



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:47 PM UTC

PDB ID : 6MAS / pdb_00006mas
Title : X-ray Structure of Branchiostoma floridae fluorescent protein lanFP10G
Authors : Muslinkina, L.; Pletneva, N.; Pletnev, V.; Pletnev, S.
Deposited on : 2018-08-28
Resolution : 1.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

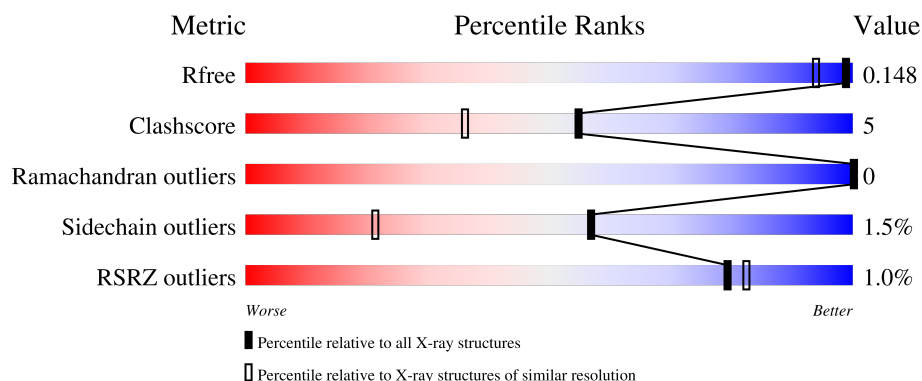
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	85% 8% 5%
1	B	227	84% 11% 5%
1	C	227	80% 15% 5%
1	D	227	83% 11% 5%
1	E	227	89% 5% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	 % 87% 7% • 5%
1	G	227	 % 87% 7% • 5%
1	H	227	 2% 83% 11% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	G	301	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17339 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	16	0
			1878	1199	318	349	12			
1	B	216	Total	C	N	O	S	0	13	0
			1849	1183	308	345	13			
1	C	216	Total	C	N	O	S	0	20	0
			1905	1221	317	352	15			
1	D	216	Total	C	N	O	S	0	16	0
			1874	1198	313	349	14			
1	E	216	Total	C	N	O	S	0	12	0
			1840	1178	303	346	13			
1	F	216	Total	C	N	O	S	0	11	0
			1834	1174	307	340	13			
1	G	216	Total	C	N	O	S	0	9	0
			1813	1159	303	338	13			
1	H	216	Total	C	N	O	S	0	13	0
			1843	1178	305	346	14			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP C3YRA2
A	58	CR2	GLY	chromophore	UNP C3YRA2
A	58	CR2	TYR	chromophore	UNP C3YRA2
A	58	CR2	ALA	chromophore	UNP C3YRA2
A	220	SER	-	expression tag	UNP C3YRA2
A	221	GLY	-	expression tag	UNP C3YRA2
A	222	GLY	-	expression tag	UNP C3YRA2
A	223	SER	-	expression tag	UNP C3YRA2
A	224	HIS	-	expression tag	UNP C3YRA2
A	225	HIS	-	expression tag	UNP C3YRA2
A	226	HIS	-	expression tag	UNP C3YRA2
A	227	HIS	-	expression tag	UNP C3YRA2
A	228	HIS	-	expression tag	UNP C3YRA2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	HIS	-	expression tag	UNP C3YRA2
B	1	MET	-	expression tag	UNP C3YRA2
B	58	CR2	GLY	chromophore	UNP C3YRA2
B	58	CR2	TYR	chromophore	UNP C3YRA2
B	58	CR2	ALA	chromophore	UNP C3YRA2
B	220	SER	-	expression tag	UNP C3YRA2
B	221	GLY	-	expression tag	UNP C3YRA2
B	222	GLY	-	expression tag	UNP C3YRA2
B	223	SER	-	expression tag	UNP C3YRA2
B	224	HIS	-	expression tag	UNP C3YRA2
B	225	HIS	-	expression tag	UNP C3YRA2
B	226	HIS	-	expression tag	UNP C3YRA2
B	227	HIS	-	expression tag	UNP C3YRA2
B	228	HIS	-	expression tag	UNP C3YRA2
B	229	HIS	-	expression tag	UNP C3YRA2
C	1	MET	-	expression tag	UNP C3YRA2
C	58	CR2	GLY	chromophore	UNP C3YRA2
C	58	CR2	TYR	chromophore	UNP C3YRA2
C	58	CR2	ALA	chromophore	UNP C3YRA2
C	220	SER	-	expression tag	UNP C3YRA2
C	221	GLY	-	expression tag	UNP C3YRA2
C	222	GLY	-	expression tag	UNP C3YRA2
C	223	SER	-	expression tag	UNP C3YRA2
C	224	HIS	-	expression tag	UNP C3YRA2
C	225	HIS	-	expression tag	UNP C3YRA2
C	226	HIS	-	expression tag	UNP C3YRA2
C	227	HIS	-	expression tag	UNP C3YRA2
C	228	HIS	-	expression tag	UNP C3YRA2
C	229	HIS	-	expression tag	UNP C3YRA2
D	1	MET	-	expression tag	UNP C3YRA2
D	58	CR2	GLY	chromophore	UNP C3YRA2
D	58	CR2	TYR	chromophore	UNP C3YRA2
D	58	CR2	ALA	chromophore	UNP C3YRA2
D	220	SER	-	expression tag	UNP C3YRA2
D	221	GLY	-	expression tag	UNP C3YRA2
D	222	GLY	-	expression tag	UNP C3YRA2
D	223	SER	-	expression tag	UNP C3YRA2
D	224	HIS	-	expression tag	UNP C3YRA2
D	225	HIS	-	expression tag	UNP C3YRA2
D	226	HIS	-	expression tag	UNP C3YRA2
D	227	HIS	-	expression tag	UNP C3YRA2
D	228	HIS	-	expression tag	UNP C3YRA2

Continued on next page...

Continued from previous page...

