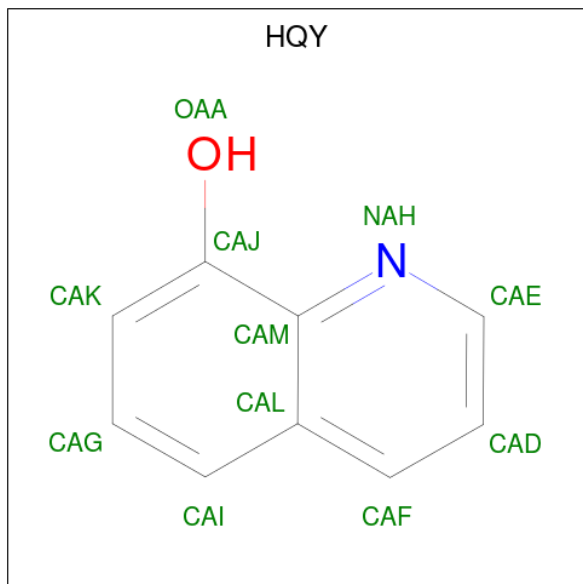
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P42212
F	30	ARG	SER	engineered mutation	UNP P42212
F	39	ASN	TYR	engineered mutation	UNP P42212
F	80	ARG	GLN	engineered mutation	UNP P42212
F	99	SER	PHE	engineered mutation	UNP P42212
F	105	THR	ASN	engineered mutation	UNP P42212
F	145	PHE	TYR	engineered mutation	UNP P42212
F	153	THR	MET	engineered mutation	UNP P42212
F	163	ALA	VAL	engineered mutation	UNP P42212
F	171	VAL	ILE	engineered mutation	UNP P42212
F	206	VAL	ALA	engineered mutation	UNP P42212
G	-7	GLY	-	expression tag	UNP P42212
G	-6	SER	-	expression tag	UNP P42212
G	-5	HIS	-	expression tag	UNP P42212
G	-4	HIS	-	expression tag	UNP P42212
G	-3	HIS	-	expression tag	UNP P42212
G	-2	HIS	-	expression tag	UNP P42212
G	-1	HIS	-	expression tag	UNP P42212
G	0	HIS	-	expression tag	UNP P42212
G	30	ARG	SER	engineered mutation	UNP P42212
G	39	ASN	TYR	engineered mutation	UNP P42212
G	80	ARG	GLN	engineered mutation	UNP P42212
G	99	SER	PHE	engineered mutation	UNP P42212
G	105	THR	ASN	engineered mutation	UNP P42212
G	145	PHE	TYR	engineered mutation	UNP P42212
G	153	THR	MET	engineered mutation	UNP P42212
G	163	ALA	VAL	engineered mutation	UNP P42212
G	171	VAL	ILE	engineered mutation	UNP P42212
G	206	VAL	ALA	engineered mutation	UNP P42212
H	-7	GLY	-	expression tag	UNP P42212
H	-6	SER	-	expression tag	UNP P42212
H	-5	HIS	-	expression tag	UNP P42212
H	-4	HIS	-	expression tag	UNP P42212
H	-3	HIS	-	expression tag	UNP P42212
H	-2	HIS	-	expression tag	UNP P42212
H	-1	HIS	-	expression tag	UNP P42212
H	0	HIS	-	expression tag	UNP P42212
H	30	ARG	SER	engineered mutation	UNP P42212
H	39	ASN	TYR	engineered mutation	UNP P42212
H	80	ARG	GLN	engineered mutation	UNP P42212
H	99	SER	PHE	engineered mutation	UNP P42212
H	105	THR	ASN	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
H	145	PHE	TYR	engineered mutation	UNP P42212
H	153	THR	MET	engineered mutation	UNP P42212
H	163	ALA	VAL	engineered mutation	UNP P42212
H	171	VAL	ILE	engineered mutation	UNP P42212
H	206	VAL	ALA	engineered mutation	UNP P42212

