Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:08 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

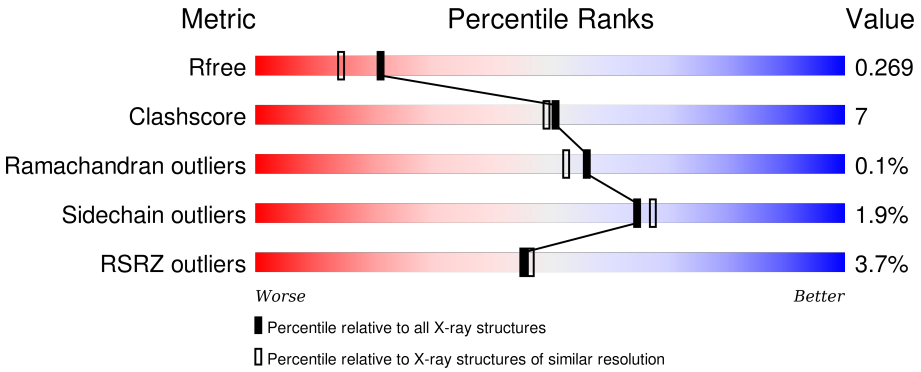
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 84% 12% •
1	B	229	2% 85% 11% • •
1	C	229	3% 86% 12% •
1	D	229	3% 84% 13% •
1	E	229	2% 85% 11% • •

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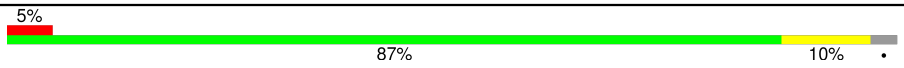
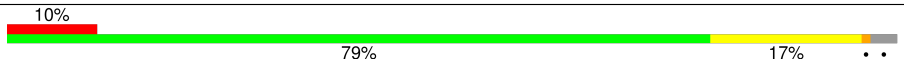
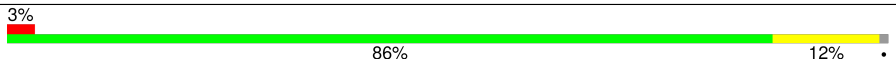
Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	

2 Entry composition

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 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	LEU	CONFLICT	UNP Q8T6U0
A	61	VAL	LEU	CONFLICT	UNP Q8T6U0
A	95	PHE	TYR	CONFLICT	UNP Q8T6U0
A	121	LYS	ASN	CONFLICT	UNP Q8T6U0
A	123	THR	MET	CONFLICT	UNP Q8T6U0
A	188	ALA	TYR	CONFLICT	UNP Q8T6U0
A	199	GLY	SER	CONFLICT	UNP Q8T6U0
A	213	ALA	GLY	CONFLICT	UNP Q8T6U0
A	224	VAL	ALA	CONFLICT	UNP Q8T6U0
B	40	ALA	LEU	CONFLICT	UNP Q8T6U0
B	61	VAL	LEU	CONFLICT	UNP Q8T6U0
B	95	PHE	TYR	CONFLICT	UNP Q8T6U0
B	121	LYS	ASN	CONFLICT	UNP Q8T6U0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	THR	MET	CONFLICT	UNP Q8T6U0
B	188	ALA	TYR	CONFLICT	UNP Q8T6U0
B	199	GLY	SER	CONFLICT	UNP Q8T6U0
B	213	ALA	GLY	CONFLICT	UNP Q8T6U0
B	224	VAL	ALA	CONFLICT	UNP Q8T6U0
C	40	ALA	LEU	CONFLICT	UNP Q8T6U0
C	61	VAL	LEU	CONFLICT	UNP Q8T6U0
C	95	PHE	TYR	CONFLICT	UNP Q8T6U0
C	121	LYS	ASN	CONFLICT	UNP Q8T6U0
C	123	THR	MET	CONFLICT	UNP Q8T6U0
C	188	ALA	TYR	CONFLICT	UNP Q8T6U0
C	199	GLY	SER	CONFLICT	UNP Q8T6U0
C	213	ALA	GLY	CONFLICT	UNP Q8T6U0
C	224	VAL	ALA	CONFLICT	UNP Q8T6U0
D	40	ALA	LEU	CONFLICT	UNP Q8T6U0
D	61	VAL	LEU	CONFLICT	UNP Q8T6U0
D	95	PHE	TYR	CONFLICT	UNP Q8T6U0
D	121	LYS	ASN	CONFLICT	UNP Q8T6U0
D	123	THR	MET	CONFLICT	UNP Q8T6U0
D	188	ALA	TYR	CONFLICT	UNP Q8T6U0
D	199	GLY	SER	CONFLICT	UNP Q8T6U0
D	213	ALA	GLY	CONFLICT	UNP Q8T6U0
D	224	VAL	ALA	CONFLICT	UNP Q8T6U0
E	40	ALA	LEU	CONFLICT	UNP Q8T6U0
E	61	VAL	LEU	CONFLICT	UNP Q8T6U0
E	95	PHE	TYR	CONFLICT	UNP Q8T6U0
E	121	LYS	ASN	CONFLICT	UNP Q8T6U0
E	123	THR	MET	CONFLICT	UNP Q8T6U0
E	188	ALA	TYR	CONFLICT	UNP Q8T6U0
E	199	GLY	SER	CONFLICT	UNP Q8T6U0
E	213	ALA	GLY	CONFLICT	UNP Q8T6U0
E	224	VAL	ALA	CONFLICT	UNP Q8T6U0
F	40	ALA	LEU	CONFLICT	UNP Q8T6U0
F	61	VAL	LEU	CONFLICT	UNP Q8T6U0
F	95	PHE	TYR	CONFLICT	UNP Q8T6U0
F	121	LYS	ASN	CONFLICT	UNP Q8T6U0
F	123	THR	MET	CONFLICT	UNP Q8T6U0
F	188	ALA	TYR	CONFLICT	UNP Q8T6U0
F	199	GLY	SER	CONFLICT	UNP Q8T6U0
F	213	ALA	GLY	CONFLICT	UNP Q8T6U0
F	224	VAL	ALA	CONFLICT	UNP Q8T6U0
G	40	ALA	LEU	CONFLICT	UNP Q8T6U0