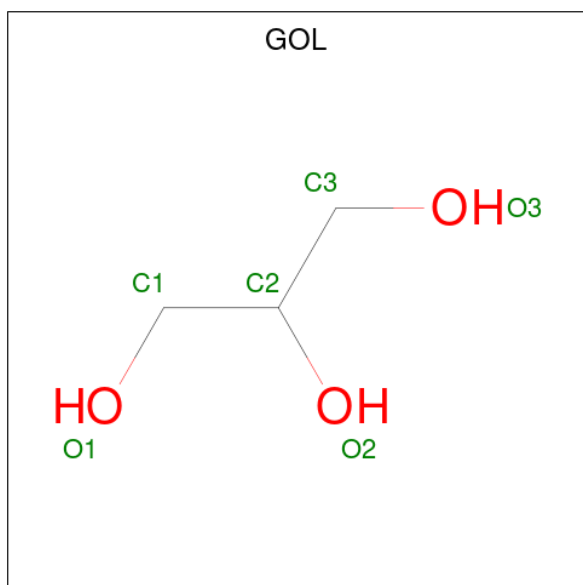
Chain	Residue	Modelled	Actual	Comment	Reference
D	229	HIS	-	expression tag	UNP C3YRA2
E	1	MET	-	expression tag	UNP C3YRA2
E	58	CR2	GLY	chromophore	UNP C3YRA2
E	58	CR2	TYR	chromophore	UNP C3YRA2
E	58	CR2	ALA	chromophore	UNP C3YRA2
E	220	SER	-	expression tag	UNP C3YRA2
E	221	GLY	-	expression tag	UNP C3YRA2
E	222	GLY	-	expression tag	UNP C3YRA2
E	223	SER	-	expression tag	UNP C3YRA2
E	224	HIS	-	expression tag	UNP C3YRA2
E	225	HIS	-	expression tag	UNP C3YRA2
E	226	HIS	-	expression tag	UNP C3YRA2
E	227	HIS	-	expression tag	UNP C3YRA2
E	228	HIS	-	expression tag	UNP C3YRA2
E	229	HIS	-	expression tag	UNP C3YRA2
F	1	MET	-	expression tag	UNP C3YRA2
F	58	CR2	GLY	chromophore	UNP C3YRA2
F	58	CR2	TYR	chromophore	UNP C3YRA2
F	58	CR2	ALA	chromophore	UNP C3YRA2
F	220	SER	-	expression tag	UNP C3YRA2
F	221	GLY	-	expression tag	UNP C3YRA2
F	222	GLY	-	expression tag	UNP C3YRA2
F	223	SER	-	expression tag	UNP C3YRA2
F	224	HIS	-	expression tag	UNP C3YRA2
F	225	HIS	-	expression tag	UNP C3YRA2
F	226	HIS	-	expression tag	UNP C3YRA2
F	227	HIS	-	expression tag	UNP C3YRA2
F	228	HIS	-	expression tag	UNP C3YRA2
F	229	HIS	-	expression tag	UNP C3YRA2
G	1	MET	-	expression tag	UNP C3YRA2
G	58	CR2	GLY	chromophore	UNP C3YRA2
G	58	CR2	TYR	chromophore	UNP C3YRA2
G	58	CR2	ALA	chromophore	UNP C3YRA2
G	220	SER	-	expression tag	UNP C3YRA2
G	221	GLY	-	expression tag	UNP C3YRA2
G	222	GLY	-	expression tag	UNP C3YRA2
G	223	SER	-	expression tag	UNP C3YRA2
G	224	HIS	-	expression tag	UNP C3YRA2
G	225	HIS	-	expression tag	UNP C3YRA2
G	226	HIS	-	expression tag	UNP C3YRA2
G	227	HIS	-	expression tag	UNP C3YRA2
G	228	HIS	-	expression tag	UNP C3YRA2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	229	HIS	-	expression tag	UNP C3YRA2
H	1	MET	-	expression tag	UNP C3YRA2
H	58	CR2	GLY	chromophore	UNP C3YRA2
H	58	CR2	TYR	chromophore	UNP C3YRA2
H	58	CR2	ALA	chromophore	UNP C3YRA2
H	220	SER	-	expression tag	UNP C3YRA2
H	221	GLY	-	expression tag	UNP C3YRA2
H	222	GLY	-	expression tag	UNP C3YRA2
H	223	SER	-	expression tag	UNP C3YRA2
H	224	HIS	-	expression tag	UNP C3YRA2
H	225	HIS	-	expression tag	UNP C3YRA2
H	226	HIS	-	expression tag	UNP C3YRA2
H	227	HIS	-	expression tag	UNP C3YRA2
H	228	HIS	-	expression tag	UNP C3YRA2
H	229	HIS	-	expression tag	UNP C3YRA2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

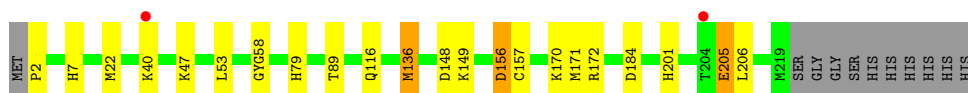
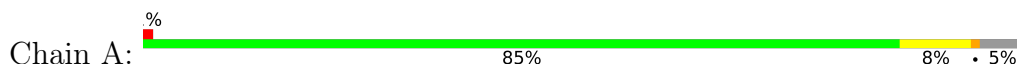
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	311	Total	O	0	0
			311	311		
3	B	321	Total	O	0	0
			321	321		
3	C	331	Total	O	0	0
			331	331		
3	D	322	Total	O	0	0
			322	322		
3	E	295	Total	O	0	0
			295	295		
3	F	300	Total	O	0	0
			300	300		
3	G	299	Total	O	0	0
			299	299		
3	H	282	Total	O	0	0
			282	282		