- Molecule 2 is quinolin-8-ol (CCD ID: HQY) (formula: C₉H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	D	1	Total	C	N	O	0	0
			11	9	1	1		
2	E	1	Total	C	N	O	0	0
			11	9	1	1		
2	F	1	Total	C	N	O	0	0
			11	9	1	1		
2	G	1	Total	C	N	O	0	0
			11	9	1	1		
2	H	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 3 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Cs 6	0	0
3	B	4	Total 4	Cs 4	0	0
3	C	4	Total 4	Cs 4	0	0
3	D	3	Total 3	Cs 3	0	0
3	E	2	Total 2	Cs 2	0	0
3	F	5	Total 5	Cs 5	0	0
3	G	5	Total 5	Cs 5	0	0
3	H	2	Total 2	Cs 2	0	0

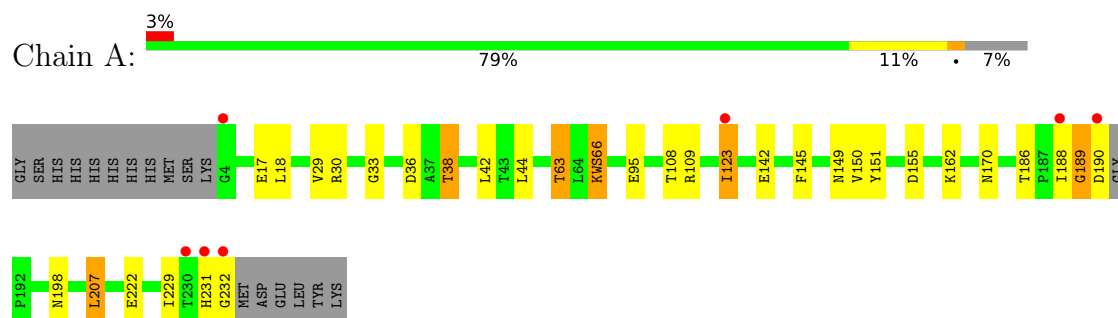
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	13	Total 13	O 13	0	0
4	C	21	Total 21	O 21	0	0
4	D	15	Total 15	O 15	0	0
4	E	16	Total 16	O 16	0	0
4	F	17	Total 17	O 17	0	0
4	G	16	Total 16	O 16	0	0
4	H	14	Total 14	O 14	0	0

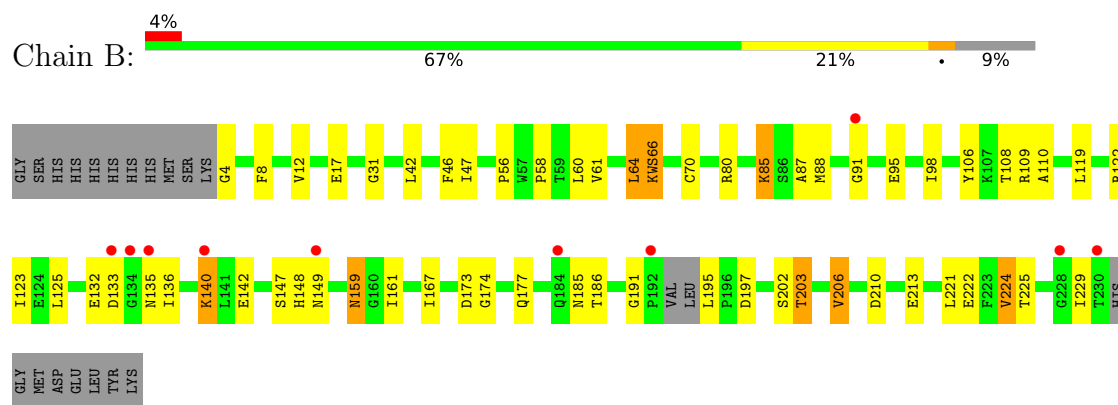
3 Residue-property plots [i](#)

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.