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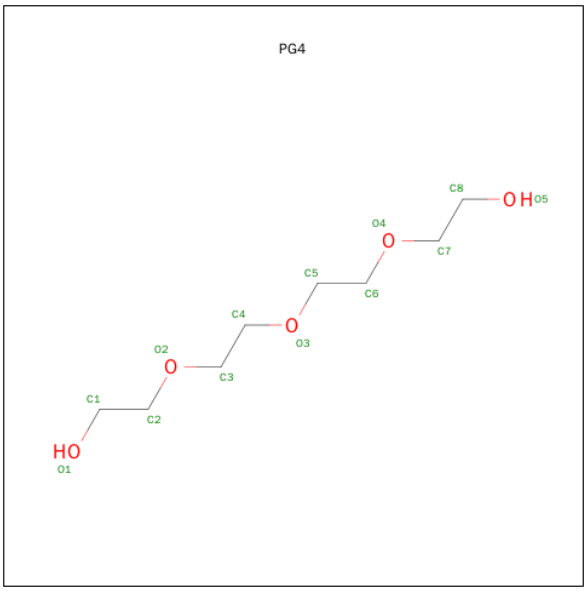
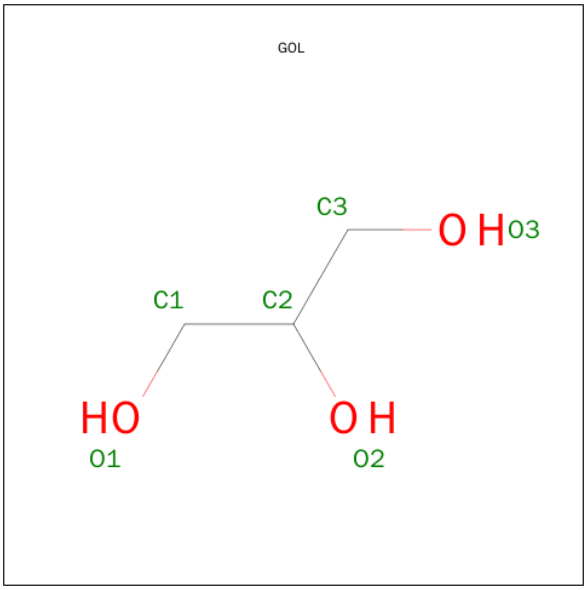
Chain	Residue	Modelled	Actual	Comment	Reference
G	61	VAL	LEU	CONFLICT	UNP Q8T6U0
G	95	PHE	TYR	CONFLICT	UNP Q8T6U0
G	121	LYS	ASN	CONFLICT	UNP Q8T6U0
G	123	THR	MET	CONFLICT	UNP Q8T6U0
G	188	ALA	TYR	CONFLICT	UNP Q8T6U0
G	199	GLY	SER	CONFLICT	UNP Q8T6U0
G	213	ALA	GLY	CONFLICT	UNP Q8T6U0
G	224	VAL	ALA	CONFLICT	UNP Q8T6U0
H	40	ALA	LEU	CONFLICT	UNP Q8T6U0
H	61	VAL	LEU	CONFLICT	UNP Q8T6U0
H	95	PHE	TYR	CONFLICT	UNP Q8T6U0
H	121	LYS	ASN	CONFLICT	UNP Q8T6U0
H	123	THR	MET	CONFLICT	UNP Q8T6U0
H	188	ALA	TYR	CONFLICT	UNP Q8T6U0
H	199	GLY	SER	CONFLICT	UNP Q8T6U0
H	213	ALA	GLY	CONFLICT	UNP Q8T6U0
H	224	VAL	ALA	CONFLICT	UNP Q8T6U0
A	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
A	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
A	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
B	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
B	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
B	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
C	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
C	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
C	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
D	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
D	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
D	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
E	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
E	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
E	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
F	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
F	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
F	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
G	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
G	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
G	64	CR8	GLY	CHROMOPHORE	UNP Q8T6U0
H	64	CR8	HIS	CHROMOPHORE	UNP Q8T6U0
H	64	CR8	TYR	CHROMOPHORE	UNP Q8T6U0
H	64	CR8	GLY	CHROMOPHORE	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.

