



Full wwPDB X-ray Structure Validation Report i

Nov 6, 2023 – 06:14 PM EST

PDB ID : 4JFG
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

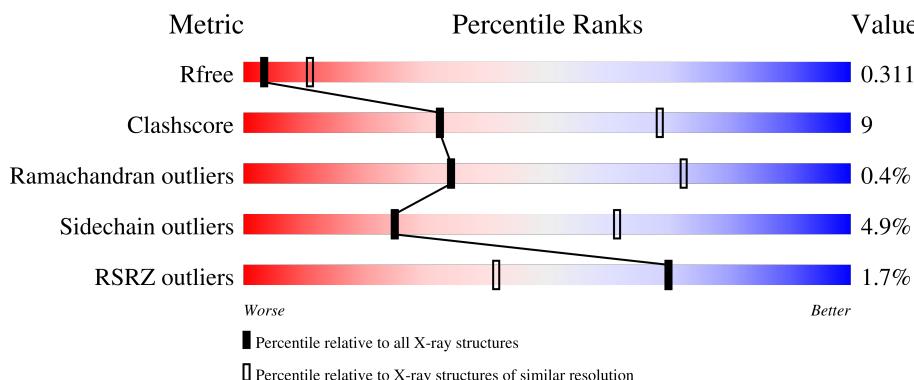
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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.



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Mol	Chain	Length	Quality of chain			
1	F	244	3%	67%	20%	• 11%
1	G	244	2%	61%	27%	• 9%
1	H	244	2%	73%	18%	• 7%

2 Entry composition (i)

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 1775	N 1122	O 306	S 342	5	0	0
1	B	223	Total	C 1746	N 1100	O 300	S 341	5	0	0
1	C	226	Total	C 1778	N 1123	O 307	S 343	5	0	0
1	D	218	Total	C 1698	N 1073	O 295	S 325	5	0	0
1	E	226	Total	C 1775	N 1120	O 306	S 344	5	0	0
1	F	218	Total	C 1710	N 1079	O 294	S 332	5	0	0
1	G	222	Total	C 1739	N 1097	O 300	S 337	5	0	0
1	H	226	Total	C 1771	N 1118	O 306	S 342	5	0	0

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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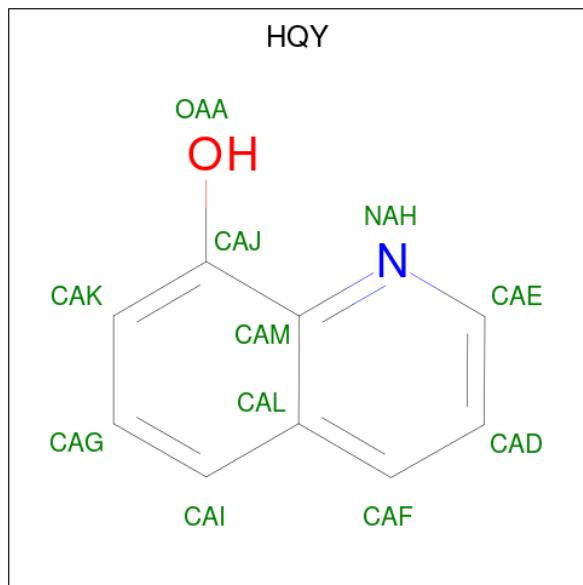
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P42212
F	30	ARG	SER	engineered mutation	UNP P42212
F	39	ASN	TYR	engineered mutation	UNP P42212
F	80	ARG	GLN	engineered mutation	UNP P42212
F	99	SER	PHE	engineered mutation	UNP P42212
F	105	THR	ASN	engineered mutation	UNP P42212
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 (three-letter code: HQY) (formula: C₉H₇NO).



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

- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

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

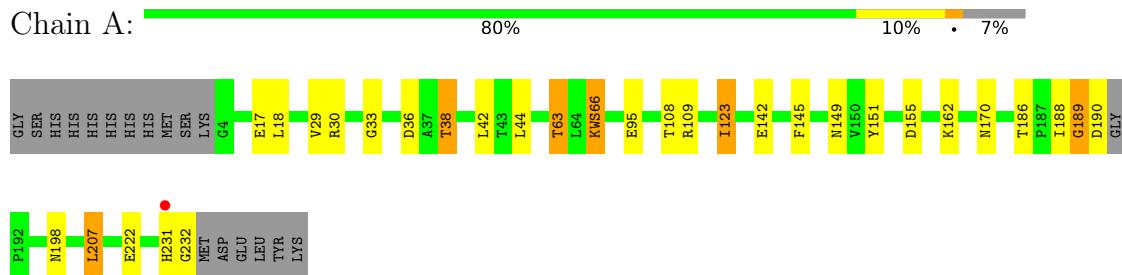
- Molecule 4 is water.

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

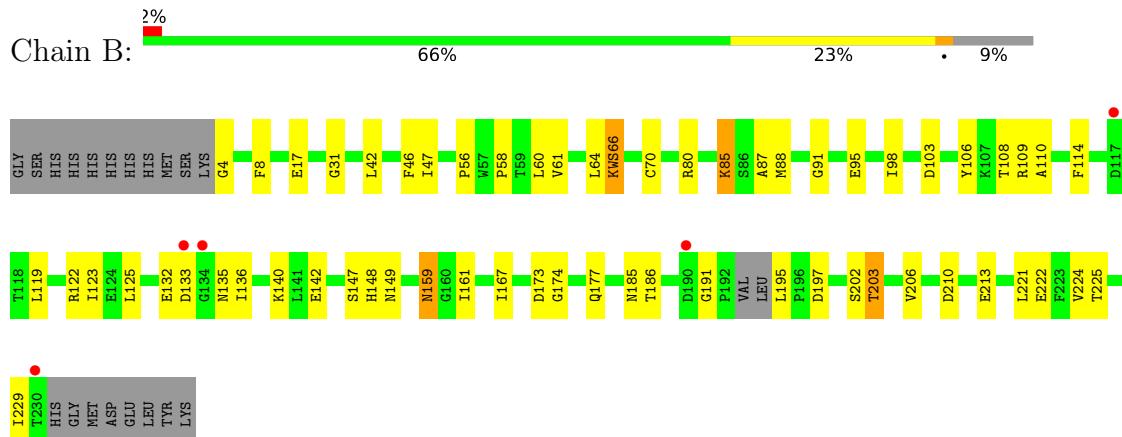
3 Residue-property plots

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



GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
MET
SER
LYS
GLY
PRO
GLY
PRO
V193
L194
Y200
L201
S202
T203
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R215
A227
G228
I1E
THR
HIS
GLY
MET
ASP
GLU
LEU
TYR
LYS