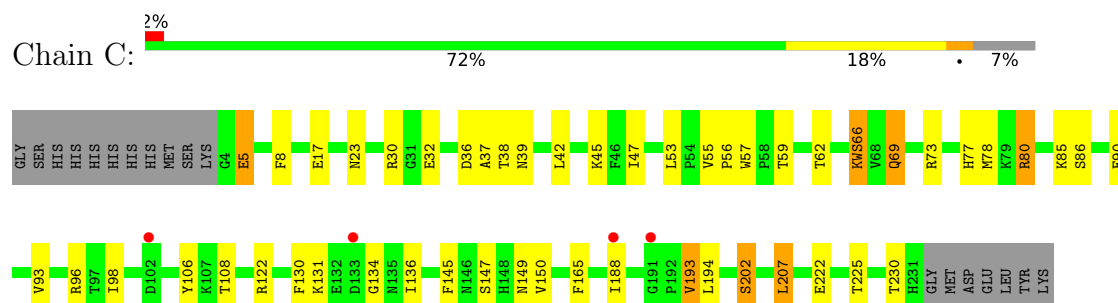
- Molecule 1: Green fluorescent protein



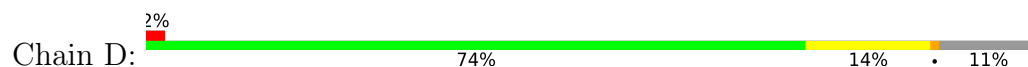
- Molecule 1: Green fluorescent protein

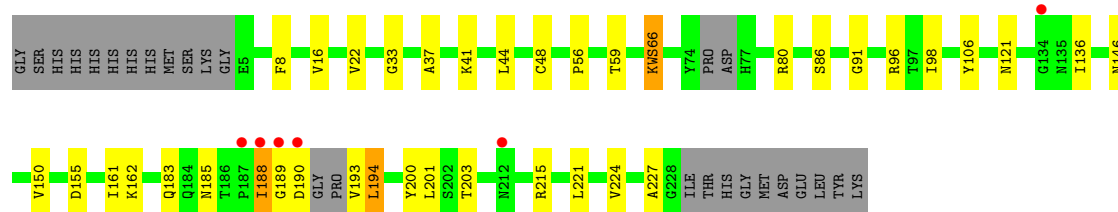


- Molecule 1: Green fluorescent protein

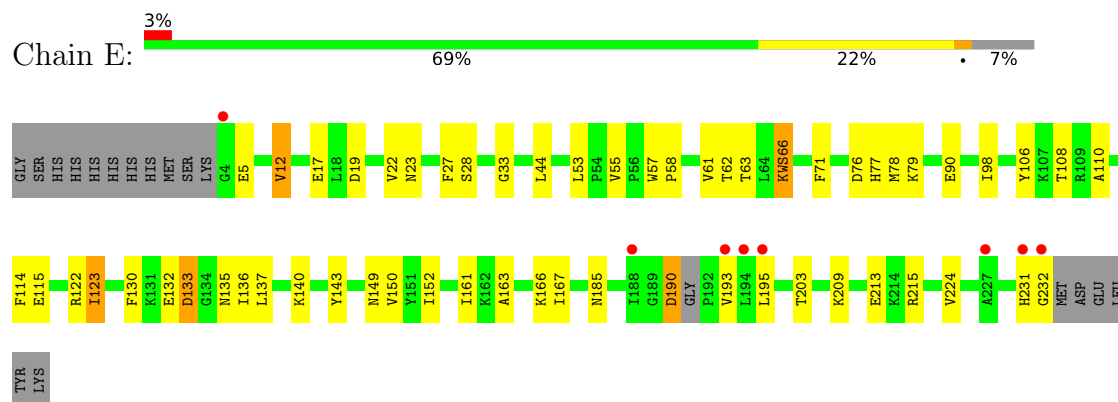


- Molecule 1: Green fluorescent protein

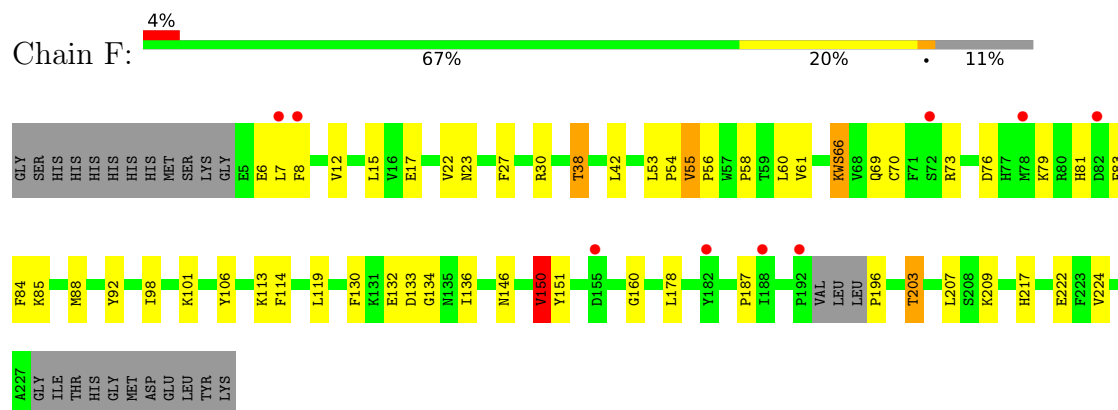




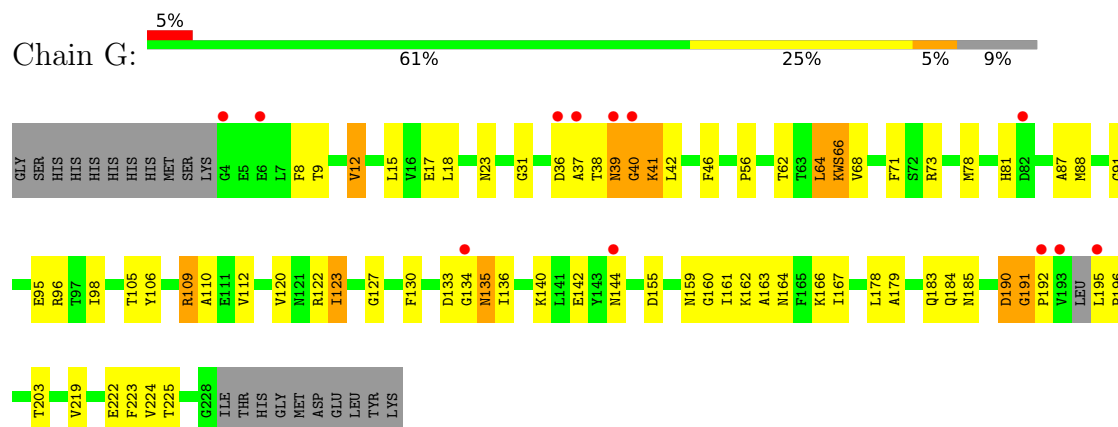
- Molecule 1: Green fluorescent protein



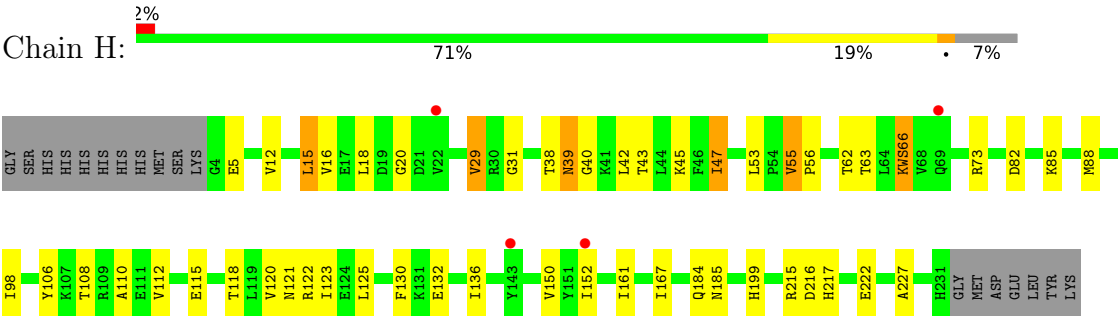
- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.17Å 148.90Å 161.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.84 – 3.00 21.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	79.7 (21.84-3.00) 83.9 (21.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.259 , 0.312 0.267 , 0.318	Depositor DCC
R_{free} test set	1835 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.63$, $\langle L^2 \rangle = 0.49$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	14241	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: KWS, HQY, CS

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	0.30	0/1798	0.71	0/2434
1	B	0.31	0/1768	0.73	1/2395 (0.0%)
1	C	0.31	0/1802	0.73	1/2442 (0.0%)
1	D	0.30	0/1717	0.71	0/2322
1	E	0.31	0/1798	0.74	0/2433
1	F	0.30	0/1732	0.72	0/2344
1	G	0.31	0/1761	0.76	3/2384 (0.1%)
1	H	0.30	0/1795	0.75	0/2432
All	All	0.31	0/14171	0.73	5/19186 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	LEU	CA-C-O	-5.81	110.93	120.80
1	G	191	GLY	CA-C-N	5.45	125.44	120.21
1	G	191	GLY	C-N-CA	5.45	125.44	120.21
1	G	41	LYS	N-CA-C	5.43	118.52	110.48
1	C	165	PHE	N-CA-C	5.32	115.56	108.38

