



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:02 am BST

PDB ID : 5MAD  
Title : GFP-binding DARPin 3G61  
Authors : Hansen, S.; Stueber, J.; Ernst, P.; Koch, A.; Bojar, D.; Batyuk, A.; Plueckthun, A.  
Deposited on : 2016-11-03  
Resolution : 1.53 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

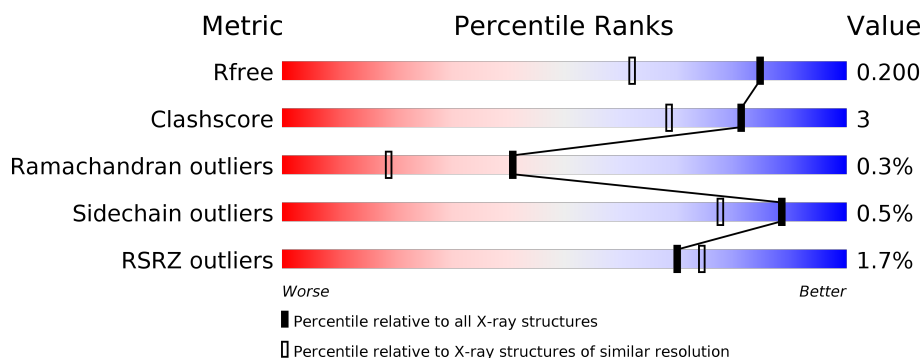
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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  $\geq 3$ , 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	160	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>• •</div> </div> </div>
1	C	160	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8% • •</div> </div> </div>
1	E	160	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div>•</div> </div> </div>
1	G	160	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>•</div> </div> </div>
2	B	243	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>5% 5%</div> </div> </div>
2	D	243	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	243	<div><div>%</div><div><div></div></div><div>88%</div><div>5%7%</div></div>
2	H	243	<div><div>%</div><div><div></div></div><div>91%</div><div>•6%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25853 atoms, of which 12176 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 3G61.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	0	9	0
			2363	757	1162	199	243	2			
1	C	155	Total	C	H	N	O	S	0	10	0
			2401	767	1193	201	238	2			
1	E	160	Total	C	H	N	O	S	0	2	0
			2389	764	1181	204	239	1			
1	G	160	Total	C	H	N	O	S	0	5	0
			2415	773	1192	205	244	1			

- Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	232	Total	C	H	N	O	S	0	17	0
			3805	1220	1885	322	370	8			
2	D	232	Total	C	H	N	O	S	0	8	0
			3709	1191	1833	315	362	8			
2	F	226	Total	C	H	N	O	S	1	13	0
			3661	1178	1807	311	358	7			
2	H	229	Total	C	H	N	O	S	0	14	0
			3727	1196	1843	319	362	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P42212
B	-3	PRO	-	expression tag	UNP P42212
B	-2	GLY	-	expression tag	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	MET	-	expression tag	UNP P42212
B	1	VAL	-	expression tag	UNP P42212
B	64	LEU	PHE	conflict	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212