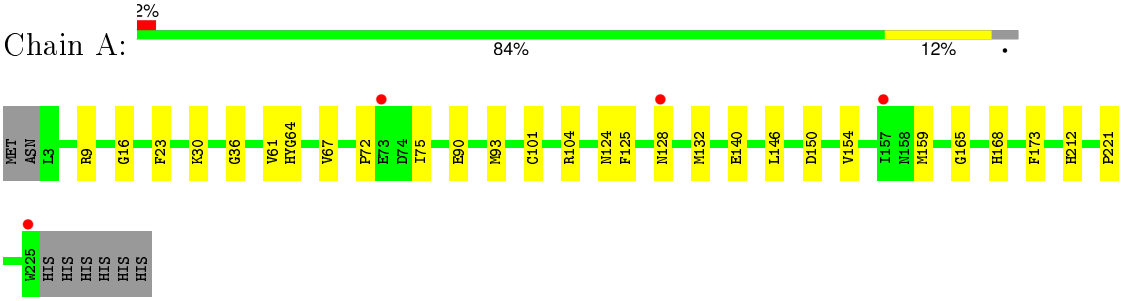
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	185	Total O 185 185	0	0
4	B	189	Total O 189 189	0	0
4	C	183	Total O 183 183	0	0
4	D	148	Total O 148 148	0	0
4	E	173	Total O 173 173	0	0
4	F	128	Total O 128 128	0	0
4	G	113	Total O 113 113	0	0
4	H	161	Total O 161 161	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

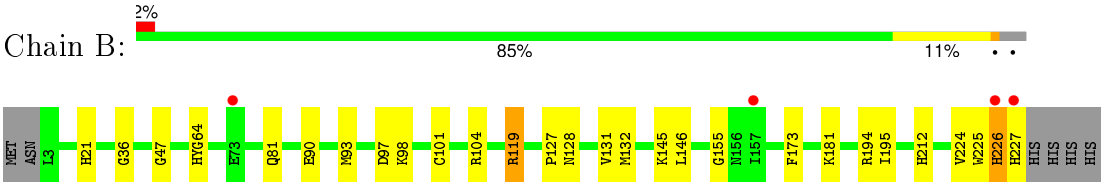
- Molecule 1: GREEN FLUORESCENT PROTEIN

Chain A:



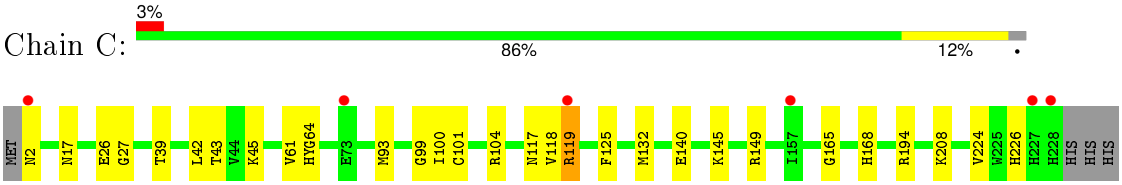
- Molecule 1: GREEN FLUORESCENT PROTEIN

Chain B:



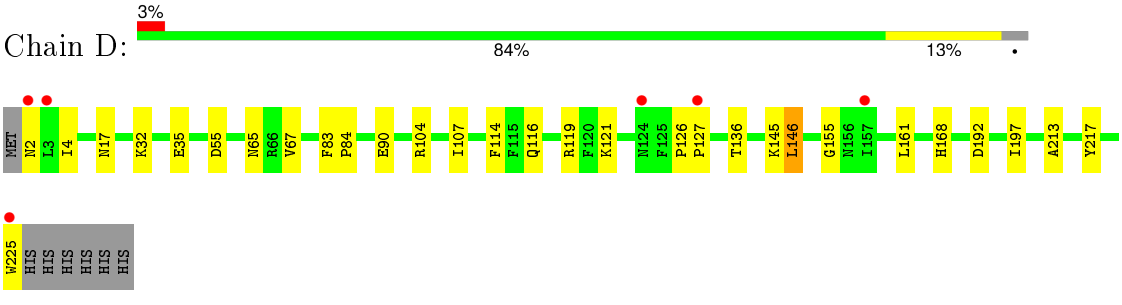
- Molecule 1: GREEN FLUORESCENT PROTEIN

Chain C:



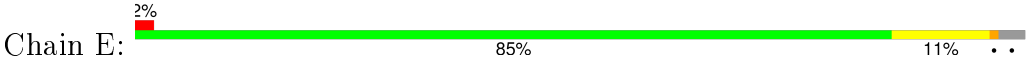
- Molecule 1: GREEN FLUORESCENT PROTEIN

Chain D:



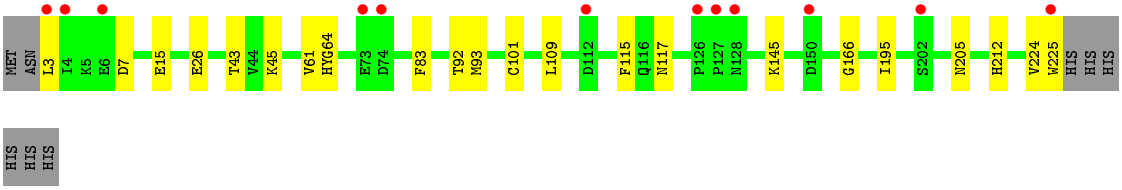
- Molecule 1: GREEN FLUORESCENT PROTEIN

Chain E:



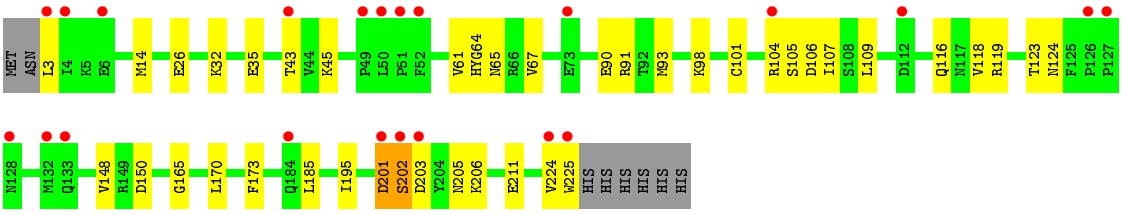
• Molecule 1: GREEN FLUORESCENT PROTEIN

Chain F:



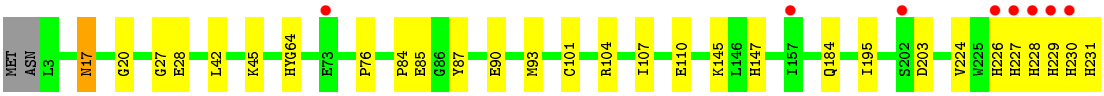
• Molecule 1: GREEN FLUORESCENT PROTEIN

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) 91.4 (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 (5.26%)	DCC
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 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 113213 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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, CR8, PG4