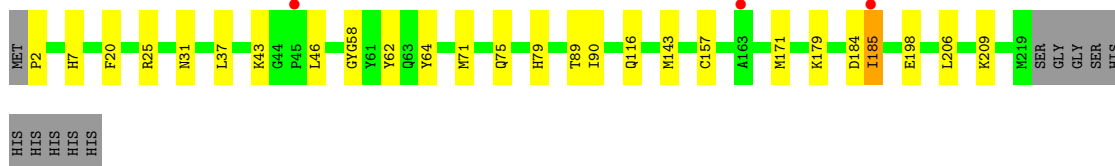
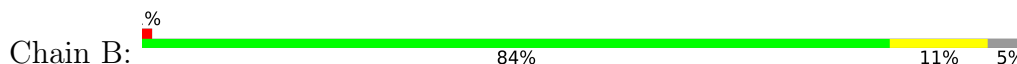
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

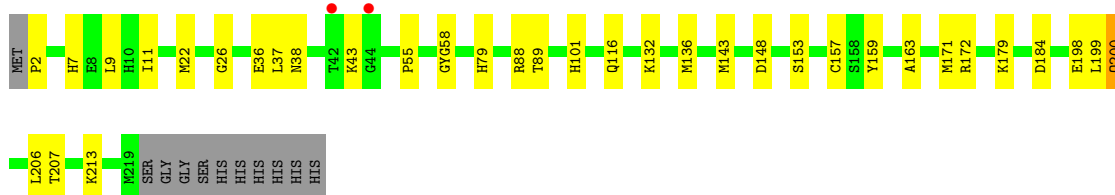
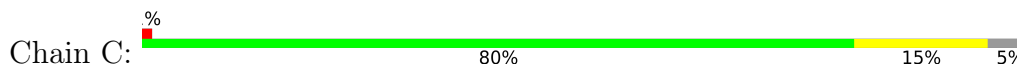
- Molecule 1: Uncharacterized protein



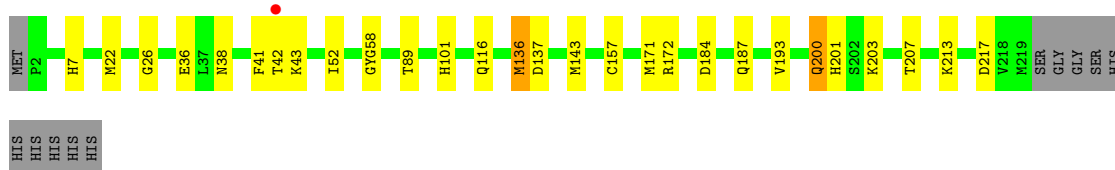
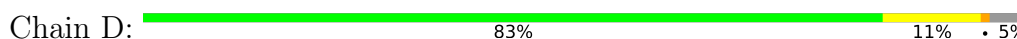
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



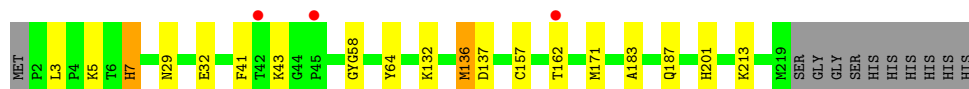
- Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein

Chain E:  89% 5% • 5%

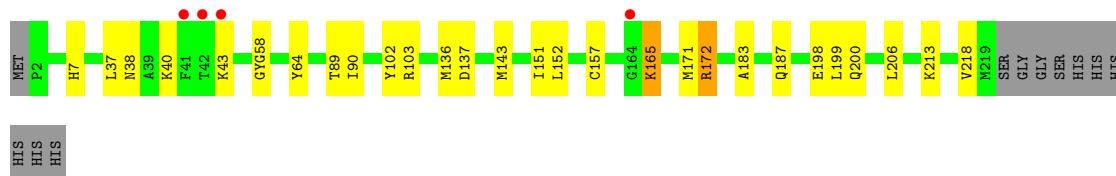
● Molecule 1: Uncharacterized protein

Chain F:  87% 7% • 5%

● Molecule 1: Uncharacterized protein

Chain G:  87% 7% • 5%

● Molecule 1: Uncharacterized protein

Chain H:  83% 11% • 5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.88Å 104.31Å 116.14Å 90.00° 95.32° 90.00°	Depositor
Resolution (Å)	29.82 – 1.30 29.82 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-1.30) 99.8 (29.82-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.119 , 0.147 0.122 , 0.148	Depositor DCC
R_{free} test set	4625 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17339	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, GOL

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	0.72	1/1910 (0.1%)	0.87	2/2573 (0.1%)
1	B	0.77	1/1882 (0.1%)	0.91	3/2540 (0.1%)
1	C	0.73	0/1938	0.86	2/2613 (0.1%)
1	D	0.73	1/1907 (0.1%)	0.87	2/2574 (0.1%)
1	E	0.73	0/1873	0.86	1/2529 (0.0%)
1	F	0.75	1/1867 (0.1%)	0.89	2/2519 (0.1%)
1	G	0.74	1/1845 (0.1%)	0.83	0/2490
1	H	0.76	2/1875 (0.1%)	0.89	2/2532 (0.1%)
All	All	0.74	7/15097 (0.0%)	0.87	14/20370 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	ILE	N-CA	6.27	1.54	1.46
1	H	102	TYR	C-O	-5.68	1.17	1.24
1	A	156	ASP	CG-OD2	-5.65	1.14	1.25
1	H	218	VAL	C-O	-5.44	1.17	1.24
1	F	7	HIS	CE1-NE2	5.37	1.38	1.32
1	G	156	ASP	CG-OD1	-5.20	1.15	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	PHE	C-O	-5.03	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	ARG	CG-CD-NE	-6.41	97.89	112.00
1	D	217	ASP	CA-CB-CG	6.40	119.00	112.60
1	H	103	ARG	CG-CD-NE	-6.40	97.93	112.00
1	F	41	PHE	CA-C-N	6.26	128.91	120.65
1	F	41	PHE	C-N-CA	6.26	128.91	120.65
1	H	165	LYS	CB-CA-C	5.40	119.59	109.71
1	B	184	ASP	CA-C-N	5.39	130.08	121.34
1	B	184	ASP	C-N-CA	5.39	130.08	121.34
1	C	148	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	184	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	184	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	148	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	143	MET	CG-SD-CE	-5.13	89.61	100.90
1	A	184	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	172[A]	ARG	Sidechain
1	E	103	ARG	Sidechain
1	G	103[A]	ARG	Sidechain
1	H	172[A]	ARG	Sidechain