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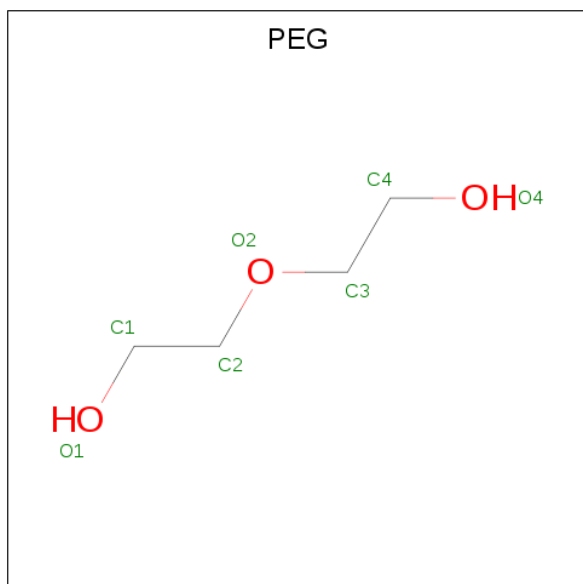
Chain	Residue	Modelled	Actual	Comment	Reference
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	231	LEU	HIS	conflict	UNP P42212
B	239	GLN	-	expression tag	UNP P42212
B	240	ALA	-	expression tag	UNP P42212
D	-4	GLY	-	expression tag	UNP P42212
D	-3	PRO	-	expression tag	UNP P42212
D	-2	GLY	-	expression tag	UNP P42212
D	-1	SER	-	expression tag	UNP P42212
D	0	MET	-	expression tag	UNP P42212
D	1	VAL	-	expression tag	UNP P42212
D	64	LEU	PHE	conflict	UNP P42212
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	231	LEU	HIS	conflict	UNP P42212
D	239	GLN	-	expression tag	UNP P42212
D	240	ALA	-	expression tag	UNP P42212
F	-4	GLY	-	expression tag	UNP P42212
F	-3	PRO	-	expression tag	UNP P42212
F	-2	GLY	-	expression tag	UNP P42212
F	-1	SER	-	expression tag	UNP P42212
F	0	MET	-	expression tag	UNP P42212
F	1	VAL	-	expression tag	UNP P42212
F	64	LEU	PHE	conflict	UNP P42212
F	66	CRO	SER	chromophore	UNP P42212
F	66	CRO	TYR	chromophore	UNP P42212
F	66	CRO	GLY	chromophore	UNP P42212
F	231	LEU	HIS	conflict	UNP P42212
F	239	GLN	-	expression tag	UNP P42212
F	240	ALA	-	expression tag	UNP P42212
H	-4	GLY	-	expression tag	UNP P42212
H	-3	PRO	-	expression tag	UNP P42212
H	-2	GLY	-	expression tag	UNP P42212
H	-1	SER	-	expression tag	UNP P42212
H	0	MET	-	expression tag	UNP P42212
H	1	VAL	-	expression tag	UNP P42212
H	64	LEU	PHE	conflict	UNP P42212
H	66	CRO	SER	chromophore	UNP P42212
H	66	CRO	TYR	chromophore	UNP P42212
H	66	CRO	GLY	chromophore	UNP P42212
H	231	LEU	HIS	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
H	239	GLN	-	expression tag	UNP P42212
H	240	ALA	-	expression tag	UNP P42212

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		
3	G	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	B	202	Total O 202 202	0	0
5	C	127	Total O 127 127	0	0
5	D	192	Total O 192 192	0	0
5	E	117	Total O 117 117	0	0
5	F	139	Total O 139 139	0	0
5	G	119	Total O 119 119	0	0
5	H	219	Total O 219 219	0	0

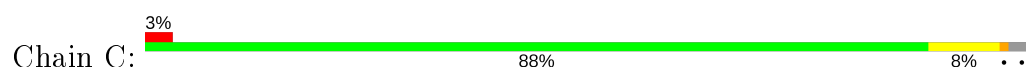
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 3G61