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	1775	0	1690	18	0
1	B	1746	0	1644	38	0
1	C	1778	0	1695	31	0
1	D	1698	0	1604	22	0
1	E	1775	0	1685	31	0
1	F	1710	0	1611	30	0
1	G	1739	0	1643	48	0
1	H	1771	0	1680	31	0
2	A	11	0	6	2	0
2	B	11	0	6	1	0
2	C	11	0	6	1	0
2	D	11	0	6	1	0
2	E	11	0	6	1	0
2	F	11	0	6	1	0
2	G	11	0	6	1	0
2	H	11	0	6	2	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	2	0	0	1	0
4	A	18	0	0	1	0
4	B	13	0	0	0	0
4	C	21	0	0	0	0
4	D	15	0	0	0	0
4	E	16	0	0	0	0
4	F	17	0	0	0	0
4	G	16	0	0	1	0
4	H	14	0	0	1	0
All	All	14241	0	13300	244	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 9.

The worst 5 of 244 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:H:184:GLN:HE22	3:H:303:CS:CS	1.68	1.03
1:F:61:VAL:O	1:F:66:KWS:OG1	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ILE:HD11	1:H:215:ARG:HB2	1.64	0.77
1:B:148:HIS:NE2	1:B:203:THR:O	2.18	0.76
1:C:98:ILE:HB	1:C:106:TYR:HB2	1.67	0.75

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	219/244 (90%)	212 (97%)	6 (3%)	1 (0%)	24	60
1	B	216/244 (88%)	203 (94%)	12 (6%)	1 (0%)	24	60
1	C	221/244 (91%)	212 (96%)	9 (4%)	0	100	100
1	D	209/244 (86%)	199 (95%)	9 (4%)	1 (0%)	24	60
1	E	219/244 (90%)	211 (96%)	7 (3%)	1 (0%)	24	60
1	F	211/244 (86%)	201 (95%)	9 (4%)	1 (0%)	24	60
1	G	215/244 (88%)	201 (94%)	12 (6%)	2 (1%)	14	48
1	H	221/244 (91%)	215 (97%)	6 (3%)	0	100	100
All	All	1731/1952 (89%)	1654 (96%)	70 (4%)	7 (0%)	30	65

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	193	VAL
1	D	189	GLY
1	G	40	GLY
1	A	189	GLY
1	G	135	ASN

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	191/213 (90%)	184 (96%)	7 (4%)	30	64
1	B	187/213 (88%)	175 (94%)	12 (6%)	16	48
1	C	192/213 (90%)	183 (95%)	9 (5%)	23	58
1	D	180/213 (84%)	176 (98%)	4 (2%)	45	74
1	E	191/213 (90%)	179 (94%)	12 (6%)	16	48
1	F	183/213 (86%)	169 (92%)	14 (8%)	12	40
1	G	186/213 (87%)	172 (92%)	14 (8%)	12	41
1	H	190/213 (89%)	178 (94%)	12 (6%)	16	48
All	All	1500/1704 (88%)	1416 (94%)	84 (6%)	19	52

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	207	LEU
1	G	225	THR
1	G	12	VAL
1	G	123	ILE
1	H	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	69	GLN
1	H	184	GLN
1	D	146	ASN
1	D	169	HIS
1	E	121	ASN

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	KWS	E	66	2,1	13,15,16	2.26	2 (15%)	17,21,23	2.81	7 (41%)
1	KWS	H	66	2,1	13,15,16	2.28	2 (15%)	17,21,23	2.49	5 (29%)
1	KWS	C	66	2,1	13,15,16	2.25	2 (15%)	17,21,23	2.35	4 (23%)
1	KWS	A	66	2,1	13,15,16	2.36	4 (30%)	17,21,23	2.85	7 (41%)
1	KWS	F	66	2,1	13,15,16	2.53	5 (38%)	17,21,23	2.83	4 (23%)
1	KWS	B	66	2,1	13,15,16	2.20	2 (15%)	17,21,23	2.74	6 (35%)
1	KWS	D	66	2,1	13,15,16	3.17	5 (38%)	17,21,23	3.78	10 (58%)
1	KWS	G	66	2,1	13,15,16	2.39	4 (30%)	17,21,23	2.85	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KWS	E	66	2,1	-	6/8/27/28	0/1/1/1
1	KWS	H	66	2,1	-	6/8/27/28	0/1/1/1
1	KWS	C	66	2,1	-	7/8/27/28	0/1/1/1
1	KWS	A	66	2,1	-	7/8/27/28	0/1/1/1
1	KWS	F	66	2,1	-	6/8/27/28	0/1/1/1
1	KWS	B	66	2,1	-	6/8/27/28	0/1/1/1
1	KWS	D	66	2,1	-	6/8/27/28	0/1/1/1
1	KWS	G	66	2,1	-	6/8/27/28	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	KWS	C1-N3	7.06	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	66	KWS	C1-N3	6.95	1.48	1.37
1	D	66	KWS	C1-N3	6.83	1.48	1.37
1	E	66	KWS	C1-N3	6.74	1.48	1.37
1	H	66	KWS	C1-N3	6.74	1.48	1.37