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	1771	18	0
1	B	1819	0	1772	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1845	0	1798	34	0
1	D	1807	0	1764	24	0
1	E	1811	0	1759	29	0
1	F	1799	0	1758	12	0
1	G	1802	0	1763	39	0
1	H	1859	0	1800	18	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	14237	199	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 (199) 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:HH21	1:C:119[A]:ARG:HG3	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:HH21	1:G:104[B]:ARG:HB2	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:CG	1:C:119[A]:ARG:HH21	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:HH21	1:G:104[B]:ARG:CB	1.76	0.94
1:E:145:LYS:HE2	4:F:2068:HOH:O	1.68	0.94
1:E:64:CR8:H23	4:E:2158:HOH:O	1.68	0.93
1:C:119[A]:ARG:NH2	1:C:119[A]:ARG:HG3	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:D:90:GLU:HG2	1:D:104[A]:ARG:HG2	1.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG21	1:C:208:LYS:HE3	1.79	0.63
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:NH2	1:D:119:ARG:HG3	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:E:144:GLU:HG2	1:E:146:LEU:HD21	1.86	0.58
1:C:194:ARG:HH22	2:D:1226:PG4:H31	1.68	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:61:VAL:O	1:G:64:CR8:H171	2.08	0.54
1:G:106:ASP:HB2	4:G:2046:HOH:O	2.07	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:E:225:TRP:CH2	1:E:227:HIS:C	2.81	0.54
1:C:117:ASN:OD1	1:C:119[B]:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PHE:HB2	1:C:132:MET:CE	2.37	0.54
1:B:127:PRO:HB2	4:B:2104:HOH:O	2.08	0.54
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
1:E:64:CR8:H2	1:E:195:ILE:HB	1.91	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:146:LEU:HD22	1:B:155:GLY:CA	2.40	0.52
1:B:81:GLN:O	1:B:181:LYS:HE3	2.09	0.52
1:G:14:MET:HG3	1:G:118:VAL:HB	1.92	0.51
1:H:64:CR8:H2	1:H:195:ILE:HB	1.93	0.51
1:D:121:LYS:HE2	4:D:2010:HOH:O	2.09	0.51
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:D:65:ASN:OD1	1:D:67:VAL:HG23	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:G:64:CR8:H2	1:G:195:ILE:HB	1.94	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:E:76:PRO:HG3	1:E:184:GLN:HE21	1.78	0.48
1:A:90:GLU:OE2	1:A:104[A]:ARG:NE	2.46	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:G:170:LEU:HD11	1:H:147:HIS:CE1	2.49	0.47
1:E:220:LEU:HD22	1:F:212:HIS:CE1	2.50	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:B:64:CR8:H2	1:B:195:ILE:HB	1.97	0.47
1:G:202:SER:CB	1:G:203:ASP:CA	2.93	0.46
1:E:17:ASN:HD21	1:E:20:GLY:HA2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:O	1:A:212:HIS:HA	2.15	0.46
1:F:64:CR8:H2	1:F:195:ILE:HB	1.97	0.46
1:A:124:ASN:HB2	4:A:2102:HOH:O	2.16	0.46
1:H:228:HIS:CG	1:H:229:HIS:N	2.83	0.46
1:F:93:MET:HB2	1:F:101:CYS:HB2	1.98	0.46
1:C:140:GLU:OE2	1:C:168:HIS:HE1	1.97	0.46
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:A:61:VAL:O	1:A:64:CR8:H171	2.18	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:D:55:ASP:HB3	1:D:161:LEU:HD21	2.00	0.43
1:C:224:VAL:O	1:C:226:HIS:CD2	2.71	0.43
1:B:21:HIS:HE1	1:B:47:GLY:O	2.01	0.43
1:G:202:SER:HB3	1:G:203:ASP:CB	2.18	0.43
1:B:93:MET:HB2	1:B:101:CYS:HB2	2.01	0.43
1:E:17:ASN:HD21	1:E:20:GLY:CA	2.31	0.43
1:C:2:ASN:N	1:C:2:ASN:HD22	2.15	0.43
1:C:93:MET:HB2	1:C:101:CYS:HB2	1.99	0.43
1:D:67:VAL:HG11	1:D:114:PHE:CZ	2.54	0.43
1:A:146:LEU:HA	1:A:154:VAL:O	2.18	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:C:61:VAL:O	1:C:64:CR8:H171	2.19	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:VAL:O	1:F:64:CR8:H171	2.20	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:D:197:ILE:HD12	4:D:2031:HOH:O	2.19	0.41
1:B:97:ASP:O	1:B:98:LYS:HB2	2.21	0.41
1:F:83:PHE:CE1	1:F:109:LEU:HB2	2.56	0.41
1:H:224:VAL:O	1:H:226:HIS:HD2	2.04	0.41
1:H:27:GLY:HA3	1:H:42:LEU:HD23	2.02	0.41
1:E:144:GLU:CG	1:E:146:LEU:HD21	2.50	0.41
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:F:224:VAL:O	1:F:225:TRP:C	2.59	0.40
1:A:72:PRO:HG2	1:A:75:ILE:HG13	2.04	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	220/229 (96%)	218 (99%)	2 (1%)	0	100	100
1	B	221/229 (96%)	219 (99%)	2 (1%)	0	100	100
1	C	224/229 (98%)	219 (98%)	5 (2%)	0	100	100
1	D	220/229 (96%)	218 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	220/229 (96%)	219 (100%)	1 (0%)	0	100 100
1	F	219/229 (96%)	217 (99%)	2 (1%)	0	100 100
1	G	220/229 (96%)	216 (98%)	3 (1%)	1 (0%)	34 26
1	H	225/229 (98%)	220 (98%)	5 (2%)	0	100 100
All	All	1769/1832 (97%)	1746 (99%)	22 (1%)	1 (0%)	56 53