- Molecule 1: 3G61



- Molecule 1: 3G61



- Molecule 1: 3G61

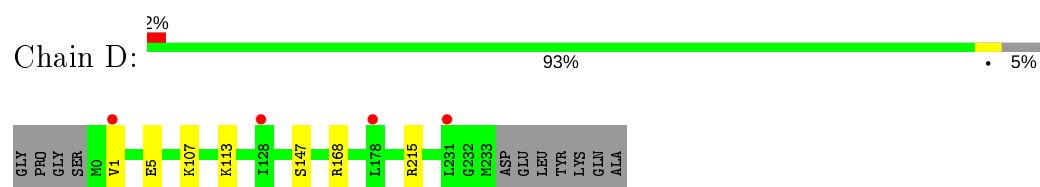


- Molecule 2: Green fluorescent protein

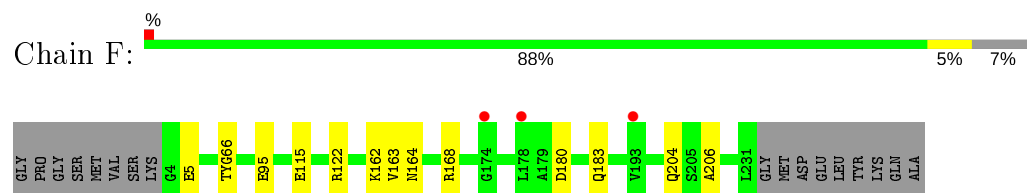


- Molecule 2: Green fluorescent protein

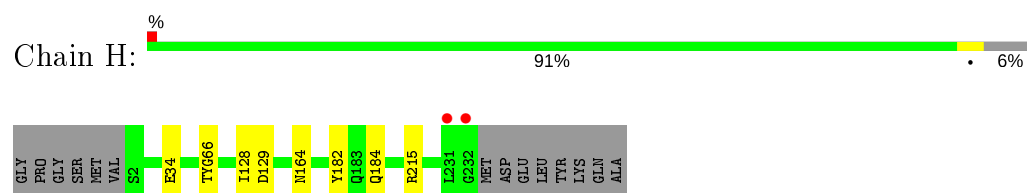




- Molecule 2: Green fluorescent protein



- Molecule 2: Green fluorescent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.42Å 83.07Å 162.00Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	48.76 – 1.53 48.76 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.76-1.53) 98.8 (48.76-1.53)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.53Å)	Xtriage
Refinement program	PHENIX (1.11 _2567: ???)	Depositor
R, $R_{free}$	0.171 , 0.199 0.172 , 0.200	Depositor DCC
$R_{free}$ test set	11883 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	25853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8209e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PEG, CRO

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	0.31	0/1250	0.50	0/1700
1	C	0.32	0/1262	0.52	0/1716
1	E	0.30	0/1232	0.49	0/1675
1	G	0.32	0/1251	0.52	0/1702
2	B	0.37	0/1995	0.58	0/2694
2	D	0.36	0/1924	0.59	0/2599
2	F	0.33	0/1930	0.56	0/2610
2	H	0.38	0/1959	0.59	0/2646
All	All	0.34	0/12803	0.55	0/17342

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	173[B]	ASP	Peptide

## 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	1201	1162	1128	6	2
1	C	1208	1193	1155	11	0
1	E	1208	1181	1177	6	0
1	G	1223	1192	1172	4	0
2	B	1920	1885	1829	11	2
2	D	1876	1833	1802	6	0
2	F	1854	1807	1740	11	0
2	H	1884	1843	1794	7	0
3	A	14	20	20	0	0
3	B	7	10	10	1	0
3	C	14	20	20	2	0
3	D	7	10	10	0	0
3	E	7	10	10	0	0
3	G	7	10	10	0	0
4	E	1	0	0	0	0
5	A	131	0	0	1	0
5	B	202	0	0	8	0
5	C	127	0	0	5	0
5	D	192	0	0	5	1
5	E	117	0	0	6	0
5	F	139	0	0	7	0
5	G	119	0	0	3	0
5	H	219	0	0	4	1
All	All	13677	12176	11877	64	3

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 3.

