Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:08 am GMT

PDB ID	:	2VZX
Title	:	Structural and spectroscopic characterization of photoconverting fluorescent protein Dendra2
Authors	:	Adam, V.; Nienhaus, K.; Bourgeois, D.; Nienhaus, G.U.
Deposited on	:	2008-08-06
Resolution	:	2.00 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 ⓘ 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:

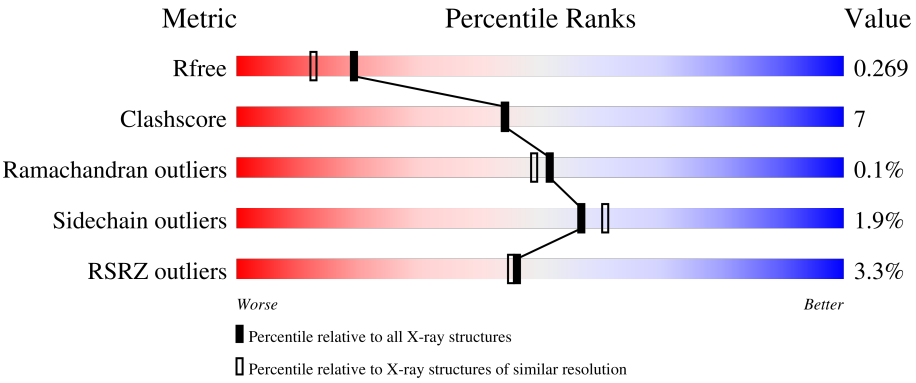
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	229	2% 85% 12%
1	B	229	2% 86% 11%
1	C	229	3% 86% 12%
1	D	229	2% 83% 13%
1	E	229	2% 85% 10%

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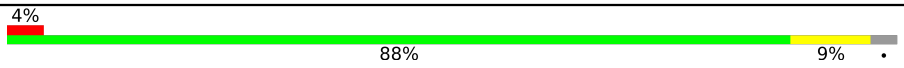
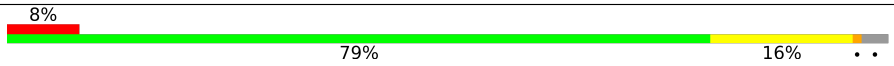
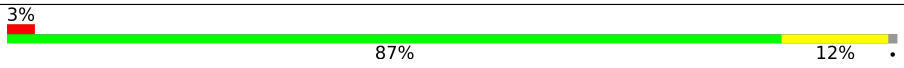
Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15867 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	221	Total	C	N	O	S	0	2	0
			1807	1160	308	331	8			
1	B	223	Total	C	N	O	S	0	1	0
			1819	1167	311	333	8			
1	C	225	Total	C	N	O	S	0	2	0
			1845	1182	319	336	8			
1	D	222	Total	C	N	O	S	0	1	0
			1807	1159	307	333	8			
1	E	223	Total	C	N	O	S	0	0	0
			1811	1162	308	333	8			
1	F	221	Total	C	N	O	S	0	1	0
			1799	1155	305	331	8			
1	G	221	Total	C	N	O	S	0	2	0
			1802	1157	305	332	8			
1	H	227	Total	C	N	O	S	0	1	0
			1859	1191	323	337	8			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	LEU	engineered mutation	UNP Q8T6U0
A	61	VAL	LEU	engineered mutation	UNP Q8T6U0
A	64	5SQ	HIS	chromophore	UNP Q8T6U0
A	64	5SQ	TYR	chromophore	UNP Q8T6U0
A	64	5SQ	GLY	chromophore	UNP Q8T6U0
A	95	PHE	TYR	engineered mutation	UNP Q8T6U0
A	121	LYS	ASN	engineered mutation	UNP Q8T6U0
A	123	THR	MET	engineered mutation	UNP Q8T6U0
A	188	ALA	TYR	engineered mutation	UNP Q8T6U0
A	199	GLY	SER	engineered mutation	UNP Q8T6U0
A	213	ALA	GLY	engineered mutation	UNP Q8T6U0
A	224	VAL	ALA	engineered mutation	UNP Q8T6U0
A	226	HIS	-	expression tag	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	-	expression tag	UNP Q8T6U0
A	228	HIS	-	expression tag	UNP Q8T6U0
A	229	HIS	-	expression tag	UNP Q8T6U0
A	230	HIS	-	expression tag	UNP Q8T6U0
A	231	HIS	-	expression tag	UNP Q8T6U0
B	40	ALA	LEU	engineered mutation	UNP Q8T6U0
B	61	VAL	LEU	engineered mutation	UNP Q8T6U0
B	64	5SQ	HIS	chromophore	UNP Q8T6U0
B	64	5SQ	TYR	chromophore	UNP Q8T6U0
B	64	5SQ	GLY	chromophore	UNP Q8T6U0
B	95	PHE	TYR	engineered mutation	UNP Q8T6U0
B	121	LYS	ASN	engineered mutation	UNP Q8T6U0
B	123	THR	MET	engineered mutation	UNP Q8T6U0
B	188	ALA	TYR	engineered mutation	UNP Q8T6U0
B	199	GLY	SER	engineered mutation	UNP Q8T6U0
B	213	ALA	GLY	engineered mutation	UNP Q8T6U0
B	224	VAL	ALA	engineered mutation	UNP Q8T6U0
B	226	HIS	-	expression tag	UNP Q8T6U0
B	227	HIS	-	expression tag	UNP Q8T6U0
B	228	HIS	-	expression tag	UNP Q8T6U0
B	229	HIS	-	expression tag	UNP Q8T6U0
B	230	HIS	-	expression tag	UNP Q8T6U0
B	231	HIS	-	expression tag	UNP Q8T6U0
C	40	ALA	LEU	engineered mutation	UNP Q8T6U0
C	61	VAL	LEU	engineered mutation	UNP Q8T6U0
C	64	5SQ	HIS	chromophore	UNP Q8T6U0
C	64	5SQ	TYR	chromophore	UNP Q8T6U0
C	64	5SQ	GLY	chromophore	UNP Q8T6U0
C	95	PHE	TYR	engineered mutation	UNP Q8T6U0
C	121	LYS	ASN	engineered mutation	UNP Q8T6U0
C	123	THR	MET	engineered mutation	UNP Q8T6U0
C	188	ALA	TYR	engineered mutation	UNP Q8T6U0
C	199	GLY	SER	engineered mutation	UNP Q8T6U0
C	213	ALA	GLY	engineered mutation	UNP Q8T6U0
C	224	VAL	ALA	engineered mutation	UNP Q8T6U0
C	226	HIS	-	expression tag	UNP Q8T6U0
C	227	HIS	-	expression tag	UNP Q8T6U0
C	228	HIS	-	expression tag	UNP Q8T6U0
C	229	HIS	-	expression tag	UNP Q8T6U0
C	230	HIS	-	expression tag	UNP Q8T6U0
C	231	HIS	-	expression tag	UNP Q8T6U0
D	40	ALA	LEU	engineered mutation	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	61	VAL	LEU	engineered mutation	UNP Q8T6U0
D	64	5SQ	HIS	chromophore	UNP Q8T6U0
D	64	5SQ	TYR	chromophore	UNP Q8T6U0
D	64	5SQ	GLY	chromophore	UNP Q8T6U0
D	95	PHE	TYR	engineered mutation	UNP Q8T6U0
D	121	LYS	ASN	engineered mutation	UNP Q8T6U0
D	123	THR	MET	engineered mutation	UNP Q8T6U0
D	188	ALA	TYR	engineered mutation	UNP Q8T6U0
D	199	GLY	SER	engineered mutation	UNP Q8T6U0
D	213	ALA	GLY	engineered mutation	UNP Q8T6U0
D	224	VAL	ALA	engineered mutation	UNP Q8T6U0
D	226	HIS	-	expression tag	UNP Q8T6U0
D	227	HIS	-	expression tag	UNP Q8T6U0
D	228	HIS	-	expression tag	UNP Q8T6U0
D	229	HIS	-	expression tag	UNP Q8T6U0
D	230	HIS	-	expression tag	UNP Q8T6U0
D	231	HIS	-	expression tag	UNP Q8T6U0
E	40	ALA	LEU	engineered mutation	UNP Q8T6U0
E	61	VAL	LEU	engineered mutation	UNP Q8T6U0
E	64	5SQ	HIS	chromophore	UNP Q8T6U0
E	64	5SQ	TYR	chromophore	UNP Q8T6U0
E	64	5SQ	GLY	chromophore	UNP Q8T6U0
E	95	PHE	TYR	engineered mutation	UNP Q8T6U0
E	121	LYS	ASN	engineered mutation	UNP Q8T6U0
E	123	THR	MET	engineered mutation	UNP Q8T6U0
E	188	ALA	TYR	engineered mutation	UNP Q8T6U0
E	199	GLY	SER	engineered mutation	UNP Q8T6U0
E	213	ALA	GLY	engineered mutation	UNP Q8T6U0
E	224	VAL	ALA	engineered mutation	UNP Q8T6U0
E	226	HIS	-	expression tag	UNP Q8T6U0
E	227	HIS	-	expression tag	UNP Q8T6U0
E	228	HIS	-	expression tag	UNP Q8T6U0
E	229	HIS	-	expression tag	UNP Q8T6U0
E	230	HIS	-	expression tag	UNP Q8T6U0
E	231	HIS	-	expression tag	UNP Q8T6U0
F	40	ALA	LEU	engineered mutation	UNP Q8T6U0
F	61	VAL	LEU	engineered mutation	UNP Q8T6U0
F	64	5SQ	HIS	chromophore	UNP Q8T6U0
F	64	5SQ	TYR	chromophore	UNP Q8T6U0
F	64	5SQ	GLY	chromophore	UNP Q8T6U0
F	95	PHE	TYR	engineered mutation	UNP Q8T6U0
F	121	LYS	ASN	engineered mutation	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	123	THR	MET	engineered mutation	UNP Q8T6U0
F	188	ALA	TYR	engineered mutation	UNP Q8T6U0
F	199	GLY	SER	engineered mutation	UNP Q8T6U0
F	213	ALA	GLY	engineered mutation	UNP Q8T6U0
F	224	VAL	ALA	engineered mutation	UNP Q8T6U0
F	226	HIS	-	expression tag	UNP Q8T6U0
F	227	HIS	-	expression tag	UNP Q8T6U0
F	228	HIS	-	expression tag	UNP Q8T6U0
F	229	HIS	-	expression tag	UNP Q8T6U0
F	230	HIS	-	expression tag	UNP Q8T6U0
F	231	HIS	-	expression tag	UNP Q8T6U0
G	40	ALA	LEU	engineered mutation	UNP Q8T6U0
G	61	VAL	LEU	engineered mutation	UNP Q8T6U0
G	64	5SQ	HIS	chromophore	UNP Q8T6U0
G	64	5SQ	TYR	chromophore	UNP Q8T6U0
G	64	5SQ	GLY	chromophore	UNP Q8T6U0
G	95	PHE	TYR	engineered mutation	UNP Q8T6U0
G	121	LYS	ASN	engineered mutation	UNP Q8T6U0
G	123	THR	MET	engineered mutation	UNP Q8T6U0
G	188	ALA	TYR	engineered mutation	UNP Q8T6U0
G	199	GLY	SER	engineered mutation	UNP Q8T6U0
G	213	ALA	GLY	engineered mutation	UNP Q8T6U0
G	224	VAL	ALA	engineered mutation	UNP Q8T6U0
G	226	HIS	-	expression tag	UNP Q8T6U0
G	227	HIS	-	expression tag	UNP Q8T6U0
G	228	HIS	-	expression tag	UNP Q8T6U0
G	229	HIS	-	expression tag	UNP Q8T6U0
G	230	HIS	-	expression tag	UNP Q8T6U0
G	231	HIS	-	expression tag	UNP Q8T6U0
H	40	ALA	LEU	engineered mutation	UNP Q8T6U0
H	61	VAL	LEU	engineered mutation	UNP Q8T6U0
H	64	5SQ	HIS	chromophore	UNP Q8T6U0
H	64	5SQ	TYR	chromophore	UNP Q8T6U0
H	64	5SQ	GLY	chromophore	UNP Q8T6U0
H	95	PHE	TYR	engineered mutation	UNP Q8T6U0
H	121	LYS	ASN	engineered mutation	UNP Q8T6U0
H	123	THR	MET	engineered mutation	UNP Q8T6U0
H	188	ALA	TYR	engineered mutation	UNP Q8T6U0
H	199	GLY	SER	engineered mutation	UNP Q8T6U0
H	213	ALA	GLY	engineered mutation	UNP Q8T6U0
H	224	VAL	ALA	engineered mutation	UNP Q8T6U0
H	226	HIS	-	expression tag	UNP Q8T6U0