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	1878	0	1811	18	0
1	B	1849	0	1767	21	0
1	C	1905	0	1839	34	0
1	D	1874	0	1797	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1840	0	1752	9	0
1	F	1834	0	1761	11	0
1	G	1813	0	1736	12	0
1	H	1843	0	1761	17	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	12	0	16	0	0
2	G	6	0	8	0	0
3	A	311	0	0	8	0
3	B	321	0	0	7	0
3	C	331	0	0	8	0
3	D	322	0	0	11	0
3	E	295	0	0	3	0
3	F	300	0	0	5	0
3	G	299	0	0	4	0
3	H	282	0	0	6	0
All	All	17339	0	14280	141	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 5.

All (141) 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:88:ARG:CD	1:C:171[A]:MET:HE3	1.52	1.39
1:C:88:ARG:HD3	1:C:171[A]:MET:CE	1.81	1.09
1:E:47:LYS:HE2	3:E:628:HOH:O	1.61	0.99
1:C:88:ARG:CD	1:C:171[A]:MET:CE	2.45	0.91
1:C:88:ARG:NE	1:C:171[A]:MET:HE3	1.85	0.90
1:A:116:GLN:HE22	1:B:116:GLN:HE22	1.20	0.90
1:A:22:MET:HE1	1:A:53:LEU:HD13	1.55	0.89
1:C:88:ARG:HD3	1:C:171[A]:MET:HE3	0.89	0.88
1:C:88:ARG:NE	1:C:171[A]:MET:CE	2.38	0.86
1:C:88:ARG:CZ	1:C:171[A]:MET:CE	2.55	0.84
1:C:116:GLN:HE22	1:D:116:GLN:HE22	1.29	0.80
1:B:20[B]:PHE:HE1	1:B:46:LEU:HD21	1.46	0.79
1:C:38[B]:ASN:ND2	1:C:207[B]:THR:HG22	2.02	0.74
1:D:207[B]:THR:HG23	3:D:493:HOH:O	1.89	0.72
1:B:179:LYS:NZ	3:B:403:HOH:O	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40[B]:LYS:HG2	3:A:348:HOH:O	1.93	0.69
1:B:89[B]:THR:HG23	3:B:564:HOH:O	1.93	0.69
1:C:89[A]:THR:HG21	3:D:401:HOH:O	1.92	0.68
1:B:198[B]:GLU:HG2	1:B:209:LYS:HB2	1.75	0.66
1:B:20[B]:PHE:HE1	1:B:46:LEU:CD2	2.09	0.66
1:D:101:HIS:HD2	3:D:604:HOH:O	1.77	0.66
1:D:89[B]:THR:HG23	3:D:591:HOH:O	1.97	0.65
1:F:157:CYS:SG	1:F:171[B]:MET:HE3	2.39	0.63
1:A:89:THR:HG21	3:B:405:HOH:O	1.97	0.62
1:H:157:CYS:SG	1:H:171[B]:MET:HE3	2.41	0.61
1:A:136:MET:HE3	3:A:314:HOH:O	2.01	0.61
1:C:88:ARG:CZ	1:C:171[A]:MET:HE2	2.30	0.60
1:E:213[B]:LYS:HE3	3:E:658:HOH:O	2.00	0.60
1:H:183:ALA:O	1:H:187:GLN:HG3	2.01	0.60
3:A:429:HOH:O	1:B:89[A]:THR:HG21	2.01	0.60
1:B:2:PRO:N	1:B:79:HIS:HD1	2.01	0.59
1:F:213[B]:LYS:HE2	3:F:552:HOH:O	2.02	0.59
1:D:38:ASN:HD22	1:D:207[B]:THR:HG22	1.67	0.59
1:G:89:THR:HG21	3:H:307:HOH:O	2.02	0.58
1:F:132:LYS:HB3	1:F:162[B]:THR:HG22	1.86	0.58
1:E:157:CYS:SG	1:E:171[B]:MET:HE3	2.43	0.58
1:G:2:PRO:N	1:G:79:HIS:HD1	2.01	0.58
1:H:89[B]:THR:HG23	3:H:459:HOH:O	2.05	0.57
1:A:157:CYS:SG	1:A:171[B]:MET:HE3	2.45	0.56
1:D:157:CYS:SG	1:D:171[B]:MET:HE3	2.45	0.56
1:H:7:HIS:HE1	3:H:336:HOH:O	1.89	0.56
1:C:163:ALA:N	3:C:407:HOH:O	2.38	0.55
1:C:157:CYS:SG	1:C:171[B]:MET:HE3	2.46	0.55
1:A:22:MET:HE1	1:A:53:LEU:CD1	2.32	0.55
1:D:7:HIS:HE1	3:D:429:HOH:O	1.90	0.54
1:G:201:HIS:HD2	3:G:405:HOH:O	1.89	0.54
1:H:90:ILE:HG12	1:H:171[A]:MET:HG3	1.90	0.54
1:C:2:PRO:N	1:C:79:HIS:HD1	2.06	0.53
1:B:7:HIS:HE1	3:B:423:HOH:O	1.90	0.53
1:H:213:LYS:HE3	3:H:537:HOH:O	2.07	0.53
1:C:38[B]:ASN:HD22	1:C:207[B]:THR:HG22	1.74	0.53
1:C:9[B]:LEU:HD21	1:C:11[B]:ILE:HG13	1.91	0.52
1:G:157:CYS:SG	1:G:171[B]:MET:HE3	2.49	0.52
1:C:7:HIS:HE1	3:C:444:HOH:O	1.93	0.52
1:C:132:LYS:HD3	3:C:407:HOH:O	2.08	0.51