All (64) 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)
2:F:164[B]:ASN:OD1	5:F:301:HOH:O	1.76	1.03
2:H:215[B]:ARG:NH2	5:H:303:HOH:O	1.91	1.02
2:H:34[B]:GLU:OE2	5:H:301:HOH:O	1.84	0.94
2:H:164[B]:ASN:OD1	5:H:302:HOH:O	1.86	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:OE2	5:C:301:HOH:O	1.90	0.88
2:F:164[B]:ASN:ND2	5:F:302:HOH:O	2.07	0.86
2:B:215:ARG:NH2	5:B:1304:HOH:O	2.09	0.84
3:B:301:PEG:O1	5:B:1301:HOH:O	1.94	0.84
1:E:155[B]:ASN:ND2	5:E:304:HOH:O	2.10	0.82
1:E:166:LYS:O	5:E:301:HOH:O	1.97	0.81
1:E:133:LYS:O	5:E:302:HOH:O	2.00	0.77
1:E:167:LEU:O	5:E:303:HOH:O	2.02	0.76
2:B:36:ASP:OD1	5:B:1302:HOH:O	2.03	0.76
1:G:167:LEU:O	5:G:301:HOH:O	2.05	0.74
1:A:109[A]:ASP:OD2	5:A:301:HOH:O	2.06	0.72
2:B:147[A]:SER:OG	5:B:1303:HOH:O	2.08	0.69
2:F:180:ASP:OD1	5:F:301:HOH:O	2.09	0.69
2:F:95:GLU:OE2	5:F:303:HOH:O	2.11	0.69
1:E:155[B]:ASN:OD1	5:E:305:HOH:O	2.12	0.68
2:D:107:LYS:NZ	5:D:403:HOH:O	2.26	0.67
2:D:147[B]:SER:OG	5:D:401:HOH:O	2.12	0.67
2:F:168:ARG:NH2	5:F:304:HOH:O	2.21	0.65
1:C:154[A]:ASP:OD1	5:C:302:HOH:O	2.15	0.64
1:E:66:LEU:O	5:E:306:HOH:O	2.17	0.61
2:H:184:GLN:NE2	5:H:306:HOH:O	2.32	0.61
2:F:204:GLN:NE2	5:F:308:HOH:O	2.35	0.57
1:C:34[A]:MET:HE1	1:C:64:VAL:HG12	1.88	0.56
2:D:215:ARG:NH1	5:D:405:HOH:O	2.39	0.55
2:F:162:LYS:NZ	5:F:311:HOH:O	2.40	0.54
2:B:162:LYS:NZ	5:B:1309:HOH:O	2.40	0.50
2:B:47[A]:ILE:HD11	2:B:49:THR:HG22	1.92	0.50
1:A:34[A]:MET:HE1	1:A:64:VAL:HG12	1.93	0.49
2:F:115:GLU:OE2	2:F:122:ARG:NH1	2.44	0.49
3:C:202:PEG:H21	5:C:306:HOH:O	2.12	0.48
2:D:1:VAL:CG1	2:D:5:GLU:HB3	2.44	0.48
1:C:125[B]:LEU:HD11	1:C:163:ILE:HD12	1.94	0.48
1:C:26:GLN:OE1	5:C:303:HOH:O	2.20	0.47
2:B:171:ILE:O	2:B:173[B]:ASP:N	2.47	0.47
1:G:23:ARG:NH2	5:G:303:HOH:O	2.32	0.45
1:G:146:LYS:NZ	1:G:154:ASP:OD2	2.44	0.43
1:A:34[A]:MET:CE	1:A:64:VAL:HG12	2.49	0.43
1:C:146:LYS:NZ	1:C:154[A]:ASP:OD2	2.45	0.43
2:B:132:GLU:OE1	5:B:1305:HOH:O	2.21	0.43
2:B:47[A]:ILE:HD13	5:B:1304:HOH:O	2.18	0.43
2:D:113:LYS:NZ	5:D:412:HOH:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:CRO:HD2	2:F:66:CRO:N2	2.35	0.42
2:H:66:CRO:N2	2:H:66:CRO:HD2	2.35	0.42
1:G:97[A]:VAL:HG23	5:G:363:HOH:O	2.19	0.42
1:C:34[B]:MET:HE2	1:C:40:VAL:HG23	2.01	0.42
2:D:168:ARG:NH2	5:D:402:HOH:O	2.22	0.42
2:B:38:THR:HG23	5:B:1302:HOH:O	2.19	0.42
2:B:66:CRO:N2	2:B:66:CRO:HD2	2.36	0.41
2:B:109:ARG:HD3	1:C:166:LYS:HB3	2.02	0.41
1:C:89:SER:OG	1:C:91:HIS:HD2	2.04	0.41
2:H:164[A]:ASN:ND2	2:H:182:TYR:CD2	2.88	0.41
1:C:125[B]:LEU:HD11	1:C:163:ILE:CD1	2.51	0.40
1:C:120:ALA:HA	1:C:160[A]:LEU:HD11	2.03	0.40
3:C:201:PEG:C2	5:C:414:HOH:O	2.69	0.40
2:F:163:VAL:HB	2:F:183:GLN:HB3	2.03	0.40
2:H:128:ILE:O	2:H:129:ASP:HB2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:547:HOH:O	5:H:449:HOH:O[2_847]	1.89	0.31
1:A:66:LEU:O	2:B:215:ARG:NH1[1_455]	2.00	0.20
1:A:66:LEU:O	2:B:215:ARG:HH12[1_455]	1.60	0.00