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%)	82 85
1	B	196/201 (98%)	194 (99%)	2 (1%)	82 85
1	C	199/201 (99%)	196 (98%)	3 (2%)	72 75
1	D	195/201 (97%)	194 (100%)	1 (0%)	92 94
1	E	195/201 (97%)	189 (97%)	6 (3%)	47 46
1	F	194/201 (96%)	191 (98%)	3 (2%)	72 75
1	G	195/201 (97%)	186 (95%)	9 (5%)	33 28
1	H	200/201 (100%)	196 (98%)	4 (2%)	63 65
All	All	1569/1608 (98%)	1539 (98%)	30 (2%)	65 67

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

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Mol	Chain	Res	Type
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
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

Some 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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CR8	A	64	1	20,27,28	1.72	4 (20%)	16,37,39	1.91	4 (25%)
1	CR8	B	64	1	20,27,28	1.69	4 (20%)	16,37,39	2.08	4 (25%)
1	CR8	C	64	1	20,27,28	1.64	5 (25%)	16,37,39	1.90	6 (37%)
1	CR8	D	64	1	20,27,28	1.72	7 (35%)	16,37,39	2.00	4 (25%)
1	CR8	E	64	1	20,27,28	1.67	5 (25%)	16,37,39	2.18	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CR8	F	64	1	20,27,28	1.78	6 (30%)	16,37,39	1.65	3 (18%)
1	CR8	G	64	1	20,27,28	1.83	5 (25%)	16,37,39	1.42	3 (18%)
1	CR8	H	64	1	20,27,28	1.69	3 (15%)	16,37,39	2.18	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	A	64	1	-	0/8/25/26	0/3/3/3
1	CR8	B	64	1	-	0/8/25/26	0/3/3/3
1	CR8	C	64	1	-	0/8/25/26	0/3/3/3
1	CR8	D	64	1	-	0/8/25/26	0/3/3/3
1	CR8	E	64	1	-	0/8/25/26	0/3/3/3
1	CR8	F	64	1	-	0/8/25/26	0/3/3/3
1	CR8	G	64	1	-	0/8/25/26	0/3/3/3
1	CR8	H	64	1	-	0/8/25/26	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CR8	C4-C1	-2.95	1.39	1.45
1	D	64	CR8	C4-C1	-2.73	1.39	1.45
1	A	64	CR8	C4-C1	-2.71	1.39	1.45
1	G	64	CR8	C4-C1	-2.64	1.39	1.45
1	F	64	CR8	C4-C1	-2.52	1.40	1.45
1	B	64	CR8	C4-C1	-2.48	1.40	1.45
1	D	64	CR8	C2-C1	-2.33	1.40	1.45
1	G	64	CR8	C2-C1	-2.32	1.40	1.45
1	C	64	CR8	C4-C1	-2.31	1.40	1.45
1	F	64	CR8	C2-C1	-2.27	1.40	1.45
1	E	64	CR8	C4-C1	-2.26	1.40	1.45
1	A	64	CR8	C2-C1	-2.17	1.40	1.45
1	C	64	CR8	C2-C1	-2.04	1.41	1.45
1	E	64	CR8	C2-C1	-2.01	1.41	1.45
1	C	64	CR8	C14-N15	2.01	1.38	1.34
1	D	64	CR8	C5-C4	2.04	1.40	1.35
1	F	64	CR8	C14-N15	2.05	1.38	1.34
1	D	64	CR8	C9-C8	2.08	1.48	1.40
1	D	64	CR8	C6-C2	2.10	1.40	1.35
1	B	64	CR8	C9-C8	2.18	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	CR8	C14-N15	2.20	1.39	1.34
1	E	64	CR8	C9-C8	2.21	1.48	1.40
1	G	64	CR8	C9-C8	2.29	1.49	1.40
1	H	64	CR8	C9-C8	2.37	1.49	1.40
1	E	64	CR8	C6-C2	2.52	1.41	1.35
1	F	64	CR8	C6-C2	2.54	1.41	1.35
1	G	64	CR8	C6-C2	2.60	1.41	1.35
1	A	64	CR8	C6-C2	2.61	1.41	1.35
1	F	64	CR8	C9-C8	2.65	1.50	1.40
1	C	64	CR8	C6-C2	2.67	1.41	1.35
1	B	64	CR8	C6-C2	2.93	1.41	1.35
1	H	64	CR8	C8-C7	4.72	1.48	1.36
1	C	64	CR8	C8-C7	4.83	1.48	1.36
1	D	64	CR8	C8-C7	4.83	1.48	1.36
1	B	64	CR8	C8-C7	4.84	1.48	1.36
1	E	64	CR8	C8-C7	5.01	1.48	1.36
1	A	64	CR8	C8-C7	5.10	1.48	1.36
1	F	64	CR8	C8-C7	5.23	1.49	1.36
1	G	64	CR8	C8-C7	5.50	1.49	1.36