1:G:7:HIS:HE1	3:G:426:HOH:O	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:CYS:SG	1:B:171[B]:MET:HE3	2.50	0.51
1:F:201:HIS:HE1	3:F:621:HOH:O	1.94	0.51
1:H:136[A]:MET:HG3	1:H:137:ASP:N	2.25	0.51
1:B:20[B]:PHE:CE1	1:B:46:LEU:HD21	2.36	0.50
1:D:136[B]:MET:HG3	1:D:137:ASP:N	2.22	0.50
1:H:143[B]:MET:HE3	1:H:151:ILE:HG21	1.93	0.50
1:A:7:HIS:HE1	3:A:331:HOH:O	1.94	0.50
1:F:5:LYS:HD2	3:F:572:HOH:O	2.11	0.50
1:A:40[A]:LYS:HG2	1:A:205:GLU:HB3	1.94	0.50
1:F:7:HIS:HE1	3:F:440:HOH:O	1.94	0.49
1:A:156:ASP:OD1	1:A:170[B]:LYS:HD2	2.12	0.49
1:E:7:HIS:HE1	3:E:443:HOH:O	1.95	0.49
1:A:2:PRO:N	1:A:79:HIS:HD1	2.10	0.49
1:C:55:PRO:HB2	1:C:171[A]:MET:HE1	1.95	0.49
1:C:213[B]:LYS:HE2	3:C:414:HOH:O	2.12	0.49
1:B:71[A]:MET:HG2	1:B:75:GLN:HB3	1.94	0.48
1:C:88:ARG:NE	1:C:171[A]:MET:HE2	2.25	0.48
1:F:183:ALA:O	1:F:187:GLN:HG3	2.14	0.48
1:C:199[A]:LEU:HD22	1:C:207[A]:THR:O	2.14	0.47
1:H:198[B]:GLU:CD	1:H:200:GLN:HE22	2.22	0.47
1:B:71[A]:MET:HG2	1:B:75:GLN:CB	2.45	0.47
1:F:136[B]:MET:HG3	1:F:137:ASP:N	2.30	0.47
1:H:152:LEU:HD21	1:H:172[B]:ARG:NH2	2.30	0.47
1:D:201:HIS:HE1	3:D:632:HOH:O	1.98	0.47
1:C:136[B]:MET:HE3	1:C:159:TYR:CZ	2.50	0.46
1:E:136[B]:MET:HG3	1:E:137:ASP:N	2.30	0.46
1:A:47:LYS:NZ	3:A:301:HOH:O	2.31	0.46
1:D:187:GLN:HG3	3:D:546:HOH:O	2.16	0.46
1:C:200:GLN:NE2	3:C:410:HOH:O	2.50	0.45
1:D:207[A]:THR:HG23	3:D:539:HOH:O	2.15	0.45
1:B:31:ASN:ND2	3:B:406:HOH:O	2.44	0.45
1:B:206:LEU:C	1:B:206:LEU:HD12	2.41	0.45
1:D:213[B]:LYS:HE3	3:D:564:HOH:O	2.17	0.45
1:A:136:MET:CE	3:A:314:HOH:O	2.61	0.45
1:D:143:MET:HE2	1:D:193:VAL:HG23	1.99	0.45
1:C:143[A]:MET:HG2	1:C:153:SER:OG	2.16	0.45
1:D:42:THR:HG22	1:D:43:LYS:HG3	1.99	0.44
1:D:136[B]:MET:HB2	1:D:136[B]:MET:HE2	1.78	0.44
1:G:131:ASN:ND2	3:G:403:HOH:O	2.40	0.44
1:G:200[A]:GLN:HA	1:G:200[A]:GLN:OE1	2.18	0.44
1:B:90:ILE:HG12	1:B:171[A]:MET:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199[A]:LEU:C	1:H:199[A]:LEU:HD13	2.43	0.44
1:B:89[B]:THR:HG22	3:B:543:HOH:O	2.18	0.43
1:C:22[B]:MET:HB2	1:C:22[B]:MET:HE3	1.75	0.43
1:D:200:GLN:NE2	3:D:402:HOH:O	2.26	0.43
3:A:484:HOH:O	1:C:172[A]:ARG:HD2	2.18	0.43
1:G:101:HIS:HE1	3:G:502:HOH:O	2.01	0.43
1:H:172[B]:ARG:NH1	3:H:305:HOH:O	2.48	0.43
1:G:136[B]:MET:HB2	1:G:136[B]:MET:HE2	1.75	0.43
1:E:136[B]:MET:HE2	1:E:136[B]:MET:HB2	1.80	0.43
1:A:149[A]:LYS:HE3	3:A:328:HOH:O	2.18	0.43
1:H:198[B]:GLU:CG	1:H:200:GLN:HE22	2.32	0.43
1:B:7:HIS:HD2	1:B:64:TYR:OH	2.02	0.43
1:D:203:LYS:HD3	1:D:203:LYS:HA	1.88	0.43
1:F:3:LEU:HD23	3:F:536:HOH:O	2.18	0.43
1:C:198[B]:GLU:HG2	1:C:200:GLN:OE1	2.19	0.43
1:A:206:LEU:HD12	1:A:206:LEU:C	2.44	0.43
1:C:101:HIS:HE1	3:C:530:HOH:O	2.02	0.43
1:B:7:HIS:CD2	1:B:64:TYR:OH	2.72	0.42
1:D:207[A]:THR:CG2	3:D:539:HOH:O	2.67	0.42
1:G:136[B]:MET:HG3	1:G:137:ASP:N	2.33	0.42
1:D:26:GLY:HA3	1:D:36:GLU:O	2.19	0.42
1:H:206:LEU:C	1:H:206:LEU:HD12	2.45	0.42
1:A:22:MET:HE2	1:A:22:MET:HB2	1.72	0.41
1:C:200:GLN:HE21	1:C:200:GLN:HB2	1.67	0.41
1:G:7:HIS:CD2	1:G:64:TYR:OH	2.74	0.41
1:C:206:LEU:HD12	1:C:206:LEU:C	2.45	0.41
1:D:52:ILE:HD12	1:D:52:ILE:HA	1.95	0.41
1:A:201:HIS:CD2	1:A:201:HIS:C	2.98	0.41
1:C:200:GLN:NE2	3:C:403:HOH:O	2.33	0.41