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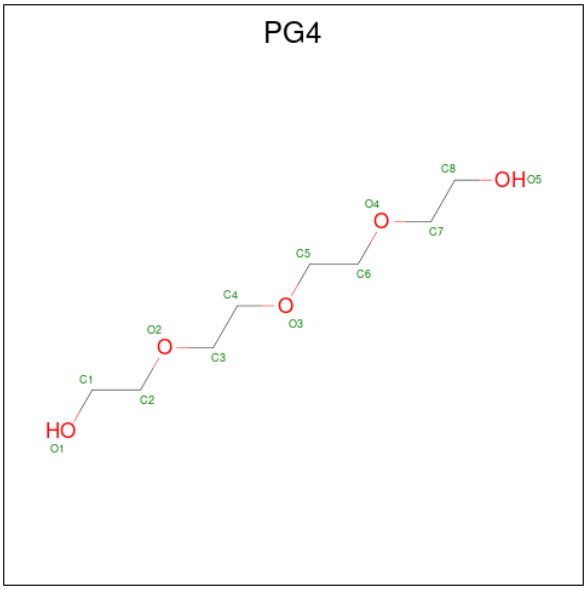
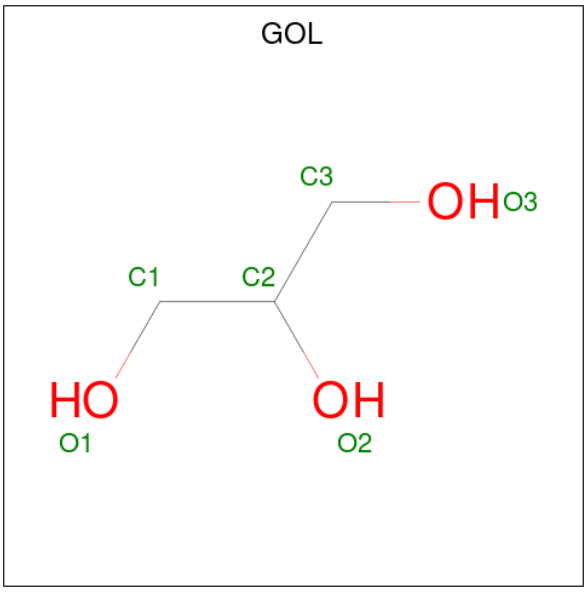
Chain	Residue	Modelled	Actual	Comment	Reference
H	227	HIS	-	expression tag	UNP Q8T6U0
H	228	HIS	-	expression tag	UNP Q8T6U0
H	229	HIS	-	expression tag	UNP Q8T6U0
H	230	HIS	-	expression tag	UNP Q8T6U0
H	231	HIS	-	expression tag	UNP Q8T6U0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	D	1	Total C O 13 8 5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