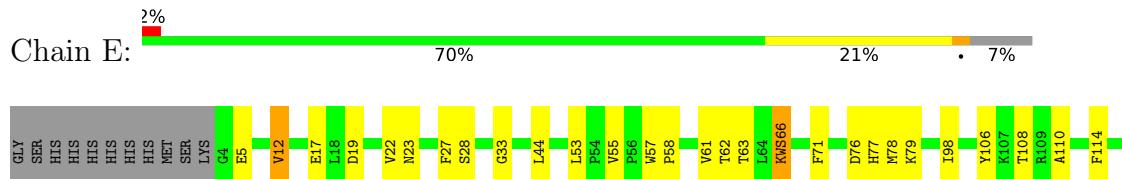
K156 I161 K162 M185 I188 C189 D190 G193 L194 Y200 L201 S202 T203 N212 R215 A227 G228 I1E THR HIS GLY MET ASP GLU LEU TYR LYS

F8 V16 G33 A37 K41 L44 C48 K52 P56 Y74 PRO ASP H77 R80 S86 G91 Y106 N121 I136 M146 V150 D165

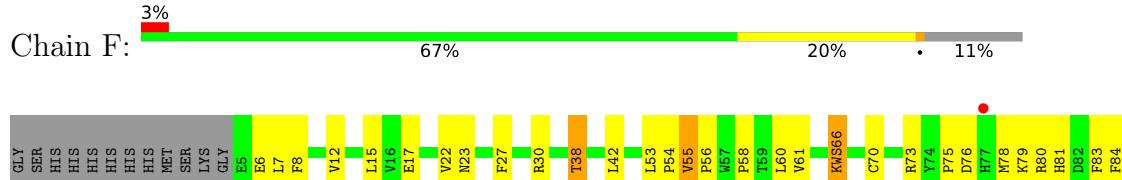
Y16 G33 A37 K41 L44 C48 K52 P56 Y74 PRO ASP H77 R80 S86 G91 Y106 N121 I136 M146 V150 D165

Y16 G33 A37 K41 L44 C48 K52 P56 Y74 PRO ASP H77 R80 S86 G91 Y106 N121 I136 M146 V150 D165

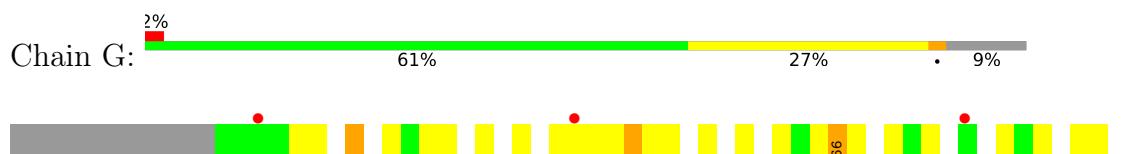
- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



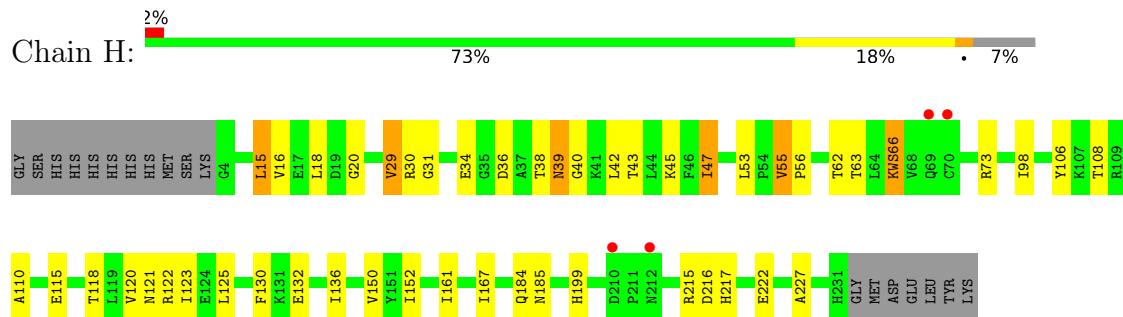
- Molecule 1: Green fluorescent protein



The diagram illustrates the SARS-CoV-2 spike protein's receptor-binding domain (RBD) with various mutations highlighted. The mutations are color-coded by their impact on the spike protein's structure or function:

- Red mutations:** D118N, E484K, N501Y, R144K, D185G, P679T, F704L, and V804A.
- Yellow mutations:** E95Q, R96P, T97M, Y106F, R122C, I123S, G127D, F130L, D133G, G134E, N135S, I136M, K140Q, L141Q, F142Q, Y143S, N144A, F145S, M146I, D155G, N159S, G160D, I161V, K162R, A163S, N164D, K165E, I166T, I167V, L178P, A179Q, S183P, Q184A, N185S, D190G, G191A, P192R, V193A, and L195S.
- Green mutation:** C145R.
- Blue mutation:** E119Q.
- Orange mutation:** V115I.
- Purple mutation:** E117Q.
- Black mutation:** N23D.
- Grey mutation:** S23P.

- Molecule 1: Green fluorescent protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.17 Å 148.90 Å 161.35 Å 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) 84.2 (21.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^{\text{1}}$	3.61 (at 2.99 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R , R_{free}	0.259 , 0.312 0.262 , 0.311	Depositor DCC
R_{free} test set	1835 reflections (5.06%)	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)	0.37 , 58.1	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CS, KWS, HQY

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	0.24	0/1798	0.44	0/2434
1	B	0.26	0/1768	0.46	0/2395
1	C	0.24	0/1802	0.44	0/2442
1	D	0.24	0/1717	0.44	0/2322
1	E	0.24	0/1798	0.47	0/2433
1	F	0.24	0/1732	0.45	0/2344
1	G	0.25	0/1761	0.46	0/2384
1	H	0.24	0/1795	0.45	0/2432
All	All	0.24	0/14171	0.45	0/19186

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	1775	0	1690	18	0
1	B	1746	0	1644	38	0
1	C	1778	0	1695	32	0
1	D	1698	0	1604	20	0
1	E	1775	0	1685	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1710	0	1611	29	0
1	G	1739	0	1643	47	0
1	H	1771	0	1680	29	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	238	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.