1:G:65:LEU:HD13	1:G:212:GLN:HB2	2.02	0.41
1:A:172[A]:ARG:HD2	3:C:590:HOH:O	2.21	0.41
1:C:88:ARG:CZ	1:C:171[A]:MET:HE1	2.48	0.41
1:E:7:HIS:HD2	1:E:64:TYR:OH	2.03	0.41
1:E:73:PRO:HD3	1:E:185[A]:ILE:HD12	2.03	0.41
1:B:62:TYR:OH	3:B:402:HOH:O	2.19	0.41
1:E:7:HIS:CD2	1:E:64:TYR:OH	2.74	0.41
1:F:29:ASN:ND2	1:F:32:GLU:HG3	2.37	0.41
1:D:22[B]:MET:HE3	1:D:22[B]:MET:HB2	1.72	0.40
1:H:38:ASN:HB2	3:H:517:HOH:O	2.20	0.40
1:B:71[B]:MET:HE2	1:B:75:GLN:HB3	2.03	0.40
1:C:26:GLY:HA3	1:C:36:GLU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:HIS:HD2	1:H:64:TYR:OH	2.05	0.40
1:H:198[B]:GLU:HG2	1:H:200:GLN:NE2	2.36	0.40
1:F:7:HIS:CD2	1:F:64:TYR:OH	2.74	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	227/227 (100%)	226 (100%)	1 (0%)	0	100	100
1	B	224/227 (99%)	223 (100%)	1 (0%)	0	100	100
1	C	231/227 (102%)	229 (99%)	2 (1%)	0	100	100
1	D	227/227 (100%)	225 (99%)	2 (1%)	0	100	100
1	E	223/227 (98%)	221 (99%)	2 (1%)	0	100	100
1	F	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
1	G	220/227 (97%)	220 (100%)	0	0	100	100
1	H	224/227 (99%)	222 (99%)	2 (1%)	0	100	100
All	All	1798/1816 (99%)	1786 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/195 (104%)	200 (99%)	2 (1%)	68	37
1	B	199/195 (102%)	194 (98%)	5 (2%)	42	8
1	C	206/195 (106%)	202 (98%)	4 (2%)	50	14
1	D	202/195 (104%)	199 (98%)	3 (2%)	57	21
1	E	198/195 (102%)	195 (98%)	3 (2%)	57	21
1	F	197/195 (101%)	194 (98%)	3 (2%)	57	21
1	G	195/195 (100%)	192 (98%)	3 (2%)	57	21
1	H	199/195 (102%)	195 (98%)	4 (2%)	48	12
All	All	1598/1560 (102%)	1571 (98%)	27 (2%)	57	17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	MET
1	A	205	GLU
1	B	25[A]	ARG
1	B	25[B]	ARG
1	B	37	LEU
1	B	43	LYS
1	B	185	ILE
1	C	37	LEU
1	C	43	LYS
1	C	179	LYS
1	C	200	GLN
1	D	136[A]	MET
1	D	136[B]	MET
1	D	200	GLN
1	E	25	ARG
1	E	136[A]	MET
1	E	136[B]	MET
1	F	43	LYS
1	F	136[A]	MET
1	F	136[B]	MET
1	G	136[A]	MET
1	G	136[B]	MET
1	G	212	GLN
1	H	37	LEU
1	H	40	LYS
1	H	43	LYS
1	H	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	101	HIS
1	A	131	ASN
1	A	175	ASN
1	A	201	HIS
1	B	7	HIS
1	B	101	HIS
1	B	116	GLN
1	B	175	ASN
1	C	7	HIS
1	C	101	HIS
1	C	175	ASN
1	C	201	HIS
1	D	7	HIS
1	D	38	ASN
1	D	101	HIS
1	D	116	GLN
1	D	175	ASN
1	D	187	GLN
1	D	201	HIS
1	E	7	HIS
1	E	79	HIS
1	E	101	HIS
1	E	175	ASN
1	F	7	HIS
1	F	85	GLN
1	F	101	HIS
1	F	116	GLN
1	F	175	ASN
1	F	201	HIS
1	G	7	HIS
1	G	85	GLN
1	G	101	HIS
1	G	175	ASN
1	G	201	HIS
1	H	7	HIS
1	H	101	HIS
1	H	116	GLN
1	H	174	ASN
1	H	175	ASN
1	H	200	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	201	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	CR2	G	58	1	20,20,21	2.42	4 (20%)	25,27,29	1.66	5 (20%)
1	CR2	D	58	1	20,20,21	2.82	5 (25%)	25,27,29	2.43	10 (40%)
1	CR2	A	58	1	20,20,21	2.49	4 (20%)	25,27,29	1.69	7 (28%)
1	CR2	H	58	1	20,20,21	2.60	4 (20%)	25,27,29	2.29	11 (44%)
1	CR2	C	58	1	20,20,21	2.01	3 (15%)	25,27,29	1.53	7 (28%)
1	CR2	B	58	1	20,20,21	2.26	3 (15%)	25,27,29	1.40	6 (24%)
1	CR2	E	58	1	20,20,21	2.74	4 (20%)	25,27,29	2.33	5 (20%)
1	CR2	F	58	1	20,20,21	3.06	4 (20%)	25,27,29	2.38	10 (40%)