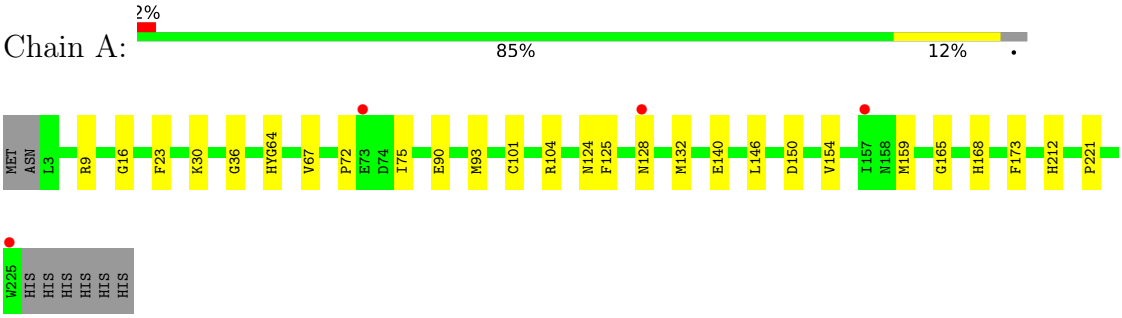
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	185	Total O 185 185	0	0
4	B	189	Total O 189 189	0	0
4	C	183	Total O 183 183	0	0
4	D	148	Total O 148 148	0	0
4	E	173	Total O 173 173	0	0
4	F	128	Total O 128 128	0	0
4	G	113	Total O 113 113	0	0
4	H	161	Total O 161 161	0	0

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.

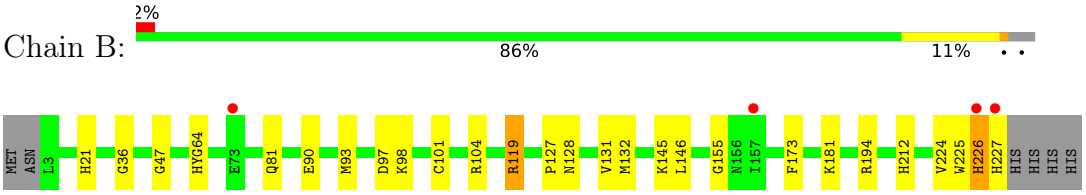
• Molecule 1: Green fluorescent protein

Chain A:



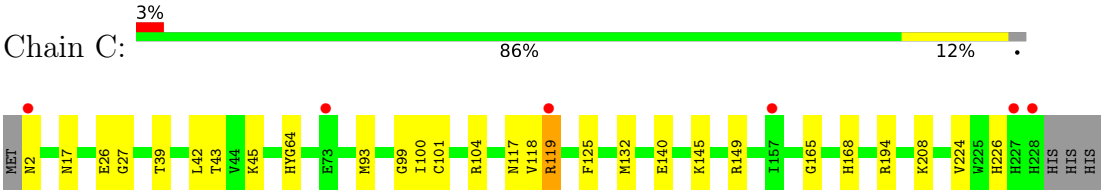
• Molecule 1: Green fluorescent protein

Chain B:



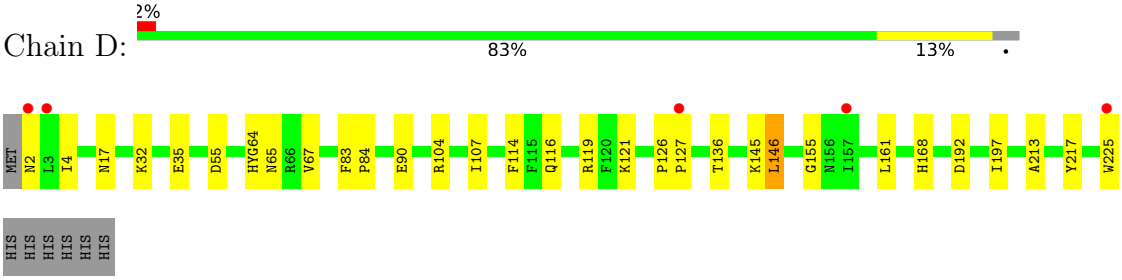
• Molecule 1: Green fluorescent protein

Chain C:



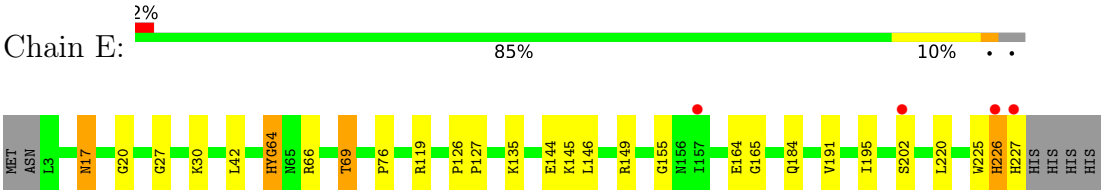
• Molecule 1: Green fluorescent protein

Chain D:



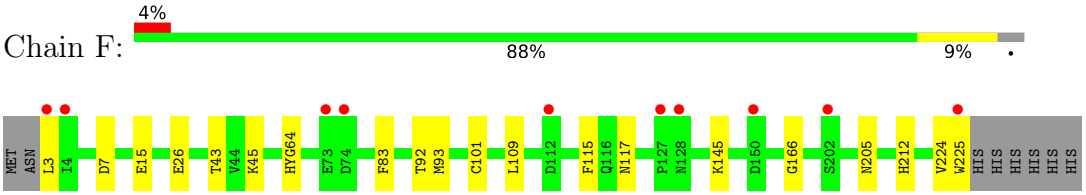
• Molecule 1: Green fluorescent protein

Chain E:



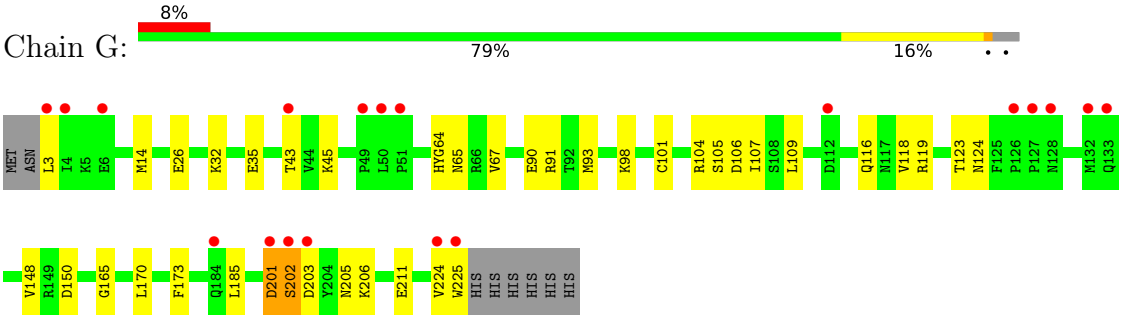
• Molecule 1: Green fluorescent protein

Chain F:



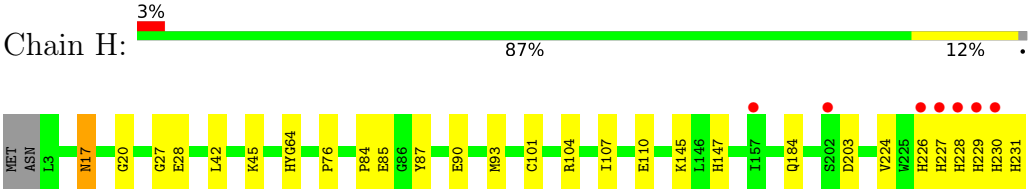
• Molecule 1: Green fluorescent protein

Chain G:



• Molecule 1: Green fluorescent protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.26Å 76.85Å 92.50Å 90.05° 108.17° 106.58°	Depositor
Resolution (Å)	33.50 – 2.00 33.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.50-2.00) 94.2 (33.49-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.212 , 0.269 0.211 , 0.269	Depositor DCC
R_{free} test set	5661 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15867	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PG4, 5SQ

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	0.49	0/1834	0.60	0/2479
1	B	0.51	0/1845	0.61	0/2495
1	C	0.48	0/1875	0.61	0/2535
1	D	0.48	0/1831	0.63	1/2476 (0.0%)
1	E	0.49	0/1834	0.62	0/2481
1	F	0.45	0/1823	0.59	0/2465
1	G	0.44	0/1829	0.61	0/2473
1	H	0.46	0/1889	0.60	0/2555
All	All	0.48	0/14760	0.61	1/19959 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	146	LEU	CA-CB-CG	6.39	130.01	115.30

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	1807	0	1757	17	0
1	B	1819	0	1758	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1845	0	1784	33	0
1	D	1807	0	1750	24	0
1	E	1811	0	1745	28	0
1	F	1799	0	1744	10	0
1	G	1802	0	1749	37	0
1	H	1859	0	1786	17	0
2	A	13	0	18	3	0
2	D	13	0	18	2	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	185	0	0	2	0
4	B	189	0	0	4	0
4	C	183	0	0	4	0
4	D	148	0	0	6	0
4	E	173	0	0	9	0
4	F	128	0	0	3	0
4	G	113	0	0	5	0
4	H	161	0	0	4	0
All	All	15867	0	14125	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (190) 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:104[A]:ARG:HH11	1:C:119[A]:ARG:CZ	1.24	1.50
1:G:104[B]:ARG:NH2	1:G:104[B]:ARG:HB2	1.57	1.20
1:C:104[A]:ARG:NH1	1:C:119[A]:ARG:CZ	2.03	1.18
1:G:202:SER:HB3	1:G:203:ASP:HB2	1.26	1.18
1:C:104[A]:ARG:HH11	1:C:119[A]:ARG:NE	1.42	1.17
1:C:104[A]:ARG:NH1	1:C:119[A]:ARG:NE	1.93	1.16
1:C:104[A]:ARG:HH11	1:C:119[A]:ARG:NH1	1.45	1.15
1:C:119[A]:ARG:HG3	1:C:119[A]:ARG:HH21	1.01	1.14
1:G:104[B]:ARG:NH2	1:G:104[B]:ARG:CB	2.12	1.13
1:G:104[B]:ARG:HB2	1:G:104[B]:ARG:HH21	1.02	1.10
1:G:202:SER:CB	1:G:203:ASP:HB2	1.80	1.09
1:D:107:ILE:HA	4:D:2074:HOH:O	1.58	1.03
1:G:224:VAL:HG12	1:G:225:TRP:HA	1.42	1.01
1:C:119[A]:ARG:HH21	1:C:119[A]:ARG:CG	1.76	0.99
1:H:227:HIS:HB2	1:H:228:HIS:HA	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104[B]:ARG:CB	1:G:104[B]:ARG:HH21	1.76	0.94
1:E:145:LYS:HE2	4:F:2068:HOH:O	1.68	0.94
1:C:119[A]:ARG:HG3	1:C:119[A]:ARG:NH2	1.82	0.92
1:G:104[B]:ARG:HB3	1:G:104[B]:ARG:CZ	2.02	0.90
1:E:195:ILE:HG13	4:E:2158:HOH:O	1.71	0.88
1:D:116:GLN:HA	4:D:2074:HOH:O	1.77	0.82
1:B:131:VAL:HG12	1:B:132:MET:HE2	1.60	0.82
1:G:104[B]:ARG:NH2	1:G:104[B]:ARG:HB3	1.93	0.81
1:C:104[A]:ARG:NH1	1:C:119[A]:ARG:NH1	2.17	0.80
1:D:119:ARG:HH21	1:D:119:ARG:HG3	1.45	0.80
1:B:119:ARG:HH21	1:B:119:ARG:HG2	1.46	0.80
1:A:125:PHE:HB2	1:A:132:MET:HE2	1.62	0.79
1:G:90:GLU:HG2	1:G:104[A]:ARG:HG2	1.65	0.79
1:G:224:VAL:CG1	1:G:225:TRP:HA	2.13	0.78
1:G:202:SER:HB2	1:G:203:ASP:HB2	1.66	0.77
1:G:65:ASN:HD22	1:G:116:GLN:HE21	1.32	0.77
1:G:104[B]:ARG:CB	1:G:104[B]:ARG:CZ	2.58	0.76
1:C:104[A]:ARG:HE	1:C:119[A]:ARG:NH1	1.85	0.75
1:G:202:SER:CB	1:G:203:ASP:CB	2.64	0.74
1:A:140:GLU:OE2	1:A:168:HIS:HE1	1.70	0.73
1:C:104[A]:ARG:NH1	1:C:119[A]:ARG:HE	1.85	0.73
1:D:90:GLU:HG2	1:D:104[B]:ARG:HG2	1.71	0.73
2:A:1226:PG4:H41	1:B:194:ARG:HH22	1.54	0.71
1:C:145:LYS:HD3	4:C:2043:HOH:O	1.90	0.71
1:D:107:ILE:HD13	4:D:2074:HOH:O	1.91	0.70
4:G:2015:HOH:O	1:H:145:LYS:HD3	1.91	0.70
4:A:2057:HOH:O	1:B:145:LYS:HD3	1.90	0.69
1:B:227:HIS:CD2	4:C:2099:HOH:O	2.45	0.69
1:B:227:HIS:HD2	4:C:2099:HOH:O	1.75	0.69
1:D:90:GLU:HG2	1:D:104[A]:ARG:HG2	1.73	0.69
1:B:146:LEU:CD2	1:B:155:GLY:CA	2.70	0.69
1:B:146:LEU:HD23	1:B:155:GLY:HA2	1.73	0.69
1:D:145:LYS:HE2	4:D:2093:HOH:O	1.93	0.69
1:G:65:ASN:HD22	1:G:116:GLN:NE2	1.92	0.68
1:E:164:GLU:O	4:E:2133:HOH:O	2.11	0.68
1:B:146:LEU:CD2	1:B:155:GLY:HA2	2.25	0.66
1:B:131:VAL:HG12	1:B:132:MET:CE	2.26	0.66
1:C:118:VAL:C	1:C:119[B]:ARG:HE	2.00	0.65
1:H:227:HIS:CB	1:H:228:HIS:HA	2.25	0.64
1:G:173:PHE:HA	4:G:2033:HOH:O	1.97	0.63
1:C:39:THR:HG21	1:C:208:LYS:HE3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119[A]:ARG:CG	1:C:119[A]:ARG:NH2	2.47	0.62
1:B:104[A]:ARG:NH2	1:B:119:ARG:HH12	1.98	0.62
1:G:14:MET:HG2	4:G:2003:HOH:O	1.98	0.62
1:C:104[A]:ARG:NE	1:C:119[A]:ARG:NH1	2.48	0.61
1:G:202:SER:HB2	1:G:203:ASP:CB	2.28	0.61
1:C:43:THR:HB	1:C:45:LYS:HE2	1.81	0.61
1:C:125:PHE:HB2	1:C:132:MET:HE3	1.82	0.61
1:D:119:ARG:HG3	1:D:119:ARG:NH2	2.15	0.60
1:E:146:LEU:HD22	1:E:155:GLY:CA	2.32	0.60
1:H:110:GLU:HG3	4:H:2080:HOH:O	2.02	0.60
1:E:146:LEU:HD22	1:E:155:GLY:HA2	1.82	0.59
1:H:76:PRO:HG3	1:H:184:GLN:HE21	1.67	0.59
1:A:165:GLY:H	1:C:165:GLY:H	1.50	0.58
1:C:194:ARG:HH22	2:D:1226:PG4:H31	1.68	0.58
1:E:144:GLU:HG2	1:E:146:LEU:HD21	1.86	0.58
1:B:146:LEU:CD2	1:B:155:GLY:HA3	2.33	0.58
1:E:66:ARG:O	1:E:69:THR:HG22	2.03	0.58
1:B:104[A]:ARG:HH22	1:B:119:ARG:HH12	1.51	0.57
1:E:184:GLN:NE2	4:E:2143:HOH:O	2.36	0.57
1:B:226:HIS:CE1	4:B:2182:HOH:O	2.57	0.57
1:A:140:GLU:OE2	1:A:168:HIS:CE1	2.56	0.57
1:E:144:GLU:HG2	1:E:146:LEU:CD2	2.34	0.57
1:E:145:LYS:HD3	4:E:2039:HOH:O	2.04	0.57
1:C:104[A]:ARG:CZ	1:C:119[A]:ARG:NH1	2.67	0.57
1:G:202:SER:HB2	1:G:203:ASP:C	2.25	0.56