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	KWS	CA2-N2-C1	8.12	112.66	105.39
1	D	66	KWS	CA2-N2-C1	7.71	112.30	105.39
1	G	66	KWS	CA2-N2-C1	7.05	111.71	105.39
1	F	66	KWS	N3-C1-N2	-6.94	106.02	111.48
1	E	66	KWS	CA2-N2-C1	6.52	111.23	105.39

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	KWS	N2-C1-CA1-CB
1	A	66	KWS	N3-C1-CA1-CB
1	A	66	KWS	N1-CA1-CB-OG1
1	A	66	KWS	N1-CA1-CB-CG2
1	A	66	KWS	C1-CA1-CB-OG1

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	66	KWS	2	0
1	H	66	KWS	1	0
1	C	66	KWS	1	0
1	A	66	KWS	1	0
1	F	66	KWS	2	0
1	B	66	KWS	1	0
1	D	66	KWS	1	0
1	G	66	KWS	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 31 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HQY	A	301	1	12,12,12	0.94	0	16,16,16	1.48	3 (18%)
2	HQY	B	301	1	12,12,12	0.97	0	16,16,16	1.46	3 (18%)
2	HQY	E	301	1	12,12,12	0.98	0	16,16,16	1.47	3 (18%)
2	HQY	G	301	1	12,12,12	0.95	0	16,16,16	1.49	3 (18%)
2	HQY	C	301	1	12,12,12	0.97	0	16,16,16	1.45	3 (18%)
2	HQY	H	301	1	12,12,12	1.03	1 (8%)	16,16,16	1.48	3 (18%)
2	HQY	F	301	1	12,12,12	0.99	0	16,16,16	1.53	3 (18%)
2	HQY	D	301	1	12,12,12	0.99	0	16,16,16	1.50	3 (18%)

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
2	HQY	A	301	1	-	-	0/2/2/2
2	HQY	B	301	1	-	-	0/2/2/2
2	HQY	E	301	1	-	-	0/2/2/2
2	HQY	G	301	1	-	-	0/2/2/2
2	HQY	C	301	1	-	-	0/2/2/2
2	HQY	H	301	1	-	-	0/2/2/2
2	HQY	F	301	1	-	-	0/2/2/2
2	HQY	D	301	1	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	HQY	CAM-NAH	-2.01	1.34	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	HQY	CAE-NAH-CAM	3.81	121.80	117.31
2	G	301	HQY	CAE-NAH-CAM	3.80	121.79	117.31
2	D	301	HQY	CAE-NAH-CAM	3.75	121.73	117.31
2	E	301	HQY	CAE-NAH-CAM	3.69	121.66	117.31
2	B	301	HQY	CAE-NAH-CAM	3.69	121.66	117.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	HQY	2	0
2	B	301	HQY	1	0
2	E	301	HQY	1	0
2	G	301	HQY	1	0
2	C	301	HQY	1	0
2	H	301	HQY	2	0
2	F	301	HQY	1	0
2	D	301	HQY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	225/244 (92%)	0.13	7 (3%)	51	30	12, 31, 60, 75	0
1	B	222/244 (90%)	0.41	10 (4%)	38	20	10, 34, 69, 98	0
1	C	225/244 (92%)	0.16	4 (1%)	67	44	13, 32, 54, 79	0
1	D	217/244 (88%)	0.38	6 (2%)	55	32	17, 39, 76, 99	0
1	E	225/244 (92%)	0.44	8 (3%)	46	26	20, 45, 68, 93	0
1	F	217/244 (88%)	0.52	9 (4%)	41	23	19, 43, 85, 108	0
1	G	221/244 (90%)	0.41	12 (5%)	31	16	13, 37, 72, 105	0
1	H	225/244 (92%)	0.53	4 (1%)	67	44	27, 53, 76, 82	0
All	All	1777/1952 (91%)	0.37	60 (3%)	48	27	10, 40, 72, 108	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	GLY	4.7
1	G	193	VAL	4.6
1	B	133	ASP	4.4
1	G	37	ALA	4.0
1	A	190	ASP	3.9