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	CR2	G	58	1	-	0/6/25/26	0/2/2/2
1	CR2	D	58	1	-	0/6/25/26	0/2/2/2
1	CR2	A	58	1	-	0/6/25/26	0/2/2/2
1	CR2	H	58	1	-	0/6/25/26	0/2/2/2
1	CR2	C	58	1	-	0/6/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	B	58	1	-	0/6/25/26	0/2/2/2
1	CR2	E	58	1	-	0/6/25/26	0/2/2/2
1	CR2	F	58	1	-	0/6/25/26	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	CR2	CB2-CA2	10.15	1.44	1.35
1	D	58	CR2	CB2-CA2	9.05	1.43	1.35
1	E	58	CR2	CB2-CA2	8.78	1.43	1.35
1	A	58	CR2	CB2-CA2	8.77	1.43	1.35
1	H	58	CR2	CB2-CA2	8.09	1.42	1.35
1	B	58	CR2	CB2-CA2	8.02	1.42	1.35
1	G	58	CR2	CB2-CA2	7.65	1.42	1.35
1	F	58	CR2	CA2-C2	-7.47	1.40	1.48
1	H	58	CR2	CA2-C2	-6.67	1.41	1.48
1	E	58	CR2	CA2-C2	-6.58	1.41	1.48
1	C	58	CR2	CB2-CA2	6.39	1.41	1.35
1	D	58	CR2	CA2-C2	-6.33	1.41	1.48
1	G	58	CR2	CA2-C2	-5.71	1.42	1.48
1	A	58	CR2	CA2-C2	-4.86	1.43	1.48
1	C	58	CR2	CA2-C2	-4.46	1.43	1.48
1	E	58	CR2	C2-N3	-3.67	1.31	1.40
1	B	58	CR2	CA2-C2	-3.60	1.44	1.48
1	B	58	CR2	OH-CZ	-3.29	1.29	1.37
1	F	58	CR2	OH-CZ	-3.27	1.29	1.37
1	D	58	CR2	O2-C2	3.03	1.29	1.23
1	D	58	CR2	OH-CZ	-2.91	1.30	1.37
1	A	58	CR2	OH-CZ	-2.86	1.30	1.37
1	F	58	CR2	C2-N3	-2.80	1.33	1.40
1	G	58	CR2	C2-N3	-2.77	1.33	1.40
1	C	58	CR2	C2-N3	-2.72	1.33	1.40
1	E	58	CR2	OH-CZ	-2.64	1.31	1.37
1	D	58	CR2	C2-N3	-2.55	1.34	1.40
1	H	58	CR2	CG2-CB2	-2.32	1.42	1.46
1	G	58	CR2	OH-CZ	-2.19	1.32	1.37
1	A	58	CR2	C2-N3	-2.17	1.35	1.40
1	H	58	CR2	OH-CZ	-2.05	1.32	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	58	CR2	O2-C2-CA2	-7.84	126.01	131.02
1	H	58	CR2	O2-C2-CA2	-6.56	126.83	131.02
1	F	58	CR2	O2-C2-CA2	-6.35	126.97	131.02
1	D	58	CR2	CA2-C2-N3	6.15	108.66	103.50
1	F	58	CR2	CA2-C2-N3	5.72	108.31	103.50
1	D	58	CR2	O2-C2-CA2	-5.35	127.61	131.02
1	H	58	CR2	CA2-C2-N3	5.13	107.81	103.50
1	E	58	CR2	CA2-C2-N3	5.00	107.70	103.50
1	E	58	CR2	C3-CA3-N3	4.60	122.89	112.43
1	G	58	CR2	O2-C2-CA2	-4.52	128.13	131.02
1	A	58	CR2	O2-C2-CA2	-3.85	128.56	131.02
1	A	58	CR2	CA2-C2-N3	3.80	106.69	103.50
1	D	58	CR2	C2-CA2-N2	-3.71	106.29	108.95
1	G	58	CR2	CA2-C2-N3	3.57	106.50	103.50
1	D	58	CR2	C3-CA3-N3	3.48	120.34	112.43
1	C	58	CR2	O2-C2-CA2	-3.39	128.85	131.02
1	H	58	CR2	C1-CA1-N1	-3.17	105.83	112.85
1	F	58	CR2	C3-CA3-N3	3.17	119.64	112.43
1	D	58	CR2	C1-CA1-N1	-3.07	106.05	112.85
1	C	58	CR2	C3-CA3-N3	3.02	119.29	112.43
1	F	58	CR2	C1-CA1-N1	-2.96	106.31	112.85
1	G	58	CR2	C3-CA3-N3	2.93	119.09	112.43
1	B	58	CR2	C1-CA1-N1	-2.89	106.47	112.85
1	F	58	CR2	C2-N3-C1	-2.88	106.78	108.08
1	B	58	CR2	C3-CA3-N3	2.85	118.91	112.43
1	D	58	CR2	CA1-C1-N3	2.84	126.33	122.52
1	H	58	CR2	C3-CA3-N3	2.69	118.55	112.43
1	G	58	CR2	C1-CA1-N1	-2.67	106.94	112.85
1	H	58	CR2	C2-CA2-N2	-2.65	107.06	108.95
1	A	58	CR2	C1-CA1-N1	-2.62	107.05	112.85
1	C	58	CR2	CG2-CB2-CA2	2.53	132.87	129.87
1	F	58	CR2	CA1-C1-N3	2.50	125.87	122.52
1	E	58	CR2	C1-CA1-N1	-2.50	107.32	112.85
1	D	58	CR2	CD2-CE2-CZ	2.50	122.52	119.88
1	A	58	CR2	C3-CA3-N3	2.48	118.08	112.43
1	F	58	CR2	CD2-CE2-CZ	2.44	122.45	119.88
1	A	58	CR2	C2-CA2-N2	-2.39	107.24	108.95
1	C	58	CR2	CA2-C2-N3	2.38	105.50	103.50
1	C	58	CR2	CA1-C1-N3	2.36	125.68	122.52
1	C	58	CR2	C1-CA1-N1	-2.36	107.64	112.85
1	A	58	CR2	O3-C3-CA3	-2.32	115.03	125.47
1	H	58	CR2	CA1-C1-N3	2.31	125.61	122.52
1	D	58	CR2	C2-N3-C1	-2.30	107.04	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	CR2	O2-C2-CA2	-2.28	129.56	131.02
1	F	58	CR2	O3-C3-CA3	-2.26	115.29	125.47
1	H	58	CR2	C2-N3-C1	-2.26	107.06	108.08
1	D	58	CR2	CD1-CE1-CZ	2.23	122.24	119.88
1	H	58	CR2	CD1-CE1-CZ	2.23	122.23	119.88
1	D	58	CR2	CE2-CZ-CE1	-2.19	116.28	119.77