1:G:90:GLU:OE2	1:G:104[B]:ARG:NH1	2.36	0.56
1:A:221:PRO:HB3	2:A:1226:PG4:H81	1.86	0.56
1:B:145:LYS:HE3	4:B:2119:HOH:O	2.04	0.56
1:E:66:ARG:O	1:E:69:THR:CG2	2.54	0.55
1:B:128:ASN:N	4:B:2104:HOH:O	2.40	0.55
1:F:26:GLU:OE1	1:F:45:LYS:HE2	2.06	0.55
1:G:202:SER:HB2	1:G:203:ASP:CA	2.36	0.55
1:C:99:GLY:O	1:C:100:ILE:HD13	2.07	0.54
1:C:104[A]:ARG:HH12	1:C:119[A]:ARG:NE	1.98	0.54
1:G:106:ASP:HB2	4:G:2046:HOH:O	2.07	0.54
1:E:225:TRP:CH2	1:E:227:HIS:C	2.81	0.54
1:G:201:ASP:HB2	1:G:206:LYS:HB2	1.89	0.54
1:H:17:ASN:ND2	4:H:2007:HOH:O	2.32	0.54
1:B:127:PRO:HB2	4:B:2104:HOH:O	2.08	0.54
1:C:117:ASN:OD1	1:C:119[B]:ARG:NH1	2.41	0.54
1:C:125:PHE:HB2	1:C:132:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:NH2	1:D:168:HIS:O	2.39	0.54
1:B:224:VAL:O	1:B:226:HIS:CE1	2.61	0.54
4:E:2045:HOH:O	1:F:145:LYS:HD3	2.08	0.53
4:C:2114:HOH:O	1:D:145:LYS:HE3	2.09	0.52
1:A:9:ARG:HH11	1:A:30:LYS:HB3	1.74	0.52
1:B:81:GLN:O	1:B:181:LYS:HE3	2.09	0.52
1:B:146:LEU:HD22	1:B:155:GLY:CA	2.40	0.52
1:G:14:MET:HG3	1:G:118:VAL:HB	1.92	0.51
1:D:121:LYS:HE2	4:D:2010:HOH:O	2.09	0.51
1:D:65:ASN:OD1	1:D:67:VAL:HG23	2.11	0.50
1:E:146:LEU:CD2	1:E:155:GLY:HA2	2.41	0.50
1:G:43:THR:HA	1:G:205:ASN:O	2.11	0.50
1:E:191:VAL:CG2	4:E:2050:HOH:O	2.59	0.50
1:E:191:VAL:HG22	4:E:2050:HOH:O	2.11	0.50
2:A:1226:PG4:H41	1:B:194:ARG:NH2	2.24	0.50
1:C:26:GLU:OE1	1:C:45:LYS:HE3	2.12	0.49
1:A:16:GLY:HA3	1:A:23:PHE:CZ	2.47	0.49
1:C:104[A]:ARG:HE	1:C:119[A]:ARG:HH12	1.59	0.49
1:D:146:LEU:HD13	1:D:155:GLY:CA	2.43	0.49
1:E:226:HIS:O	1:E:227:HIS:HB2	2.12	0.49
1:D:192:ASP:O	1:D:213:ALA:HA	2.11	0.49
1:A:90:GLU:OE2	1:A:104[A]:ARG:NE	2.46	0.48
1:E:76:PRO:HG3	1:E:184:GLN:HE21	1.78	0.48
1:B:90:GLU:HG2	1:B:104[A]:ARG:HG2	1.95	0.48
1:E:27:GLY:HA3	1:E:42:LEU:HD23	1.95	0.48
1:B:119:ARG:HG2	1:B:119:ARG:NH2	2.21	0.48
1:D:136:THR:HG21	1:D:161:LEU:HD13	1.95	0.48
1:E:64:5SQ:C2H	4:E:2158:HOH:O	2.61	0.48
1:E:220:LEU:HD22	1:F:212:HIS:CE1	2.50	0.47
1:G:170:LEU:HD11	1:H:147:HIS:CE1	2.49	0.47
1:E:135:LYS:HE3	1:E:164:GLU:OE1	2.14	0.47
1:G:32:LYS:HD2	1:G:35:GLU:OE1	2.14	0.47
1:G:91:ARG:HG3	4:G:2033:HOH:O	2.14	0.47
1:C:27:GLY:HA3	1:C:42:LEU:HD23	1.96	0.47
1:A:36:GLY:O	1:A:212:HIS:HA	2.15	0.46
1:E:17:ASN:HD21	1:E:20:GLY:HA2	1.80	0.46
1:G:202:SER:CB	1:G:203:ASP:CA	2.93	0.46
1:A:124:ASN:HB2	4:A:2102:HOH:O	2.16	0.46
1:F:93:MET:HB2	1:F:101:CYS:HB2	1.98	0.46
1:H:228:HIS:CG	1:H:229:HIS:N	2.83	0.46
1:C:140:GLU:OE2	1:C:168:HIS:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG2	1:A:104[A]:ARG:HG2	1.97	0.45
1:F:92:THR:HG23	4:F:2092:HOH:O	2.16	0.45
1:G:107:ILE:HD12	1:G:116:GLN:HG2	1.98	0.45
1:A:128:ASN:HB3	1:D:225:TRP:CH2	2.51	0.45
1:E:145:LYS:C	1:E:146:LEU:HD23	2.37	0.45
1:H:93:MET:HB2	1:H:101:CYS:HB2	1.98	0.45
1:E:165:GLY:H	1:G:165:GLY:H	1.64	0.44
1:G:148:VAL:HG11	1:G:185:LEU:HD13	2.00	0.44
1:B:225:TRP:CZ2	1:B:227:HIS:HA	2.53	0.44
1:G:93:MET:HB2	1:G:101:CYS:HB2	2.00	0.44
1:A:93:MET:HB2	1:A:101:CYS:HB2	2.00	0.43
1:H:90:GLU:HG2	1:H:104:ARG:HG2	2.01	0.43
1:B:21:HIS:HE1	1:B:47:GLY:O	2.01	0.43
1:C:224:VAL:O	1:C:226:HIS:CD2	2.71	0.43
1:D:55:ASP:HB3	1:D:161:LEU:HD21	2.00	0.43
1:B:93:MET:HB2	1:B:101:CYS:HB2	2.01	0.43
1:G:202:SER:HB3	1:G:203:ASP:CB	2.18	0.43
1:C:2:ASN:HD22	1:C:2:ASN:N	2.15	0.43
1:E:17:ASN:HD21	1:E:20:GLY:CA	2.31	0.43
1:C:93:MET:HB2	1:C:101:CYS:HB2	1.99	0.43
1:A:146:LEU:HA	1:A:154:VAL:O	2.18	0.43
1:D:67:VAL:HG11	1:D:114:PHE:CZ	2.54	0.43
1:B:93:MET:HG2	1:B:173:PHE:CE1	2.54	0.42
1:E:149:ARG:NH2	4:E:2124:HOH:O	2.44	0.42
1:F:115:PHE:CE2	1:F:117:ASN:HB2	2.54	0.42
1:B:104[A]:ARG:NH2	1:B:119:ARG:NH1	2.66	0.42
1:D:2:ASN:N	1:D:4:ILE:H	2.18	0.42
1:G:26:GLU:OE2	1:G:45:LYS:HG3	2.19	0.42
1:D:217:TYR:HB3	2:D:1226:PG4:H32	2.02	0.42
1:H:17:ASN:HD21	1:H:20:GLY:CA	2.33	0.42
1:H:87:TYR:CZ	1:H:107:ILE:HG13	2.55	0.42
1:D:126:PRO:HA	1:D:127:PRO:HD3	1.84	0.41
1:G:3:LEU:HD23	1:G:109:LEU:HD23	2.01	0.41
1:H:203:ASP:N	4:H:2142:HOH:O	2.12	0.41
1:A:159:MET:HG3	1:A:173:PHE:CD1	2.56	0.41
1:B:97:ASP:O	1:B:98:LYS:HB2	2.21	0.41
1:D:197:ILE:HD12	4:D:2031:HOH:O	2.19	0.41
1:F:83:PHE:CE1	1:F:109:LEU:HB2	2.56	0.41
1:H:27:GLY:HA3	1:H:42:LEU:HD23	2.02	0.41
1:H:224:VAL:O	1:H:226:HIS:HD2	2.04	0.41
1:E:144:GLU:CG	1:E:146:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:HIS:HB3	4:H:2159:HOH:O	2.20	0.41
1:H:84:PRO:HD2	1:H:85:GLU:OE1	2.21	0.41
1:A:125:PHE:HB2	1:A:132:MET:CE	2.43	0.40
1:D:83:PHE:HB3	1:D:84:PRO:HA	2.03	0.40
1:F:43:THR:HA	1:F:205:ASN:O	2.21	0.40
1:D:32:LYS:HE3	1:D:35:GLU:CD	2.41	0.40
1:E:126:PRO:HA	1:E:127:PRO:HD3	1.93	0.40
1:F:166:GLY:HA2	4:F:2087:HOH:O	2.20	0.40
1:B:36:GLY:O	1:B:212:HIS:HA	2.21	0.40
1:A:72:PRO:HG2	1:A:75:ILE:HG13	2.04	0.40
1:F:224:VAL:O	1:F:225:TRP:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/229 (95%)	216 (99%)	2 (1%)	0	100	100
1	B	219/229 (96%)	217 (99%)	2 (1%)	0	100	100
1	C	222/229 (97%)	217 (98%)	5 (2%)	0	100	100
1	D	218/229 (95%)	216 (99%)	2 (1%)	0	100	100
1	E	218/229 (95%)	217 (100%)	1 (0%)	0	100	100
1	F	217/229 (95%)	215 (99%)	2 (1%)	0	100	100
1	G	218/229 (95%)	214 (98%)	3 (1%)	1 (0%)	29	23
1	H	223/229 (97%)	218 (98%)	5 (2%)	0	100	100
All	All	1753/1832 (96%)	1730 (99%)	22 (1%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	202	SER