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(Å ²)	Q<0.9
1	KWS	F	66	15/16	0.66	0.14	34,38,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KWS	D	66	15/16	0.79	0.13	38,43,46,47	0
1	KWS	G	66	15/16	0.82	0.12	32,40,46,50	0
1	KWS	A	66	15/16	0.83	0.11	14,25,26,27	0
1	KWS	C	66	15/16	0.87	0.10	35,39,45,48	0
1	KWS	E	66	15/16	0.90	0.09	34,38,42,44	0
1	KWS	H	66	15/16	0.90	0.10	46,50,52,54	0
1	KWS	B	66	15/16	0.91	0.08	28,33,34,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CS	H	302	1/1	0.63	0.17	144,144,144,144	0
3	CS	G	303	1/1	0.65	0.18	202,202,202,202	0
3	CS	F	305	1/1	0.75	0.12	167,167,167,167	0
3	CS	A	307	1/1	0.77	0.18	167,167,167,167	0
2	HQY	H	301	11/11	0.81	0.18	48,51,58,58	0
3	CS	F	306	1/1	0.81	0.16	168,168,168,168	0
3	CS	C	302	1/1	0.83	0.09	117,117,117,117	0
3	CS	H	303	1/1	0.83	0.11	132,132,132,132	0
2	HQY	D	301	11/11	0.84	0.15	51,53,55,57	0
2	HQY	G	301	11/11	0.85	0.16	53,54,55,55	0
3	CS	D	304	1/1	0.86	0.09	148,148,148,148	0
3	CS	A	306	1/1	0.87	0.11	121,121,121,121	0
2	HQY	B	301	11/11	0.87	0.16	54,55,56,56	0
3	CS	A	304	1/1	0.87	0.16	202,202,202,202	0
3	CS	G	306	1/1	0.88	0.08	162,162,162,162	0
3	CS	A	305	1/1	0.88	0.07	111,111,111,111	0
2	HQY	C	301	11/11	0.88	0.18	52,53,56,56	0
2	HQY	F	301	11/11	0.89	0.14	55,58,59,60	0
3	CS	F	302	1/1	0.89	0.08	129,129,129,129	0
2	HQY	A	301	11/11	0.90	0.13	34,36,40,42	0
2	HQY	E	301	11/11	0.91	0.13	33,35,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CS	B	304	1/1	0.91	0.09	85,85,85,85	0
3	CS	G	305	1/1	0.91	0.11	161,161,161,161	0
3	CS	F	304	1/1	0.92	0.10	121,121,121,121	0
3	CS	D	303	1/1	0.92	0.11	154,154,154,154	0
3	CS	A	303	1/1	0.92	0.07	122,122,122,122	0
3	CS	C	305	1/1	0.92	0.08	118,118,118,118	0
3	CS	E	303	1/1	0.93	0.11	154,154,154,154	0
3	CS	E	302	1/1	0.93	0.06	110,110,110,110	0
3	CS	D	302	1/1	0.94	0.08	86,86,86,86	0
3	CS	A	302	1/1	0.95	0.07	100,100,100,100	0
3	CS	B	302	1/1	0.95	0.07	100,100,100,100	0
3	CS	C	304	1/1	0.95	0.06	109,109,109,109	0
3	CS	C	303	1/1	0.96	0.05	85,85,85,85	0
3	CS	G	304	1/1	0.96	0.06	96,96,96,96	0
3	CS	B	303	1/1	0.96	0.07	110,110,110,110	0
3	CS	F	303	1/1	0.97	0.04	75,75,75,75	0
3	CS	B	305	1/1	0.97	0.08	146,146,146,146	0
3	CS	G	302	1/1	0.98	0.08	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.