All (238) 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
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
1:B:135:ASN:OD1	1:B:140:LYS:NZ	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:GLU:OE1	1:G:122:ARG:NH1	2.22	0.72
1:G:41:LYS:O	1:G:73:ARG:NH1	2.24	0.71
1:G:135:ASN:H	1:G:140:LYS:HE2	1.56	0.71
1:H:115:GLU:OE2	1:H:122:ARG:NH1	2.24	0.71
1:A:63:THR:HG21	1:A:108:THR:HG21	1.73	0.69
1:D:48:CYS:O	1:D:215:ARG:NH1	2.25	0.69
1:D:150:VAL:HG12	1:D:201:LEU:HB2	1.75	0.68
1:F:98:ILE:HB	1:F:106:TYR:HB2	1.75	0.68
1:G:98:ILE:HB	1:G:106:TYR:HB2	1.76	0.68
1:B:135:ASN:ND2	1:B:177:GLN:OE1	2.26	0.68
1:B:8:PHE:HZ	1:B:88:MET:HG3	1.59	0.67
1:G:39:ASN:H	1:G:73:ARG:HH21	1.40	0.66
1:H:98:ILE:HB	1:H:106:TYR:HB2	1.77	0.66
1:E:98:ILE:HG13	1:E:106:TYR:HB2	1.77	0.66
1:B:17:GLU:OE2	1:B:122:ARG:NH1	2.29	0.65
1:G:133:ASP:N	1:G:134:GLY:HA2	2.09	0.65
1:B:135:ASN:HD22	1:B:177:GLN:HB2	1.62	0.65
1:G:42:LEU:HB2	1:G:222:GLU:HB3	1.78	0.65
1:D:98:ILE:HB	1:D:106:TYR:HB2	1.79	0.65
1:D:86:SER:HB2	1:D:194:LEU:HD23	1.79	0.64
1:G:203:THR:HG22	1:G:224:VAL:HG13	1.79	0.64
1:F:70:CYS:O	1:F:85:LYS:NZ	2.31	0.64
1:B:148:HIS:HE1	1:B:203:THR:HG23	1.62	0.63
1:H:47:ILE:HD12	1:H:217:HIS:HB3	1.80	0.63
1:F:203:THR:HG23	1:F:224:VAL:HB	1.79	0.63
1:G:195:LEU:N	4:G:404:HOH:O	2.31	0.63
1:B:42:LEU:HB2	1:B:222:GLU:HB3	1.81	0.62
1:B:110:ALA:HB2	1:B:123:ILE:HG23	1.80	0.62
1:D:66:KWS:N2	2:D:301:HQY:HAG	2.13	0.62
1:G:190:ASP:OD1	1:G:190:ASP:N	2.29	0.62
1:B:203:THR:HA	1:B:224:VAL:HA	1.82	0.61
1:G:8:PHE:O	1:G:37:ALA:HB3	2.00	0.61
1:B:66:KWS:N2	2:B:301:HQY:HAG	2.15	0.61
1:F:209:LYS:NZ	1:F:217:HIS:O	2.31	0.61
1:F:55:VAL:HG13	1:F:136:ILE:HG23	1.82	0.61
1:B:206:VAL:HG13	1:B:221:LEU:HB3	1.83	0.61
1:B:203:THR:HB	1:B:224:VAL:HG22	1.82	0.60
1:F:66:KWS:N2	2:F:301:HQY:HAG	2.17	0.60
1:H:16:VAL:HG13	1:H:121:ASN:HB3	1.82	0.60
1:G:18:LEU:HD22	1:G:64:LEU:HD11	1.83	0.60
1:C:90:GLU:O	1:C:188:ILE:HD11	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:OE2	1:C:122:ARG:NH1	2.36	0.59
1:G:166:LYS:HE2	1:G:178:LEU:HD22	1.84	0.59
1:H:63:THR:HG21	1:H:125:LEU:HD12	1.85	0.58
1:G:62:THR:O	1:G:96:ARG:NH1	2.33	0.58
1:G:163:ALA:HB3	1:G:183:GLN:HB3	1.86	0.58
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.84	0.58
1:E:17:GLU:OE1	1:E:122:ARG:NH1	2.36	0.58
1:G:39:ASN:N	1:G:73:ARG:HH21	2.02	0.58
1:C:55:VAL:HG13	1:C:136:ILE:HG23	1.86	0.57
1:D:41:LYS:HE3	1:D:221:LEU:HD11	1.87	0.57
1:E:203:THR:HG22	1:E:224:VAL:HG13	1.87	0.57
1:B:159:ASN:O	1:B:159:ASN:ND2	2.38	0.57
1:H:161:ILE:HG13	1:H:185:ASN:HB2	1.86	0.56
1:A:149:ASN:ND2	1:B:142:GLU:OE2	2.38	0.56
1:H:62:THR:HG21	1:H:167:ILE:HG13	1.87	0.56
1:H:42:LEU:HB2	1:H:222:GLU:HB3	1.86	0.56
1:C:30:ARG:NH1	1:C:32:GLU:OE1	2.39	0.56
1:F:55:VAL:HG12	1:F:56:PRO:HD2	1.88	0.56
1:D:155:ASP:HB3	1:D:162:LYS:HG3	1.86	0.56
1:C:38:THR:O	1:C:73:ARG:NH1	2.39	0.56
1:H:130:PHE:HE1	1:H:136:ILE:HD13	1.70	0.56
1:B:98:ILE:HB	1:B:106:TYR:HB2	1.88	0.55
1:D:161:ILE:HG12	1:D:185:ASN:HB2	1.89	0.55
1:E:190:ASP:OD1	1:E:190:ASP:N	2.39	0.55
1:D:188:ILE:O	1:D:190:ASP:N	2.39	0.54
1:E:76:ASP:HA	1:E:79:LYS:HE2	1.88	0.54
1:G:36:ASP:HB3	1:G:73:ARG:HH22	1.71	0.54
1:A:155:ASP:HB2	1:A:162:LYS:HG3	1.89	0.54
1:C:23:ASN:ND2	1:C:130:PHE:O	2.40	0.54
1:B:108:THR:HG22	1:B:125:LEU:HD13	1.90	0.53
1:C:55:VAL:HG11	1:C:106:TYR:OH	2.06	0.53
1:C:73:ARG:HB3	1:C:225:THR:HA	1.90	0.52
1:G:110:ALA:HB2	1:G:123:ILE:HG23	1.90	0.52
1:B:210:ASP:HB3	1:B:213:GLU:HB2	1.91	0.52
1:G:66:KWS:N2	2:G:301:HQY:HAG	2.25	0.52
1:G:95:GLU:HG2	1:G:109:ARG:HG2	1.91	0.51