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	195/201 (97%)	193 (99%)	2 (1%)	76	81
1	B	196/201 (98%)	194 (99%)	2 (1%)	76	81
1	C	199/201 (99%)	196 (98%)	3 (2%)	65	69
1	D	195/201 (97%)	194 (100%)	1 (0%)	88	92
1	E	195/201 (97%)	189 (97%)	6 (3%)	40	40
1	F	194/201 (96%)	191 (98%)	3 (2%)	65	69
1	G	195/201 (97%)	186 (95%)	9 (5%)	27	23
1	H	200/201 (100%)	196 (98%)	4 (2%)	55	58
All	All	1569/1608 (98%)	1539 (98%)	30 (2%)	57	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	150	ASP
1	B	119	ARG
1	B	226	HIS
1	C	17	ASN
1	C	119[A]	ARG
1	C	119[B]	ARG
1	D	17	ASN
1	E	17	ASN
1	E	30	LYS
1	E	69	THR
1	E	119	ARG
1	E	202	SER
1	E	226	HIS
1	F	3	LEU

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Mol	Chain	Res	Type
1	F	7	ASP
1	F	15	GLU
1	G	67	VAL
1	G	98	LYS
1	G	105	SER
1	G	119	ARG
1	G	123	THR
1	G	124	ASN
1	G	150	ASP
1	G	201	ASP
1	G	211	GLU
1	H	17	ASN
1	H	28	GLU
1	H	45	LYS
1	H	231	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	133	GLN
1	A	156	ASN
1	A	168	HIS
1	B	21	HIS
1	B	184	GLN
1	B	200	ASN
1	B	205	ASN
1	B	226	HIS
1	B	227	HIS
1	C	17	ASN
1	C	168	HIS
1	C	200	ASN
1	D	17	ASN
1	D	21	HIS
1	D	128	ASN
1	E	17	ASN
1	E	21	HIS
1	E	184	GLN
1	F	41	ASN
1	F	184	GLN
1	F	205	ASN
1	G	116	GLN

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Mol	Chain	Res	Type
1	H	17	ASN
1	H	21	HIS
1	H	184	GLN
1	H	227	HIS
1	H	228	HIS

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	5SQ	F	64	1	23,27,28	4.73	6 (26%)	29,37,39	4.16	8 (27%)
1	5SQ	H	64	1	23,27,28	4.59	6 (26%)	29,37,39	4.38	8 (27%)
1	5SQ	G	64	1	23,27,28	4.45	6 (26%)	29,37,39	4.24	7 (24%)
1	5SQ	C	64	1	23,27,28	4.24	6 (26%)	29,37,39	3.96	7 (24%)
1	5SQ	A	64	1	23,27,28	4.27	6 (26%)	29,37,39	4.22	7 (24%)
1	5SQ	B	64	1	23,27,28	4.26	6 (26%)	29,37,39	4.04	9 (31%)
1	5SQ	D	64	1	23,27,28	4.34	6 (26%)	29,37,39	4.39	8 (27%)
1	5SQ	E	64	1	23,27,28	4.41	6 (26%)	29,37,39	4.12	8 (27%)