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/160 (101%)	156 (97%)	1 (1%)	4 (2%)	5	0
1	C	163/160 (102%)	158 (97%)	5 (3%)	0	100	100
1	E	160/160 (100%)	157 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	162/160 (101%)	159 (98%)	3 (2%)	0	100	100
2	B	244/243 (100%)	235 (96%)	5 (2%)	4 (2%)	9	1
2	D	235/243 (97%)	232 (99%)	3 (1%)	0	100	100
2	F	234/243 (96%)	231 (99%)	3 (1%)	0	100	100
2	H	238/243 (98%)	235 (99%)	3 (1%)	0	100	100
All	All	1597/1612 (99%)	1563 (98%)	26 (2%)	8 (0%)	41	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110[A]	GLN
1	A	110[B]	GLN
1	A	108[A]	ASP
1	A	108[B]	ASP
2	B	172[A]	GLU
2	B	172[B]	GLU
2	B	174[A]	GLY
2	B	174[B]	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/122 (103%)	126 (100%)	0	100	100
1	C	127/122 (104%)	123 (97%)	4 (3%)	40	11
1	E	123/122 (101%)	123 (100%)	0	100	100
1	G	126/122 (103%)	125 (99%)	1 (1%)	81	64
2	B	218/210 (104%)	214 (98%)	4 (2%)	59	29
2	D	209/210 (100%)	209 (100%)	0	100	100
2	F	209/210 (100%)	208 (100%)	1 (0%)	88	77
2	H	211/210 (100%)	211 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1349/1328 (102%)	1339 (99%)	10 (1%)	88	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	172[A]	GLU
2	B	172[B]	GLU
2	B	173[A]	ASP
2	B	173[B]	ASP
1	C	60	GLU
1	C	77	ILE
1	C	160[A]	LEU
1	C	160[B]	LEU
2	F	5	GLU
1	G	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	CRO	B	66	2	23,23,24	2.37	7 (30%)	30,32,34	2.06	9 (30%)
2	CRO	H	66	2	23,23,24	2.30	7 (30%)	30,32,34	1.82	9 (30%)
2	CRO	F	66	2	23,23,24	2.40	7 (30%)	30,32,34	2.45	10 (33%)
2	CRO	D	66	2	23,23,24	2.45	7 (30%)	30,32,34	2.23	9 (30%)