1:B:135:ASN:HA	1:B:140:LYS:HG2	1.93	0.51
1:E:98:ILE:CG1	1:E:106:TYR:HB2	2.40	0.51
1:C:62:THR:O	1:C:96:ARG:NH1	2.44	0.51
1:E:62:THR:HG21	1:E:167:ILE:HG13	1.93	0.51
1:G:40:GLY:HA3	1:G:223:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:CD1	1:B:85:LYS:HG3	2.46	0.51
1:E:55:VAL:HG11	1:E:106:TYR:OH	2.11	0.51
1:B:8:PHE:CZ	1:B:88:MET:HG3	2.42	0.51
1:E:19:ASP:OD1	1:E:28:SER:OG	2.24	0.50
1:B:173:ASP:OD1	1:B:174:GLY:N	2.45	0.50
1:A:95:GLU:HG2	1:A:109:ARG:HG3	1.93	0.50
1:C:53:LEU:HD22	1:C:57:TRP:CE2	2.47	0.50
1:G:23:ASN:ND2	1:G:130:PHE:O	2.44	0.50
1:F:42:LEU:HB2	1:F:222:GLU:HB3	1.93	0.49
1:G:8:PHE:HE2	1:G:88:MET:HG3	1.77	0.49
1:A:142:GLU:CD	1:B:149:ASN:HD22	2.16	0.49
1:B:60:LEU:HB3	1:B:64:LEU:HD13	1.95	0.49
1:D:203:THR:HG22	1:D:224:VAL:HG12	1.93	0.49
1:B:87:ALA:O	1:B:91:GLY:N	2.42	0.49
1:E:55:VAL:HG13	1:E:136:ILE:HG23	1.95	0.49
1:G:135:ASN:HA	1:G:140:LYS:HB2	1.94	0.49
1:G:155:ASP:HB2	1:G:162:LYS:HG3	1.95	0.49
1:G:87:ALA:O	1:G:91:GLY:N	2.46	0.49
1:G:39:ASN:H	1:G:73:ARG:NH2	2.09	0.49
1:F:92:TYR:HA	1:F:187:PRO:HA	1.94	0.48
1:C:77:HIS:CD2	1:C:78:MET:HG3	2.48	0.48
1:H:39:ASN:OD1	1:H:39:ASN:N	2.47	0.48
1:F:101:LYS:HD2	1:F:178:LEU:HD12	1.96	0.48
1:H:130:PHE:CE1	1:H:136:ILE:HD13	2.49	0.48
1:E:12:VAL:HG13	1:E:71:PHE:HE1	1.79	0.48
1:E:161:ILE:HG12	1:E:185:ASN:HB2	1.95	0.48
1:G:161:ILE:HG12	1:G:185:ASN:HB2	1.96	0.48
1:F:17:GLU:OE2	1:F:30:ARG:NH2	2.46	0.48
1:H:73:ARG:NH2	4:H:404:HOH:O	2.41	0.48
1:A:231:HIS:HA	1:A:232:GLY:HA3	1.56	0.47
1:F:83:PHE:CE1	1:F:160:GLY:HA2	2.49	0.47
1:C:147:SER:H	1:D:146:ASN:HD21	1.60	0.47
1:G:40:GLY:HA2	1:G:73:ARG:HG3	1.96	0.47
1:A:145:PHE:HB2	1:A:207:LEU:HD21	1.95	0.47
1:C:36:ASP:OD1	1:C:38:THR:HG22	2.14	0.47
1:E:23:ASN:ND2	1:E:130:PHE:O	2.43	0.47
1:A:17:GLU:OE1	1:A:30:ARG:NH2	2.47	0.47
1:F:8:PHE:CE1	1:F:88:MET:HG3	2.49	0.47
1:F:55:VAL:HG11	1:F:106:TYR:OH	2.15	0.47
1:G:38:THR:H	1:G:73:ARG:HH21	1.61	0.47
1:H:15:LEU:HD23	1:H:120:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:VAL:HG23	1:F:27:PHE:HE1	1.80	0.47
1:F:76:ASP:HA	1:F:79:LYS:HG2	1.95	0.47
1:B:95:GLU:HG2	1:B:109:ARG:HG3	1.95	0.46
1:G:8:PHE:CE2	1:G:88:MET:HG3	2.50	0.46
1:G:134:GLY:O	1:G:136:ILE:N	2.45	0.46
1:B:161:ILE:HG13	1:B:185:ASN:HB2	1.97	0.46
1:A:36:ASP:OD1	1:A:38:THR:OG1	2.33	0.46
1:C:86:SER:OG	1:C:193:VAL:O	2.28	0.46
1:B:56:PRO:HD3	1:B:136:ILE:O	2.16	0.46
1:F:38:THR:O	1:F:73:ARG:NH1	2.41	0.45
1:D:33:GLY:HA3	1:D:44:LEU:HD23	1.97	0.45
1:F:8:PHE:HE1	1:F:88:MET:HG3	1.82	0.45
1:F:150:VAL:HG12	1:F:151:TYR:H	1.81	0.45
1:C:66:KWS:HB2	2:C:301:HQY:HAF	1.73	0.45
1:D:16:VAL:HG22	1:D:121:ASN:HB3	1.98	0.45
1:A:42:LEU:HB3	1:A:222:GLU:HB3	1.97	0.45
1:D:91:GLY:O	1:D:188:ILE:HD11	2.17	0.45
1:E:66:KWS:N2	2:E:301:HQY:HAG	2.32	0.45
1:B:203:THR:HG22	1:B:224:VAL:HG13	1.98	0.45
1:A:170:ASN:ND2	1:B:147:SER:O	2.50	0.45
1:A:188:ILE:HG13	1:A:189:GLY:N	2.32	0.45
1:H:18:LEU:HD13	1:H:123:ILE:HB	1.98	0.45
1:H:150:VAL:HG21	2:H:301:HQY:HAD	1.99	0.45
1:C:69:GLN:H	1:C:69:GLN:HE21	1.63	0.45
1:D:86:SER:HG	1:D:193:VAL:N	2.15	0.45
1:C:45:LYS:HE2	1:C:47:ILE:HD11	1.99	0.45
1:C:93:VAL:HG23	1:C:188:ILE:HG22	1.99	0.45
1:D:200:TYR:CZ	1:D:227:ALA:HB3	2.52	0.45
1:A:18:LEU:HG	1:A:123:ILE:HD11	1.99	0.44
1:C:39:ASN:HA	1:C:73:ARG:NH1	2.32	0.44
1:C:42:LEU:HB2	1:C:222:GLU:HB3	1.97	0.44
1:C:56:PRO:O	1:C:59:THR:OG1	2.32	0.44
1:B:58:PRO:HA	1:B:61:VAL:HG23	2.00	0.44
1:F:53:LEU:HD21	1:F:60:LEU:HD12	1.99	0.44
1:B:80:ARG:NH1	1:B:197:ASP:OD2	2.27	0.44
1:A:18:LEU:HB3	1:A:29:VAL:HB	2.00	0.44
2:A:301:HQY:OAA	4:A:417:HOH:O	2.21	0.44