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	5SQ	F	64	1	-	4/12/31/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5SQ	H	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	G	64	1	-	3/12/31/32	0/3/3/3
1	5SQ	C	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	A	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	B	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	D	64	1	-	4/12/31/32	0/3/3/3
1	5SQ	E	64	1	-	3/12/31/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	64	5SQ	CB2-CA2	18.25	1.50	1.35
1	H	64	5SQ	CB2-CA2	16.98	1.49	1.35
1	G	64	5SQ	CB2-CA2	16.65	1.49	1.35
1	E	64	5SQ	CB2-CA2	16.29	1.48	1.35
1	B	64	5SQ	CB2-CA2	16.12	1.48	1.35
1	D	64	5SQ	CB2-CA2	15.71	1.48	1.35
1	C	64	5SQ	CB2-CA2	15.28	1.47	1.35
1	A	64	5SQ	CB2-CA2	15.14	1.47	1.35
1	H	64	5SQ	CA2-C2	-11.80	1.37	1.48
1	A	64	5SQ	CA2-C2	-11.66	1.37	1.48
1	D	64	5SQ	CA2-C2	-11.22	1.37	1.48
1	E	64	5SQ	CA2-C2	-10.95	1.37	1.48
1	F	64	5SQ	CA2-C2	-10.80	1.38	1.48
1	G	64	5SQ	CA2-C2	-10.74	1.38	1.48
1	C	64	5SQ	CA2-C2	-10.69	1.38	1.48
1	B	64	5SQ	CA2-C2	-10.05	1.38	1.48
1	E	64	5SQ	OH-CZ1	-4.69	1.26	1.37
1	F	64	5SQ	OH-CZ1	-4.60	1.26	1.37
1	D	64	5SQ	C1-N2	4.60	1.39	1.32
1	C	64	5SQ	OH-CZ1	-4.48	1.26	1.37
1	D	64	5SQ	OH-CZ1	-4.46	1.26	1.37
1	H	64	5SQ	OH-CZ1	-4.41	1.26	1.37
1	F	64	5SQ	C1-N2	4.41	1.38	1.32
1	G	64	5SQ	OH-CZ1	-4.39	1.26	1.37
1	C	64	5SQ	C1-N2	4.37	1.38	1.32
1	G	64	5SQ	C1-N2	4.24	1.38	1.32
1	E	64	5SQ	C1-N2	4.13	1.38	1.32
1	A	64	5SQ	OH-CZ1	-4.11	1.27	1.37
1	A	64	5SQ	C1-N2	4.08	1.38	1.32
1	H	64	5SQ	C1-N2	4.03	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	5SQ	C1-N2	4.01	1.38	1.32
1	B	64	5SQ	OH-CZ1	-3.55	1.28	1.37
1	C	64	5SQ	O2-C2	3.44	1.30	1.23
1	B	64	5SQ	O2-C2	3.09	1.29	1.23
1	A	64	5SQ	O2-C2	2.98	1.29	1.23
1	D	64	5SQ	O2-C2	2.90	1.29	1.23
1	E	64	5SQ	C2-N3	-2.90	1.33	1.39
1	F	64	5SQ	O2-C2	2.83	1.29	1.23
1	H	64	5SQ	O2-C2	2.72	1.28	1.23
1	F	64	5SQ	C2-N3	-2.71	1.33	1.39
1	G	64	5SQ	O2-C2	2.68	1.28	1.23
1	H	64	5SQ	C2-N3	-2.58	1.33	1.39
1	D	64	5SQ	C2-N3	-2.50	1.34	1.39
1	G	64	5SQ	C2-N3	-2.49	1.34	1.39
1	B	64	5SQ	C2-N3	-2.45	1.34	1.39
1	E	64	5SQ	O2-C2	2.37	1.28	1.23
1	C	64	5SQ	C2-N3	-2.33	1.34	1.39
1	A	64	5SQ	C2-N3	-2.30	1.34	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	64	5SQ	CA2-C2-N3	16.84	111.33	103.37
1	F	64	5SQ	CA2-C2-N3	16.75	111.29	103.37
1	E	64	5SQ	CA2-C2-N3	16.38	111.12	103.37
1	H	64	5SQ	CA2-C2-N3	15.79	110.84	103.37
1	D	64	5SQ	CA2-C2-N3	15.36	110.64	103.37
1	A	64	5SQ	O2-C2-CA2	-15.15	122.46	130.96
1	B	64	5SQ	CA2-C2-N3	15.03	110.48	103.37
1	D	64	5SQ	O2-C2-CA2	-14.74	122.69	130.96
1	H	64	5SQ	O2-C2-CA2	-14.29	122.94	130.96
1	C	64	5SQ	CA2-C2-N3	14.21	110.09	103.37
1	A	64	5SQ	CA2-C2-N3	13.96	109.97	103.37
1	C	64	5SQ	O2-C2-CA2	-12.61	123.88	130.96
1	E	64	5SQ	O2-C2-CA2	-11.29	124.62	130.96
1	G	64	5SQ	O2-C2-CA2	-11.05	124.76	130.96
1	F	64	5SQ	O2-C2-CA2	-10.76	124.92	130.96
1	B	64	5SQ	O2-C2-CA2	-10.71	124.94	130.96
1	B	64	5SQ	C2-N3-C1	-6.78	104.54	107.97
1	G	64	5SQ	C2-N3-C1	-6.52	104.67	107.97
1	H	64	5SQ	C2-N3-C1	-6.44	104.71	107.97
1	F	64	5SQ	C2-N3-C1	-6.08	104.89	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	64	5SQ	C2-N3-C1	-6.05	104.90	107.97
1	E	64	5SQ	C2-N3-C1	-5.94	104.96	107.97
1	C	64	5SQ	C2-N3-C1	-5.83	105.02	107.97
1	G	64	5SQ	CB2-CA2-C2	5.45	128.79	122.28
1	F	64	5SQ	CB2-CA2-C2	4.81	128.02	122.28
1	B	64	5SQ	CB2-CA2-C2	4.78	127.98	122.28
1	A	64	5SQ	C2-N3-C1	-4.60	105.64	107.97
1	C	64	5SQ	CB2-CA2-C2	3.85	126.88	122.28
1	E	64	5SQ	CB2-CA2-C2	3.78	126.79	122.28
1	B	64	5SQ	CB2-CA2-N2	-3.66	123.76	128.83
1	A	64	5SQ	CA3-N3-C1	-3.58	122.87	127.16
1	H	64	5SQ	O3-C3-CA3	-3.48	115.89	126.39
1	D	64	5SQ	CA3-N3-C2	3.41	131.61	123.80
1	H	64	5SQ	CB2-CA2-C2	3.37	126.30	122.28
1	G	64	5SQ	CB2-CA2-N2	-3.37	124.16	128.83
1	E	64	5SQ	O3-C3-CA3	-3.36	116.24	126.39
1	A	64	5SQ	CA3-N3-C2	3.35	131.49	123.80
1	A	64	5SQ	O3-C3-CA3	-3.21	116.69	126.39
1	B	64	5SQ	O3-C3-CA3	-3.21	116.70	126.39
1	D	64	5SQ	O3-C3-CA3	-3.19	116.76	126.39
1	C	64	5SQ	CB2-CA2-N2	-3.18	124.42	128.83
1	F	64	5SQ	O3-C3-CA3	-3.07	117.13	126.39
1	D	64	5SQ	CA3-N3-C1	-3.07	123.48	127.16
1	F	64	5SQ	CB2-CA2-N2	-3.01	124.65	128.83
1	B	64	5SQ	CA3-N3-C2	3.00	130.69	123.80
1	H	64	5SQ	CA3-N3-C2	2.96	130.58	123.80
1	G	64	5SQ	O3-C3-CA3	-2.93	117.53	126.39
1	G	64	5SQ	C2-CA2-N2	-2.68	107.05	108.93
1	A	64	5SQ	CB2-CA2-C2	2.63	125.42	122.28
1	C	64	5SQ	CA3-N3-C2	2.57	129.70	123.80
1	D	64	5SQ	CA1-C1-N3	-2.56	121.52	124.85
1	D	64	5SQ	CB2-CA2-C2	2.41	125.16	122.28
1	E	64	5SQ	CB2-CA2-N2	-2.34	125.58	128.83
1	H	64	5SQ	CB2-CA2-N2	-2.31	125.62	128.83
1	F	64	5SQ	C2-CA2-N2	-2.29	107.33	108.93
1	F	64	5SQ	CA3-N3-C2	2.22	128.90	123.80
1	C	64	5SQ	CD1-CG2-CB2	-2.18	113.78	121.22
1	H	64	5SQ	CA3-N3-C1	-2.15	124.58	127.16
1	E	64	5SQ	CD1-CG2-CB2	-2.14	113.94	121.22
1	E	64	5SQ	CA3-N3-C2	2.12	128.67	123.80
1	B	64	5SQ	CD1-CG2-CB2	-2.04	114.28	121.22
1	B	64	5SQ	CA3-N3-C1	-2.00	124.76	127.16