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	CRO	B	66	2	-	0/12/31/32	0/2/2/2
2	CRO	H	66	2	-	0/12/31/32	0/2/2/2
2	CRO	F	66	2	-	0/12/31/32	0/2/2/2
2	CRO	D	66	2	-	0/12/31/32	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	66	CRO	C1-N2	6.85	1.42	1.32
2	H	66	CRO	C1-N2	6.66	1.42	1.32
2	B	66	CRO	C1-N2	6.41	1.41	1.32
2	D	66	CRO	C1-N2	6.37	1.41	1.32
2	D	66	CRO	CA2-C2	5.28	1.53	1.48
2	B	66	CRO	CA2-C2	5.14	1.53	1.48
2	F	66	CRO	CA2-C2	4.95	1.53	1.48
2	D	66	CRO	C1-N3	4.74	1.45	1.37
2	H	66	CRO	CA2-C2	4.31	1.52	1.48
2	F	66	CRO	C1-N3	4.20	1.44	1.37
2	B	66	CRO	C1-N3	3.90	1.43	1.37
2	H	66	CRO	C1-N3	3.89	1.43	1.37
2	D	66	CRO	CB2-CA2	-3.53	1.32	1.35
2	H	66	CRO	CB2-CA2	-3.42	1.32	1.35
2	B	66	CRO	CB2-CA2	-3.37	1.32	1.35
2	F	66	CRO	CG2-CB2	3.33	1.53	1.46
2	F	66	CRO	C2-N3	3.21	1.47	1.39
2	D	66	CRO	CG2-CB2	3.08	1.52	1.46
2	B	66	CRO	C2-N3	3.08	1.47	1.39
2	B	66	CRO	CG2-CB2	2.98	1.52	1.46
2	H	66	CRO	CG2-CB2	2.89	1.52	1.46
2	D	66	CRO	CA2-N2	2.61	1.44	1.38
2	D	66	CRO	C2-N3	2.48	1.45	1.39
2	F	66	CRO	CA2-N2	2.48	1.43	1.38
2	H	66	CRO	C2-N3	2.43	1.45	1.39
2	H	66	CRO	O2-C2	-2.22	1.18	1.23
2	F	66	CRO	CB2-CA2	-2.07	1.33	1.35
2	B	66	CRO	O2-C2	-2.02	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	66	CRO	CA2-C2-N3	6.45	106.42	103.37
2	D	66	CRO	CA2-C2-N3	6.19	106.30	103.37
2	F	66	CRO	O2-C2-CA2	-5.28	127.99	130.96
2	F	66	CRO	C1-CA1-N1	-4.78	102.21	109.96
2	H	66	CRO	CA2-C2-N3	4.61	105.55	103.37
2	B	66	CRO	O2-C2-CA2	-4.46	128.46	130.96
2	B	66	CRO	CA2-C2-N3	4.42	105.46	103.37
2	D	66	CRO	C1-CA1-N1	-4.37	102.87	109.96
2	D	66	CRO	C2-N3-C1	-4.25	105.82	107.97
2	F	66	CRO	CA1-C1-N3	-3.94	120.02	124.75
2	D	66	CRO	CA1-C1-N3	-3.94	120.02	124.75
2	B	66	CRO	CA1-C1-N3	-3.94	120.03	124.75
2	F	66	CRO	CG2-CB2-CA2	-3.79	125.30	129.94
2	F	66	CRO	C2-N3-C1	-3.74	106.07	107.97
2	B	66	CRO	CG2-CB2-CA2	-3.69	125.42	129.94
2	B	66	CRO	O3-C3-CA3	-3.64	115.39	126.39
2	F	66	CRO	O3-C3-CA3	-3.62	115.47	126.39
2	H	66	CRO	CA1-C1-N3	-3.33	120.75	124.75
2	H	66	CRO	C1-CA1-N1	-3.30	104.61	109.96
2	D	66	CRO	O3-C3-CA3	-3.28	116.50	126.39
2	D	66	CRO	CG2-CB2-CA2	-3.22	126.00	129.94
2	H	66	CRO	O3-C3-CA3	-2.95	117.47	126.39
2	D	66	CRO	N3-C1-N2	2.87	113.44	111.45
2	H	66	CRO	CG2-CB2-CA2	-2.82	126.48	129.94
2	B	66	CRO	CA1-C1-N2	2.81	127.82	123.89
2	B	66	CRO	CA2-N2-C1	2.75	107.80	105.77
2	B	66	CRO	C1-CA1-N1	-2.66	105.65	109.96
2	H	66	CRO	CA1-C1-N2	2.60	127.53	123.89
2	F	66	CRO	CA1-C1-N2	2.54	127.44	123.89
2	B	66	CRO	C2-N3-C1	-2.51	106.69	107.97
2	F	66	CRO	CA2-N2-C1	2.50	107.61	105.77
2	H	66	CRO	CG1-CB1-CA1	-2.34	106.64	112.16
2	H	66	CRO	CA2-N2-C1	2.30	107.47	105.77
2	D	66	CRO	O2-C2-CA2	-2.25	129.70	130.96
2	F	66	CRO	C2-CA2-N2	-2.20	107.39	108.93
2	D	66	CRO	CA3-N3-C1	2.19	129.80	127.16
2	H	66	CRO	CD2-CG2-CD1	2.04	120.66	117.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	66	CRO	1	0
2	H	66	CRO	1	0
2	F	66	CRO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PEG	A	201	-	6,6,6	0.46	0	5,5,5	0.29	0