1:G:15:LEU:HB3	1:G:120:VAL:HG22	1.99	0.44
1:G:96:ARG:HH21	1:G:183:GLN:CD	2.21	0.44
1:G:142:GLU:O	1:G:144:ASN:N	2.51	0.44
1:E:132:GLU:HA	1:E:137:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:THR:H	1:G:73:ARG:NH2	2.16	0.44
1:B:132:GLU:HA	1:B:133:ASP:C	2.38	0.43
1:F:70:CYS:HA	1:F:84:PHE:HB3	1.99	0.43
1:G:191:GLY:HA3	1:G:192:PRO:HD3	1.69	0.43
1:F:53:LEU:HA	1:F:54:PRO:HD3	1.82	0.43
1:E:22:VAL:HG23	1:E:27:PHE:HE1	1.83	0.43
1:E:231:HIS:HA	1:E:232:GLY:HA3	1.56	0.43
1:H:55:VAL:HG23	1:H:56:PRO:HD2	2.00	0.43
1:F:81:HIS:HA	1:F:196:PRO:HA	1.99	0.43
1:G:56:PRO:HD3	1:G:136:ILE:O	2.19	0.43
1:H:199:HIS:HB2	1:H:227:ALA:O	2.18	0.43
1:A:66:KWS:HB2	2:A:301:HQY:HAF	1.72	0.43
1:F:83:PHE:CZ	1:F:187:PRO:HD3	2.53	0.43
1:H:31:GLY:HA2	1:H:45:LYS:O	2.17	0.43
1:C:53:LEU:HD22	1:C:57:TRP:CD2	2.53	0.43
1:E:53:LEU:HD22	1:E:57:TRP:CE2	2.53	0.43
1:F:23:ASN:ND2	1:F:130:PHE:O	2.47	0.43
1:G:12:VAL:HG13	1:G:71:PHE:HE1	1.82	0.43
1:B:202:SER:N	1:B:225:THR:O	2.47	0.43
1:E:135:ASN:HA	1:E:140:LYS:HG3	2.00	0.43
1:E:133:ASP:OD1	1:E:133:ASP:N	2.52	0.43
1:E:58:PRO:HA	1:E:61:VAL:HG23	2.01	0.43
1:F:79:LYS:HD3	1:F:79:LYS:HA	1.87	0.43
1:G:36:ASP:OD1	1:G:37:ALA:N	2.49	0.43
1:H:132:GLU:CD	1:H:132:GLU:H	2.23	0.42
1:C:149:ASN:OD1	1:C:202:SER:OG	2.36	0.42
1:E:213:GLU:OE2	1:E:215:ARG:HB2	2.19	0.42
1:E:33:GLY:HA3	1:E:44:LEU:HG	2.00	0.42
1:H:20:GLY:HA2	1:H:125:LEU:O	2.19	0.42
1:C:147:SER:H	1:D:146:ASN:ND2	2.16	0.42
1:H:120:VAL:HG11	1:H:122:ARG:NH1	2.35	0.42
1:E:143:TYR:CZ	1:E:209:LYS:HE2	2.55	0.42
1:E:110:ALA:HB2	1:E:123:ILE:HG23	2.02	0.42
1:C:80:ARG:HD2	1:C:194:LEU:HD22	2.02	0.42
1:F:58:PRO:HA	1:F:61:VAL:HG23	2.02	0.42
1:G:167:ILE:CG2	1:G:179:ALA:HB3	2.50	0.42
1:A:151:TYR:OH	1:A:198:ASN:HB3	2.20	0.41
1:B:148:HIS:HB3	1:B:149:ASN:ND2	2.35	0.41
1:C:88:MET:HE1	1:C:112:VAL:HG12	2.02	0.41
1:E:53:LEU:HD22	1:E:57:TRP:CD2	2.54	0.41
1:E:77:HIS:CD2	1:E:78:MET:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:THR:O	1:G:127:GLY:HA2	2.20	0.41
1:H:53:LEU:HD23	1:H:55:VAL:O	2.21	0.41
1:H:110:ALA:HB2	1:H:123:ILE:HG23	2.02	0.41
1:C:131:LYS:NZ	1:C:134:GLY:HA2	2.36	0.41
1:E:61:VAL:O	1:E:66:KWS:OG1	2.38	0.41
1:E:152:ILE:HD13	1:E:163:ALA:HB2	2.02	0.41
1:G:31:GLY:HA3	1:G:46:PHE:CD2	2.56	0.41
1:B:31:GLY:HA3	1:B:46:PHE:CD2	2.56	0.41
1:C:69:GLN:HE21	1:C:69:GLN:N	2.18	0.41
1:E:149:ASN:ND2	1:G:142:GLU:OE1	2.53	0.41
1:H:18:LEU:HB3	1:H:29:VAL:HG13	2.02	0.41
1:C:145:PHE:HB2	1:C:207:LEU:HD21	2.02	0.41
1:G:81:HIS:O	1:G:196:PRO:HB3	2.21	0.41
1:G:160:GLY:HA3	1:G:185:ASN:O	2.21	0.41
1:H:66:KWS:HB2	2:H:301:HQY:HAF	1.46	0.41
1:H:115:GLU:O	1:H:118:THR:HG22	2.21	0.41
1:G:40:GLY:HA3	1:G:223:PHE:HD1	1.86	0.40
1:H:40:GLY:HA3	1:H:73:ARG:HB2	2.03	0.40
1:F:75:PRO:HD2	1:F:78:MET:HE2	2.03	0.40
1:B:70:CYS:SG	1:B:119:LEU:HD11	2.61	0.40
1:C:8:PHE:HB3	1:C:37:ALA:HB3	2.03	0.40
1:C:5:GLU:HA	1:C:85:LYS:HD3	2.03	0.40
1:D:56:PRO:HD3	1:D:136:ILE:O	2.21	0.40
1:D:56:PRO:HG2	1:D:59:THR:HG23	2.04	0.40
1:A:189:GLY:HA2	1:A:190:ASP:C	2.42	0.40
1:B:4:GLY:HA3	1:B:85:LYS:O	2.22	0.40
1:D:8:PHE:HB3	1:D:37:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	29 68
1	B	216/244 (88%)	203 (94%)	12 (6%)	1 (0%)	29 68
1	C	221/244 (91%)	212 (96%)	9 (4%)	0	100 100
1	D	209/244 (86%)	199 (95%)	9 (4%)	1 (0%)	29 68
1	E	219/244 (90%)	211 (96%)	7 (3%)	1 (0%)	29 68
1	F	211/244 (86%)	201 (95%)	9 (4%)	1 (0%)	29 68
1	G	215/244 (88%)	201 (94%)	12 (6%)	2 (1%)	17 55
1	H	221/244 (91%)	215 (97%)	6 (3%)	0	100 100
All	All	1731/1952 (89%)	1654 (96%)	70 (4%)	7 (0%)	34 72