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	5SQ	C3-CA3-N3-C1
1	A	64	5SQ	C3-CA3-N3-C2
1	A	64	5SQ	CA1-CB1-CG1-C2H
1	A	64	5SQ	CA1-CB1-CG1-N1H
1	B	64	5SQ	C3-CA3-N3-C2
1	B	64	5SQ	CA1-CB1-CG1-N1H
1	C	64	5SQ	C3-CA3-N3-C2
1	C	64	5SQ	CA1-CB1-CG1-C2H
1	C	64	5SQ	CA1-CB1-CG1-N1H
1	D	64	5SQ	C3-CA3-N3-C1
1	D	64	5SQ	C3-CA3-N3-C2
1	D	64	5SQ	CA1-CB1-CG1-C2H
1	D	64	5SQ	CA1-CB1-CG1-N1H
1	E	64	5SQ	C3-CA3-N3-C2
1	E	64	5SQ	CA1-CB1-CG1-C2H
1	E	64	5SQ	CA1-CB1-CG1-N1H
1	F	64	5SQ	C3-CA3-N3-C2
1	F	64	5SQ	CA1-CB1-CG1-C2H
1	F	64	5SQ	CA1-CB1-CG1-N1H
1	G	64	5SQ	C3-CA3-N3-C2
1	G	64	5SQ	CA1-CB1-CG1-C2H
1	G	64	5SQ	CA1-CB1-CG1-N1H
1	H	64	5SQ	C3-CA3-N3-C2
1	H	64	5SQ	CA1-CB1-CG1-N1H
1	C	64	5SQ	C3-CA3-N3-C1
1	B	64	5SQ	CA1-CB1-CG1-C2H
1	H	64	5SQ	CA1-CB1-CG1-C2H
1	B	64	5SQ	C3-CA3-N3-C1
1	F	64	5SQ	C3-CA3-N3-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	64	5SQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
3	GOL	B	1228	-	5,5,5	0.39	0	5,5,5	0.24	0
2	PG4	A	1226	-	12,12,12	0.58	0	11,11,11	0.42	0
3	GOL	C	1229	-	5,5,5	0.43	0	5,5,5	0.34	0
2	PG4	D	1226	-	12,12,12	0.59	0	11,11,11	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
3	GOL	B	1228	-	-	4/4/4/4	-
2	PG4	A	1226	-	-	4/10/10/10	-
3	GOL	C	1229	-	-	2/4/4/4	-
2	PG4	D	1226	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1228	GOL	O1-C1-C2-C3
3	B	1228	GOL	C1-C2-C3-O3
2	D	1226	PG4	O2-C3-C4-O3
2	A	1226	PG4	O2-C3-C4-O3
2	D	1226	PG4	O3-C5-C6-O4
2	A	1226	PG4	O3-C5-C6-O4
3	B	1228	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	1226	PG4	O4-C7-C8-O5
2	D	1226	PG4	O1-C1-C2-O2
3	C	1229	GOL	C1-C2-C3-O3
3	B	1228	GOL	O1-C1-C2-O2
2	D	1226	PG4	C5-C6-O4-C7
2	D	1226	PG4	C8-C7-O4-C6
2	D	1226	PG4	C6-C5-O3-C4
2	A	1226	PG4	C8-C7-O4-C6
3	C	1229	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1226	PG4	3	0
2	D	1226	PG4	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

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, 95^{th} 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	220/229 (96%)	0.11	4 (1%)	68	66	10, 20, 28, 39	0
1	B	222/229 (96%)	0.01	4 (1%)	68	66	10, 17, 25, 32	0
1	C	224/229 (97%)	0.13	6 (2%)	54	53	10, 20, 30, 39	0
1	D	221/229 (96%)	0.14	5 (2%)	60	59	11, 20, 29, 42	0
1	E	222/229 (96%)	-0.01	4 (1%)	68	66	9, 17, 26, 39	0
1	F	220/229 (96%)	0.42	10 (4%)	33	32	13, 26, 37, 42	0
1	G	220/229 (96%)	0.76	19 (8%)	10	9	15, 30, 44, 48	0
1	H	226/229 (98%)	0.12	7 (3%)	49	48	11, 19, 31, 53	0
All	All	1775/1832 (96%)	0.21	59 (3%)	46	45	9, 20, 37, 53	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	TRP	7.1
1	A	225	TRP	7.0
1	G	225	TRP	6.6
1	F	225	TRP	6.3
1	H	228	HIS	6.0
1	D	2	ASN	5.0
1	H	227	HIS	4.7
1	C	227	HIS	4.4
1	C	228	HIS	4.3
1	E	227	HIS	4.3
1	G	128	ASN	4.3
1	H	229	HIS	4.1
1	G	201	ASP	3.8
1	B	227	HIS	3.7
1	C	2	ASN	3.7
1	E	226	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	112	ASP	3.3
1	D	127	PRO	3.3
1	H	226	HIS	3.3
1	H	230	HIS	3.2
1	G	127	PRO	2.9
1	F	202	SER	2.9
1	G	3	LEU	2.9
1	G	132	MET	2.9
1	D	3	LEU	2.8
1	G	6	GLU	2.8
1	D	157	ILE	2.8
1	G	202	SER	2.8
1	E	202	SER	2.8
1	H	202	SER	2.7
1	A	157	ILE	2.7
1	F	128	ASN	2.7
1	F	127	PRO	2.6
1	G	4	ILE	2.6
1	F	73	GLU	2.5
1	C	73	GLU	2.5
1	G	224	VAL	2.5
1	G	49	PRO	2.5
1	F	4	ILE	2.5
1	G	133	GLN	2.5
1	B	226	HIS	2.4
1	G	50	LEU	2.3
1	G	203	ASP	2.3
1	F	3	LEU	2.3
1	G	51	PRO	2.3
1	G	184	GLN	2.3
1	A	128	ASN	2.2
1	A	73	GLU	2.2
1	E	157	ILE	2.2
1	F	112	ASP	2.2
1	C	157	ILE	2.1
1	F	150	ASP	2.1
1	H	157	ILE	2.1
1	C	119[A]	ARG	2.1
1	G	43	THR	2.1
1	B	157	ILE	2.0
1	G	126	PRO	2.0
1	F	74	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	73	GLU	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, 95^{th} 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	5SQ	G	64	25/26	0.87	0.15	12,23,28,28	0
1	5SQ	C	64	25/26	0.90	0.15	6,16,18,18	0
1	5SQ	A	64	25/26	0.91	0.15	9,16,17,18	0
1	5SQ	F	64	25/26	0.91	0.14	15,20,24,24	0
1	5SQ	B	64	25/26	0.91	0.14	10,12,14,15	0
1	5SQ	D	64	25/26	0.94	0.15	9,14,17,18	0
1	5SQ	H	64	25/26	0.94	0.14	7,11,14,15	0
1	5SQ	E	64	25/26	0.95	0.15	10,12,14,14	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, 95^{th} 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	GOL	B	1228	6/6	0.71	0.15	43,43,44,44	0
3	GOL	C	1229	6/6	0.73	0.14	33,35,36,37	0
2	PG4	D	1226	13/13	0.82	0.15	32,34,35,35	0
2	PG4	A	1226	13/13	0.85	0.14	31,34,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.