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	CR8	C2-C6-C7	-3.43	118.96	122.00
1	B	64	CR8	C2-C6-C7	-3.26	119.11	122.00
1	D	64	CR8	C2-C6-C7	-3.16	119.19	122.00
1	E	64	CR8	C2-C6-C7	-2.99	119.35	122.00
1	C	64	CR8	C5-C7-C8	-2.87	113.78	121.85
1	E	64	CR8	C5-C7-C8	-2.81	113.94	121.85
1	C	64	CR8	C2-C6-C7	-2.81	119.51	122.00
1	B	64	CR8	C5-C7-C8	-2.69	114.28	121.85
1	G	64	CR8	C2-C6-C7	-2.62	119.67	122.00
1	A	64	CR8	C5-C7-C8	-2.47	114.91	121.85
1	H	64	CR8	C2-C6-C7	-2.45	119.83	122.00
1	H	64	CR8	C5-C7-C8	-2.44	114.99	121.85
1	E	64	CR8	O3-C1-C4	-2.17	118.09	121.51
1	C	64	CR8	O3-C1-C4	-2.16	118.11	121.51
1	D	64	CR8	C5-C7-C8	-2.15	115.81	121.85
1	G	64	CR8	C5-C7-C8	-2.09	115.98	121.85
1	F	64	CR8	C2-C6-C7	-2.03	120.19	122.00
1	E	64	CR8	C4-C1-C2	2.15	120.76	116.77
1	C	64	CR8	C4-C1-C2	2.19	120.83	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	64	CR8	C17-N13-C12	2.20	128.67	124.74
1	F	64	CR8	C17-N13-C12	2.33	128.90	124.74
1	G	64	CR8	C-C17-N13	2.65	116.68	112.37
1	C	64	CR8	C17-N13-C12	2.77	129.70	124.74
1	C	64	CR8	C-C17-N13	2.96	117.17	112.37
1	H	64	CR8	C17-N13-C12	3.27	130.58	124.74
1	B	64	CR8	C17-N13-C12	3.32	130.69	124.74
1	A	64	CR8	C-C17-N13	3.62	118.25	112.37
1	F	64	CR8	C-C17-N13	3.75	118.46	112.37
1	A	64	CR8	C17-N13-C12	3.77	131.49	124.74
1	D	64	CR8	C17-N13-C12	3.84	131.61	124.74
1	D	64	CR8	C-C17-N13	4.17	119.14	112.37
1	B	64	CR8	C-C17-N13	5.00	120.49	112.37
1	E	64	CR8	C-C17-N13	5.43	121.18	112.37
1	H	64	CR8	C-C17-N13	6.06	122.21	112.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	64	CR8	1	0
1	B	64	CR8	1	0
1	C	64	CR8	1	0
1	E	64	CR8	2	0
1	F	64	CR8	2	0
1	G	64	CR8	2	0
1	H	64	CR8	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	PG4	A	1226	-	12,12,12	0.58	0	11,11,11	0.42	0
3	GOL	B	1228	-	5,5,5	0.34	0	5,5,5	0.24	0
3	GOL	C	1229	-	5,5,5	0.38	0	5,5,5	0.32	0
2	PG4	D	1226	-	12,12,12	0.60	0	11,11,11	0.52	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
2	PG4	A	1226	-	-	0/10/10/10	0/0/0/0
3	GOL	B	1228	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1229	-	-	0/4/4/4	0/0/0/0
2	PG4	D	1226	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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%)	0.17	4 (1%)	71 72	10, 20, 28, 39	0
1	B	222/229 (96%)	0.07	4 (1%)	71 72	10, 17, 25, 33	0