All (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
1	B	191	GLY
1	F	150	VAL

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	191/213 (90%)	186 (97%)	5 (3%)	46 78
1	B	187/213 (88%)	177 (95%)	10 (5%)	22 58
1	C	192/213 (90%)	183 (95%)	9 (5%)	26 63
1	D	180/213 (84%)	176 (98%)	4 (2%)	52 81
1	E	191/213 (90%)	182 (95%)	9 (5%)	26 63
1	F	183/213 (86%)	170 (93%)	13 (7%)	14 46
1	G	186/213 (87%)	175 (94%)	11 (6%)	19 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	190/213 (89%)	177 (93%)	13 (7%)	16	48
All	All	1500/1704 (88%)	1426 (95%)	74 (5%)	25	61

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	63	THR
1	A	123	ILE
1	A	186	THR
1	A	207	LEU
1	B	47	ILE
1	B	85	LYS
1	B	103	ASP
1	B	114	PHE
1	B	159	ASN
1	B	167	ILE
1	B	186	THR
1	B	195	LEU
1	B	203	THR
1	B	229	ILE
1	C	5	GLU
1	C	69	GLN
1	C	80	ARG
1	C	150	VAL
1	C	193	VAL
1	C	202	SER
1	C	207	LEU
1	C	215	ARG
1	C	230	THR
1	D	52	LYS
1	D	80	ARG
1	D	188	ILE
1	D	194	LEU
1	E	5	GLU
1	E	12	VAL
1	E	63	THR
1	E	108	THR
1	E	114	PHE
1	E	133	ASP
1	E	166	LYS
1	E	190	ASP

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Mol	Chain	Res	Type
1	E	195	LEU
1	F	6	GLU
1	F	7	LEU
1	F	12	VAL
1	F	15	LEU
1	F	38	THR
1	F	55	VAL
1	F	80	ARG
1	F	114	PHE
1	F	133	ASP
1	F	146	ASN
1	F	150	VAL
1	F	207	LEU
1	F	223	PHE
1	G	9	THR
1	G	12	VAL
1	G	68	VAL
1	G	79	LYS
1	G	109	ARG
1	G	146	ASN
1	G	159	ASN
1	G	164	ASN
1	G	190	ASP
1	G	219	VAL
1	G	225	THR
1	H	15	LEU
1	H	29	VAL
1	H	30	ARG
1	H	34	GLU
1	H	36	ASP
1	H	38	THR
1	H	39	ASN
1	H	43	THR
1	H	47	ILE
1	H	55	VAL
1	H	108	THR
1	H	152	ILE
1	H	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	B	77	HIS
1	B	149	ASN
1	C	164	ASN
1	D	146	ASN
1	H	184	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	D	66	2,1	14,15,16	3.50	6 (42%)	18,21,23	3.80	9 (50%)
1	KWS	G	66	2,1	14,15,16	2.30	3 (21%)	18,21,23	2.94	7 (38%)
1	KWS	B	66	2,1	14,15,16	2.14	2 (14%)	18,21,23	2.84	8 (44%)
1	KWS	H	66	2,1	14,15,16	2.19	2 (14%)	18,21,23	2.57	6 (33%)
1	KWS	E	66	2,1	14,15,16	2.20	2 (14%)	18,21,23	2.85	8 (44%)
1	KWS	A	66	2,1	14,15,16	2.27	4 (28%)	18,21,23	2.90	9 (50%)
1	KWS	F	66	2,1	14,15,16	2.39	5 (35%)	18,21,23	2.95	4 (22%)
1	KWS	C	66	2,1	14,15,16	2.18	2 (14%)	18,21,23	2.40	4 (22%)

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	D	66	2,1	-	6/8/27/28	0/1/1/1

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	KWS	C1-N3	7.05	1.49	1.37
1	F	66	KWS	C1-N3	6.95	1.48	1.37
1	D	66	KWS	C1-N3	6.82	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
1	B	66	KWS	C1-N3	6.68	1.48	1.37
1	D	66	KWS	CA1-C1	6.62	1.60	1.51
1	C	66	KWS	C1-N3	6.59	1.48	1.37
1	A	66	KWS	C1-N3	6.51	1.48	1.37
1	D	66	KWS	CA3-C3	-5.11	1.31	1.49
1	D	66	KWS	CA3-N3	-5.04	1.37	1.47
1	D	66	KWS	O3-C3	4.10	1.43	1.19
1	F	66	KWS	CA3-N3	-3.79	1.39	1.47
1	H	66	KWS	CA3-N3	-2.65	1.42	1.47
1	C	66	KWS	CA3-N3	-2.45	1.42	1.47
1	A	66	KWS	CA3-N3	-2.43	1.42	1.47
1	A	66	KWS	OG1-CB	-2.40	1.36	1.43
1	E	66	KWS	CA3-N3	-2.35	1.42	1.47
1	F	66	KWS	C2-N3	2.20	1.45	1.39
1	A	66	KWS	CB-CA1	2.17	1.61	1.53
1	F	66	KWS	OG1-CB	-2.14	1.37	1.43
1	B	66	KWS	CA3-N3	-2.13	1.43	1.47
1	D	66	KWS	C2-N3	2.10	1.44	1.39
1	G	66	KWS	CA3-N3	-2.07	1.43	1.47
1	G	66	KWS	C2-N3	2.02	1.44	1.39
1	F	66	KWS	CG2-CB	-2.00	1.45	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	KWS	CA2-N2-C1	8.02	112.66	105.40
1	F	66	KWS	N3-C1-N2	-7.85	106.02	111.45
1	D	66	KWS	CA2-N2-C1	7.62	112.30	105.40
1	G	66	KWS	CA2-N2-C1	6.97	111.71	105.40
1	D	66	KWS	N3-C1-N2	-6.90	106.68	111.45
1	G	66	KWS	N3-C1-N2	-6.74	106.79	111.45
1	E	66	KWS	CA2-N2-C1	6.44	111.23	105.40
1	D	66	KWS	C1-CA1-N1	-6.36	99.65	109.96
1	A	66	KWS	N3-C1-N2	-6.26	107.12	111.45
1	A	66	KWS	CA2-N2-C1	6.25	111.06	105.40
1	B	66	KWS	CA2-N2-C1	6.07	110.90	105.40
1	C	66	KWS	CA2-N2-C1	5.96	110.80	105.40
1	E	66	KWS	N3-C1-N2	-5.83	107.41	111.45
1	H	66	KWS	CA2-N2-C1	5.77	110.62	105.40
1	C	66	KWS	N3-C1-N2	-5.15	107.89	111.45
1	H	66	KWS	N3-C1-N2	-5.07	107.94	111.45
1	B	66	KWS	N3-C1-N2	-5.02	107.98	111.45
1	G	66	KWS	O2-C2-CA2	-4.93	128.19	130.96
1	B	66	KWS	C1-CA1-N1	-4.89	102.03	109.96
1	D	66	KWS	CA1-C1-N3	4.87	130.59	124.75
1	D	66	KWS	OG1-CB-CA1	4.85	119.42	109.04
1	B	66	KWS	O2-C2-CA2	-4.78	128.27	130.96
1	C	66	KWS	O2-C2-CA2	-4.50	128.44	130.96
1	E	66	KWS	CG2-CB-CA1	-4.31	102.01	112.16
1	H	66	KWS	O2-C2-CA2	-4.25	128.57	130.96
1	A	66	KWS	OG1-CB-CA1	4.22	118.07	109.04
1	D	66	KWS	O3-C3-CA3	-4.13	113.91	126.39
1	D	66	KWS	O2-C2-CA2	-3.98	128.73	130.96
1	E	66	KWS	O2-C2-CA2	-3.68	128.90	130.96
1	H	66	KWS	C1-CA1-N1	-3.64	104.06	109.96
1	A	66	KWS	O2-C2-CA2	-3.57	128.95	130.96
1	F	66	KWS	CA1-C1-N2	3.23	128.41	123.89
1	D	66	KWS	CG2-CB-CA1	-3.16	104.70	112.16
1	B	66	KWS	CA1-C1-N3	3.11	128.47	124.75
1	B	66	KWS	CB-CA1-N1	-3.02	93.82	113.84
1	G	66	KWS	CA1-C1-N2	2.94	128.01	123.89
1	A	66	KWS	CA1-C1-N2	2.85	127.88	123.89
1	D	66	KWS	CB-CA1-N1	-2.85	94.95	113.84
1	E	66	KWS	OG1-CB-CA1	2.79	115.01	109.04
1	E	66	KWS	CB-CA1-N1	-2.60	96.59	113.84
1	G	66	KWS	OG1-CB-CA1	2.58	114.56	109.04
1	A	66	KWS	OG1-CB-CG2	-2.54	102.21	109.74
1	H	66	KWS	CB-CA1-N1	-2.54	97.01	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	KWS	CG2-CB-CA1	-2.51	106.25	112.16
1	F	66	KWS	O2-C2-CA2	-2.41	129.60	130.96
1	B	66	KWS	O3-C3-CA3	-2.33	119.35	126.39
1	E	66	KWS	O3-C3-CA3	-2.30	119.45	126.39
1	H	66	KWS	O3-C3-CA3	-2.26	119.56	126.39
1	A	66	KWS	O3-C3-CA3	-2.25	119.58	126.39
1	G	66	KWS	O3-C3-CA3	-2.19	119.77	126.39
1	C	66	KWS	O3-C3-CA3	-2.06	120.17	126.39
1	E	66	KWS	CB2-CA2-C2	2.04	126.50	122.76
1	B	66	KWS	CB2-CA2-C2	2.02	126.47	122.76
1	A	66	KWS	C1-CA1-N1	-2.00	106.72	109.96
1	A	66	KWS	CB-CA1-N1	-2.00	100.57	113.84