3	PEG	G	201	-	6,6,6	0.48	0	5,5,5	0.21	0
3	PEG	D	301	-	6,6,6	0.51	0	5,5,5	0.35	0
3	PEG	B	301	-	6,6,6	0.46	0	5,5,5	0.28	0
3	PEG	C	202	-	6,6,6	0.47	0	5,5,5	0.98	0
3	PEG	E	201	-	6,6,6	0.47	0	5,5,5	0.37	0
3	PEG	A	202	-	6,6,6	0.48	0	5,5,5	0.36	0
3	PEG	C	201	-	6,6,6	0.44	0	5,5,5	0.37	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	PEG	A	201	-	-	2/4/4/4	-
3	PEG	G	201	-	-	2/4/4/4	-
3	PEG	D	301	-	-	1/4/4/4	-
3	PEG	B	301	-	-	3/4/4/4	-
3	PEG	C	202	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	E	201	-	-	3/4/4/4	-
3	PEG	A	202	-	-	3/4/4/4	-
3	PEG	C	201	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	202	PEG	C4-C3-O2-C2
3	C	202	PEG	C1-C2-O2-C3
3	G	201	PEG	O2-C3-C4-O4
3	B	301	PEG	O2-C3-C4-O4
3	E	201	PEG	O2-C3-C4-O4
3	D	301	PEG	O2-C3-C4-O4
3	B	301	PEG	O1-C1-C2-O2
3	C	202	PEG	O1-C1-C2-O2
3	A	202	PEG	O2-C3-C4-O4
3	E	201	PEG	O1-C1-C2-O2
3	A	202	PEG	O1-C1-C2-O2
3	C	201	PEG	O2-C3-C4-O4
3	A	201	PEG	O1-C1-C2-O2
3	A	202	PEG	C4-C3-O2-C2
3	E	201	PEG	C4-C3-O2-C2
3	G	201	PEG	C1-C2-O2-C3
3	B	301	PEG	C4-C3-O2-C2
3	A	201	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	PEG	1	0
3	C	202	PEG	1	0
3	C	201	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	154/160 (96%)	-0.32	2 (1%) 77 81	26, 36, 60, 98	0
1	C	155/160 (96%)	-0.32	4 (2%) 56 62	22, 31, 54, 94	0
1	E	160/160 (100%)	-0.20	5 (3%) 49 56	29, 39, 76, 142	0
1	G	160/160 (100%)	-0.29	2 (1%) 77 81	24, 36, 64, 78	0
2	B	231/243 (95%)	-0.27	5 (2%) 62 67	19, 31, 57, 125	0
2	D	231/243 (95%)	-0.22	4 (1%) 70 74	21, 35, 63, 85	0
2	F	225/243 (92%)	-0.18	3 (1%) 77 81	26, 44, 77, 113	0
2	H	228/243 (93%)	-0.24	2 (0%) 84 86	21, 31, 59, 95	0
All	All	1544/1612 (95%)	-0.25	27 (1%) 70 74	19, 35, 68, 142	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173[A]	ASP	4.1
2	B	0	MET	3.9
1	A	163	ILE	3.6
1	E	9	GLY	3.5
2	B	174[A]	GLY	3.4
1	A	12	SER	3.4
1	E	168	ASN	3.3
1	E	12	SER	3.0
1	C	165	GLN	3.0
1	E	10	PRO	2.7
2	H	232	GLY	2.6
1	G	168	ASN	2.6
1	C	163	ILE	2.6
2	H	231	LEU	2.5
2	B	1	VAL	2.5
2	D	231	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	1	VAL	2.4
2	D	178	LEU	2.4
2	F	193	VAL	2.3
2	F	174	GLY	2.3
2	F	178	LEU	2.2
1	C	109	ASP	2.2
1	E	113	PHE	2.1
1	C	13	ASP	2.1
2	B	231	LEU	2.1
2	D	128	ILE	2.1
1	G	12	SER	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CRO	B	66	22/23	0.95	0.08	20,25,32,34	0
2	CRO	F	66	22/23	0.95	0.06	24,28,39,39	0
2	CRO	H	66	22/23	0.96	0.08	20,24,30,32	0
2	CRO	D	66	22/23	0.96	0.07	21,26,37,37	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	C	202	7/7	0.59	0.20	51,61,71,71	0
3	PEG	A	201	7/7	0.79	0.12	46,55,60,66	0
3	PEG	D	301	7/7	0.81	0.12	51,62,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	C	201	7/7	0.83	0.14	44,53,56,60	0
3	PEG	A	202	7/7	0.88	0.19	51,61,68,73	0
3	PEG	B	301	7/7	0.89	0.08	53,63,67,67	0
3	PEG	E	201	7/7	0.91	0.09	49,58,64,71	0
3	PEG	G	201	7/7	0.92	0.10	43,54,63,67	0
4	NA	E	202	1/1	0.98	0.04	30,30,30,30	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.