1	C	224/229 (97%)	0.19	6 (2%)	58 58	10, 20, 30, 39	0
1	D	221/229 (96%)	0.21	6 (2%)	58 58	11, 20, 29, 42	0
1	E	222/229 (96%)	0.05	4 (1%)	71 72	9, 17, 26, 39	0
1	F	220/229 (96%)	0.49	12 (5%)	29 30	13, 26, 37, 42	0
1	G	220/229 (96%)	0.84	22 (10%)	9 10	15, 30, 44, 48	0
1	H	226/229 (98%)	0.18	8 (3%)	48 49	11, 19, 31, 53	0
All	All	1775/1832 (96%)	0.27	66 (3%)	45 47	9, 20, 37, 53	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	TRP	7.4
1	A	225	TRP	7.3
1	G	225	TRP	7.0
1	F	225	TRP	6.7
1	H	228	HIS	6.1
1	D	2	ASN	5.3
1	H	227	HIS	4.8
1	C	227	HIS	4.5
1	E	227	HIS	4.5
1	C	228	HIS	4.5
1	G	128	ASN	4.4
1	H	229	HIS	4.2
1	G	201	ASP	4.0
1	B	227	HIS	3.9
1	C	2	ASN	3.8
1	E	226	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	127	PRO	3.4
1	H	226	HIS	3.4
1	G	112	ASP	3.4
1	H	230	HIS	3.3
1	G	127	PRO	3.1
1	D	157	ILE	3.1
1	D	3	LEU	3.0
1	G	3	LEU	3.0
1	G	132	MET	3.0
1	F	202	SER	3.0
1	G	6	GLU	2.9
1	A	157	ILE	2.9
1	E	202	SER	2.9
1	H	202	SER	2.9
1	G	4	ILE	2.8
1	G	202	SER	2.8
1	F	4	ILE	2.7
1	G	224	VAL	2.7
1	F	127	PRO	2.7
1	F	128	ASN	2.7
1	F	73	GLU	2.7
1	G	49	PRO	2.6
1	C	73	GLU	2.6
1	G	133	GLN	2.6
1	G	50	LEU	2.5
1	B	226	HIS	2.5
1	F	3	LEU	2.5
1	G	203	ASP	2.4
1	G	51	PRO	2.4
1	E	157	ILE	2.4
1	C	157	ILE	2.3
1	H	157	ILE	2.3
1	F	112	ASP	2.3
1	A	73	GLU	2.3
1	A	128	ASN	2.3
1	G	184	GLN	2.3
1	B	157	ILE	2.3
1	F	150	ASP	2.3
1	G	126	PRO	2.2
1	C	119[A]	ARG	2.2
1	G	43	THR	2.1
1	F	74	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	126	PRO	2.1
1	G	52	PHE	2.1
1	G	73	GLU	2.1
1	B	73	GLU	2.1
1	H	73	GLU	2.1
1	D	124	ASN	2.1
1	G	104[A]	ARG	2.1
1	F	6	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	CR8	A	64	25/26	0.91	0.15	-	9,16,17,18	0
1	CR8	H	64	25/26	0.94	0.14	-	7,11,14,15	0
1	CR8	G	64	25/26	0.87	0.15	-	12,23,28,28	0
1	CR8	D	64	25/26	0.94	0.15	-	9,14,17,18	0
1	CR8	F	64	25/26	0.91	0.14	-	15,20,24,24	0
1	CR8	C	64	25/26	0.89	0.15	-	6,16,18,18	0
1	CR8	E	64	25/26	0.95	0.15	-	10,12,14,14	0
1	CR8	B	64	25/26	0.91	0.15	-	10,12,14,15	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	C	1229	6/6	0.73	0.15	0.93	33,35,36,37	0
2	PG4	D	1226	13/13	0.82	0.15	-0.22	32,34,35,35	0
2	PG4	A	1226	13/13	0.85	0.14	-0.23	31,34,36,37	0
3	GOL	B	1228	6/6	0.70	0.15	-0.32	43,43,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.