There are no chirality outliers.

All (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
1	A	66	KWS	C1-CA1-CB-CG2
1	B	66	KWS	N2-C1-CA1-CB
1	B	66	KWS	N3-C1-CA1-CB
1	B	66	KWS	N1-CA1-CB-OG1
1	B	66	KWS	N1-CA1-CB-CG2
1	C	66	KWS	N2-C1-CA1-CB
1	C	66	KWS	N3-C1-CA1-CB
1	C	66	KWS	N1-CA1-CB-OG1
1	C	66	KWS	N1-CA1-CB-CG2
1	C	66	KWS	C1-CA1-CB-OG1
1	C	66	KWS	C1-CA1-CB-CG2
1	D	66	KWS	N2-C1-CA1-CB
1	D	66	KWS	N1-CA1-CB-OG1
1	D	66	KWS	N1-CA1-CB-CG2
1	D	66	KWS	C1-CA1-CB-OG1
1	D	66	KWS	C1-CA1-CB-CG2
1	E	66	KWS	N2-C1-CA1-CB
1	E	66	KWS	N3-C1-CA1-CB
1	E	66	KWS	N1-CA1-CB-OG1
1	E	66	KWS	C1-CA1-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	F	66	KWS	N2-C1-CA1-CB
1	F	66	KWS	N3-C1-CA1-CB
1	G	66	KWS	N2-C1-CA1-CB
1	G	66	KWS	N3-C1-CA1-CB
1	G	66	KWS	N1-CA1-CB-OG1
1	G	66	KWS	C1-CA1-CB-OG1
1	H	66	KWS	N1-CA1-CB-OG1
1	H	66	KWS	N1-CA1-CB-CG2
1	H	66	KWS	C1-CA1-CB-OG1
1	H	66	KWS	C1-CA1-CB-CG2
1	E	66	KWS	N1-CA1-CB-CG2
1	G	66	KWS	N1-CA1-CB-CG2
1	E	66	KWS	C1-CA1-CB-CG2
1	F	66	KWS	C1-CA1-CB-CG2
1	G	66	KWS	C1-CA1-CB-CG2
1	D	66	KWS	N3-C1-CA1-CB
1	H	66	KWS	N2-C1-CA1-CB
1	H	66	KWS	N3-C1-CA1-CB
1	F	66	KWS	N1-CA1-CB-CG2
1	B	66	KWS	C1-CA1-CB-OG1
1	F	66	KWS	C1-CA1-CB-OG1
1	A	66	KWS	C3-CA3-N3-C2
1	C	66	KWS	C3-CA3-N3-C2
1	F	66	KWS	C3-CA3-N3-C2
1	B	66	KWS	C1-CA1-CB-CG2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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	0.91	0	16,16,16	1.41	3 (18%)
2	HQY	C	301	1	12,12,12	0.94	0	16,16,16	1.38	3 (18%)
2	HQY	B	301	1	12,12,12	0.93	0	16,16,16	1.38	3 (18%)
2	HQY	F	301	1	12,12,12	0.95	0	16,16,16	1.44	3 (18%)
2	HQY	E	301	1	12,12,12	0.95	1 (8%)	16,16,16	1.39	3 (18%)
2	HQY	G	301	1	12,12,12	0.92	0	16,16,16	1.42	3 (18%)
2	HQY	D	301	1	12,12,12	0.95	0	16,16,16	1.42	3 (18%)
2	HQY	H	301	1	12,12,12	0.99	1 (8%)	16,16,16	1.40	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	C	301	1	-	-	0/2/2/2
2	HQY	B	301	1	-	-	0/2/2/2
2	HQY	F	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	D	301	1	-	-	0/2/2/2
2	HQY	H	301	1	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	HQY	CAM-NAH	-2.06	1.34	1.37
2	E	301	HQY	CAM-NAH	-2.02	1.34	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	HQY	CAE-NAH-CAM	3.62	121.80	117.30
2	G	301	HQY	CAE-NAH-CAM	3.60	121.79	117.30
2	D	301	HQY	CAE-NAH-CAM	3.56	121.73	117.30
2	E	301	HQY	CAE-NAH-CAM	3.50	121.66	117.30
2	B	301	HQY	CAE-NAH-CAM	3.50	121.66	117.30
2	A	301	HQY	CAE-NAH-CAM	3.30	121.40	117.30
2	C	301	HQY	CAE-NAH-CAM	3.28	121.38	117.30
2	H	301	HQY	CAE-NAH-CAM	3.19	121.28	117.30
2	D	301	HQY	CAL-CAM-NAH	-2.53	119.85	122.62
2	G	301	HQY	CAL-CAM-NAH	-2.48	119.91	122.62
2	F	301	HQY	CAL-CAM-NAH	-2.44	119.94	122.62
2	C	301	HQY	CAL-CAM-NAH	-2.36	120.04	122.62
2	B	301	HQY	CAL-CAM-NAH	-2.34	120.06	122.62
2	H	301	HQY	CAL-CAM-NAH	-2.28	120.12	122.62
2	D	301	HQY	CAJ-CAM-NAH	2.27	121.12	117.41
2	H	301	HQY	CAJ-CAM-NAH	2.25	121.08	117.41
2	E	301	HQY	CAL-CAM-NAH	-2.23	120.18	122.62
2	A	301	HQY	CAL-CAM-NAH	-2.23	120.18	122.62
2	A	301	HQY	CAJ-CAM-NAH	2.18	120.97	117.41
2	C	301	HQY	CAJ-CAM-NAH	2.15	120.91	117.41
2	E	301	HQY	CAJ-CAM-NAH	2.15	120.91	117.41
2	G	301	HQY	CAJ-CAM-NAH	2.14	120.90	117.41
2	B	301	HQY	CAJ-CAM-NAH	2.08	120.81	117.41
2	F	301	HQY	CAJ-CAM-NAH	2.02	120.71	117.41