1	B	58	CR2	CA1-C1-N3	2.19	125.45	122.52
1	H	58	CR2	O3-C3-CA3	-2.17	115.69	125.47
1	B	58	CR2	CD1-CE1-CZ	2.16	122.16	119.88
1	H	58	CR2	CE2-CZ-CE1	-2.15	116.34	119.77
1	H	58	CR2	CD2-CE2-CZ	2.10	122.10	119.88
1	F	58	CR2	C2-CA2-N2	-2.08	107.46	108.95
1	F	58	CR2	CD1-CE1-CZ	2.08	122.08	119.88
1	G	58	CR2	O3-C3-CA3	-2.07	116.14	125.47
1	A	58	CR2	CA1-C1-N3	2.06	125.28	122.52
1	B	58	CR2	O3-C3-CA3	-2.05	116.24	125.47
1	C	58	CR2	O3-C3-CA3	-2.04	116.31	125.47
1	E	58	CR2	CA1-C1-N3	2.01	125.21	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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	GOL	C	301	-	5,5,5	1.22	0	5,5,5	1.40	0
2	GOL	F	302	-	5,5,5	0.67	0	5,5,5	1.64	2 (40%)
2	GOL	B	301	-	5,5,5	1.53	1 (20%)	5,5,5	1.86	1 (20%)
2	GOL	F	301	-	5,5,5	0.33	0	5,5,5	2.47	2 (40%)
2	GOL	G	301	-	5,5,5	1.93	1 (20%)	5,5,5	2.25	3 (60%)
2	GOL	E	301	-	5,5,5	0.70	0	5,5,5	0.41	0
2	GOL	D	301	-	5,5,5	0.57	0	5,5,5	0.71	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	GOL	C	301	-	-	0/4/4/4	-
2	GOL	F	302	-	-	2/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	F	301	-	-	2/4/4/4	-
2	GOL	G	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	0/4/4/4	-
2	GOL	D	301	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	GOL	O2-C2	3.63	1.53	1.43
2	B	301	GOL	O2-C2	3.00	1.52	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	GOL	O3-C3-C2	4.59	131.03	110.38
2	B	301	GOL	C3-C2-C1	-3.58	98.67	111.80
2	G	301	GOL	O2-C2-C1	3.20	122.41	109.18
2	G	301	GOL	C3-C2-C1	-3.08	100.50	111.80
2	F	301	GOL	O2-C2-C1	-2.44	99.07	109.18
2	F	302	GOL	O2-C2-C1	2.04	117.62	109.18
2	F	302	GOL	C3-C2-C1	-2.03	104.37	111.80
2	G	301	GOL	O1-C1-C2	2.01	119.42	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	302	GOL	O1-C1-C2-C3
2	F	302	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-C3
2	G	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
2	F	301	GOL	O1-C1-C2-O2
2	G	301	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/227 (94%)	-0.40	2 (0%) 81 84	5, 11, 28, 45	16 (7%)
1	B	215/227 (94%)	-0.41	3 (1%) 73 77	4, 12, 27, 40	13 (6%)
1	C	215/227 (94%)	-0.49	2 (0%) 81 84	4, 10, 26, 47	20 (9%)
1	D	215/227 (94%)	-0.45	1 (0%) 87 90	4, 11, 25, 44	16 (7%)
1	E	215/227 (94%)	-0.43	1 (0%) 87 90	6, 13, 26, 38	12 (5%)
1	F	215/227 (94%)	-0.34	3 (1%) 73 77	6, 13, 29, 54	11 (5%)
1	G	215/227 (94%)	-0.39	2 (0%) 81 84	6, 12, 27, 42	9 (4%)
1	H	215/227 (94%)	-0.22	4 (1%) 66 70	6, 14, 31, 52	13 (6%)
All	All	1720/1816 (94%)	-0.39	18 (1%) 79 82	4, 12, 28, 54	110 (6%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	THR	3.2
1	B	45	PRO	3.2
1	G	42	THR	2.9
1	A	40[A]	LYS	2.7
1	H	41	PHE	2.6
1	H	42	THR	2.6
1	F	45	PRO	2.4
1	F	162[A]	THR	2.4
1	G	44	GLY	2.3
1	A	204	THR	2.3
1	H	43	LYS	2.3
1	C	44	GLY	2.3
1	E	183	ALA	2.2
1	F	42	THR	2.2
1	B	163	ALA	2.2
1	C	42	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	185	ILE	2.0
1	H	164	GLY	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	CR2	B	58	19/20	0.98	0.04	8,9,11,11	0
1	CR2	E	58	19/20	0.98	0.04	9,10,11,12	0
1	CR2	H	58	19/20	0.98	0.04	10,11,12,12	0
1	CR2	D	58	19/20	0.99	0.03	7,8,10,10	0
1	CR2	A	58	19/20	0.99	0.03	7,8,9,9	0
1	CR2	F	58	19/20	0.99	0.03	10,10,11,11	0
1	CR2	G	58	19/20	0.99	0.03	8,10,12,12	0
1	CR2	C	58	19/20	0.99	0.03	6,7,9,9	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	F	302	6/6	0.72	0.16	24,26,31,32	0
2	GOL	F	301	6/6	0.80	0.13	23,24,29,30	0
2	GOL	C	301	6/6	0.86	0.12	20,21,22,24	0
2	GOL	D	301	6/6	0.89	0.10	20,23,26,26	0
2	GOL	G	301	6/6	0.89	0.10	23,25,27,27	0
2	GOL	B	301	6/6	0.90	0.10	20,23,26,28	0
2	GOL	E	301	6/6	0.98	0.05	15,15,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.