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	C	301	HQY	1	0
2	B	301	HQY	1	0
2	F	301	HQY	1	0
2	E	301	HQY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	HQY	1	0
2	D	301	HQY	1	0
2	H	301	HQY	2	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 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	225/244 (92%)	-0.29	1 (0%)	92	79	12, 31, 60, 75
1	B	222/244 (90%)	-0.08	5 (2%)	60	31	10, 34, 69, 98
1	C	225/244 (92%)	-0.26	1 (0%)	92	79	13, 32, 54, 79
1	D	217/244 (88%)	-0.13	2 (0%)	84	63	17, 39, 76, 99
1	E	225/244 (92%)	-0.01	6 (2%)	54	26	20, 45, 68, 93
1	F	217/244 (88%)	0.02	7 (3%)	47	20	19, 43, 85, 108
1	G	221/244 (90%)	-0.15	5 (2%)	60	31	13, 37, 72, 105
1	H	225/244 (92%)	0.10	4 (1%)	68	40	27, 53, 76, 82
All	All	1777/1952 (91%)	-0.10	31 (1%)	70	41	10, 40, 72, 108
							0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ASP	4.6
1	C	133	ASP	3.9
1	A	231	HIS	3.6
1	E	231	HIS	3.5
1	B	230	THR	3.5
1	F	156	LYS	3.3
1	D	212	ASN	3.2
1	D	156	LYS	3.0
1	B	134	GLY	3.0
1	F	190	ASP	2.9
1	H	212	ASN	2.9
1	H	69	GLN	2.7
1	F	77	HIS	2.6
1	G	76	ASP	2.6
1	G	133	ASP	2.5
1	G	6	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	190	ASP	2.4
1	F	159	ASN	2.3
1	E	133	ASP	2.2
1	F	157	GLN	2.2
1	E	232	GLY	2.2
1	H	70	CYS	2.2
1	B	117	ASP	2.2
1	E	210	ASP	2.2
1	E	211	PRO	2.1
1	F	197	ASP	2.1
1	G	37	ALA	2.1
1	H	210	ASP	2.1
1	F	117	ASP	2.0
1	G	193	VAL	2.0
1	E	193	VAL	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(Å ²)	Q<0.9
1	KWS	F	66	15/16	0.87	0.31	34,38,40,41	0
1	KWS	D	66	15/16	0.92	0.26	38,43,46,47	0
1	KWS	A	66	15/16	0.92	0.23	14,25,26,27	0
1	KWS	H	66	15/16	0.92	0.31	46,50,52,54	0
1	KWS	G	66	15/16	0.93	0.24	32,40,46,50	0
1	KWS	E	66	15/16	0.94	0.27	34,38,42,44	0
1	KWS	C	66	15/16	0.94	0.23	35,39,45,48	0
1	KWS	B	66	15/16	0.96	0.25	28,33,34,36	0

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	CS	A	304	1/1	0.73	0.30	202,202,202,202	0
3	CS	H	302	1/1	0.76	0.12	144,144,144,144	0
3	CS	G	305	1/1	0.79	0.08	161,161,161,161	0
3	CS	A	307	1/1	0.81	0.23	167,167,167,167	0
3	CS	G	303	1/1	0.84	0.31	202,202,202,202	0
2	HQY	B	301	11/11	0.86	0.29	54,55,56,56	0
3	CS	F	305	1/1	0.87	0.09	167,167,167,167	0
2	HQY	G	301	11/11	0.88	0.25	53,54,55,55	0
2	HQY	F	301	11/11	0.89	0.23	55,58,59,60	0
2	HQY	D	301	11/11	0.89	0.25	51,53,55,57	0
2	HQY	C	301	11/11	0.90	0.25	52,53,56,56	0
2	HQY	H	301	11/11	0.90	0.26	48,51,58,58	0
3	CS	C	302	1/1	0.90	0.08	117,117,117,117	0
3	CS	E	302	1/1	0.90	0.04	110,110,110,110	0
3	CS	E	303	1/1	0.91	0.20	154,154,154,154	0
3	CS	F	302	1/1	0.91	0.05	129,129,129,129	0
3	CS	A	305	1/1	0.91	0.05	111,111,111,111	0
3	CS	H	303	1/1	0.91	0.10	132,132,132,132	0
3	CS	D	303	1/1	0.92	0.08	154,154,154,154	0
3	CS	F	306	1/1	0.92	0.14	168,168,168,168	0
3	CS	G	306	1/1	0.93	0.05	162,162,162,162	0
3	CS	D	304	1/1	0.93	0.07	148,148,148,148	0
2	HQY	A	301	11/11	0.93	0.21	34,36,40,42	0
3	CS	B	305	1/1	0.94	0.06	146,146,146,146	0
3	CS	C	305	1/1	0.94	0.06	118,118,118,118	0
2	HQY	E	301	11/11	0.95	0.16	33,35,36,37	0
3	CS	A	302	1/1	0.95	0.05	100,100,100,100	0
3	CS	A	303	1/1	0.95	0.05	122,122,122,122	0
3	CS	F	304	1/1	0.96	0.09	121,121,121,121	0
3	CS	G	304	1/1	0.97	0.05	96,96,96,96	0
3	CS	B	303	1/1	0.97	0.04	110,110,110,110	0
3	CS	C	304	1/1	0.97	0.04	109,109,109,109	0
3	CS	B	304	1/1	0.97	0.06	85,85,85,85	0
3	CS	B	302	1/1	0.97	0.05	100,100,100,100	0
3	CS	D	302	1/1	0.98	0.07	86,86,86,86	0
3	CS	A	306	1/1	0.98	0.04	121,121,121,121	0
3	CS	C	303	1/1	0.98	0.04	85,85,85,85	0
3	CS	F	303	1/1	0.99	0.03	75,75,75,75	0
3	CS	G	302	1/1	0.99	0.04	64,64,64,64	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.