Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 03:01 pm GMT

PDB ID	:	5MA9
Title	:	GFP-binding DARPin fusion gc_R11
Authors	:	Hansen, S.; Stueber, J.; Ernst, P.; Koch, A.; Bojar, D.; Batyuk, A.; Plueckthun, A.
Deposited on	:	2016-11-03
Resolution	:	1.57 Å(reported)

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

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

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

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

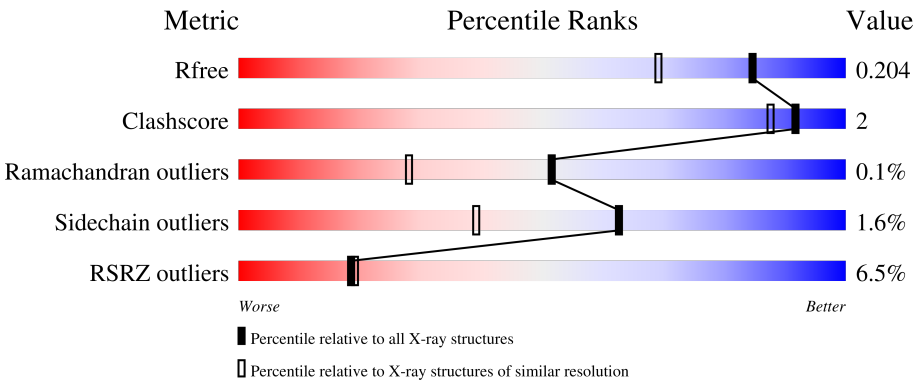
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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

Mol	Chain	Length	Quality of chain
1	B	243	% 88% 5% • 7%
1	D	243	91% • 7%
1	F	243	90% • 7%
1	H	243	89% • 7%
2	A	305	12% 94% • •

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Mol	Chain	Length	Quality of chain
2	C	305	16% 92%
2	E	305	9% 93%
2	G	305	6% 94%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33807 atoms, of which 15558 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
			Total	C	H	N	O	S			
1	B	227	3561	1159	1737	307	352	6	0	2	0
1	D	227	3561	1159	1737	307	352	6	0	1	0
1	H	227	3562	1159	1738	307	352	6	0	1	0
1	F	227	3562	1159	1738	307	352	6	0	2	0

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	?	-	SER	deletion	UNP P42212
B	?	-	TYR	deletion	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	?	-	SER	deletion	UNP P42212

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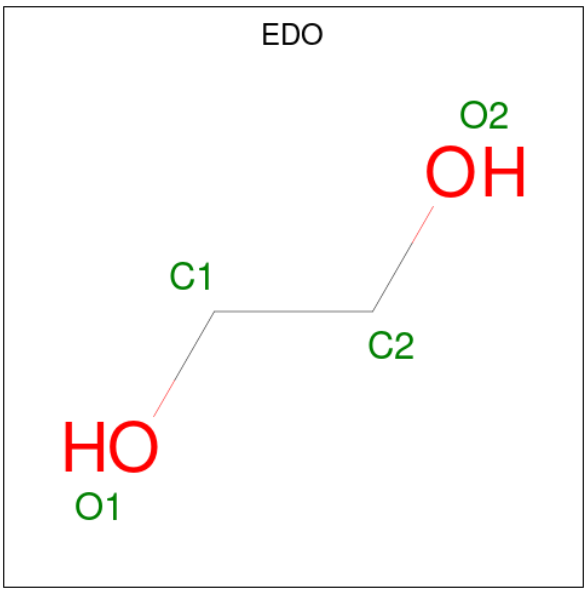
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	TYR	deletion	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	231	LEU	HIS	conflict	UNP P42212
D	239	GLN	-	expression tag	UNP P42212
D	240	ALA	-	expression tag	UNP P42212
H	-4	GLY	-	expression tag	UNP P42212
H	-3	PRO	-	expression tag	UNP P42212
H	-2	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	?	-	SER	deletion	UNP P42212
H	?	-	TYR	deletion	UNP P42212
H	66	CRO	GLY	chromophore	UNP P42212
H	231	LEU	HIS	conflict	UNP P42212
H	239	GLN	-	expression tag	UNP P42212
H	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	?	-	SER	deletion	UNP P42212
F	?	-	TYR	deletion	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

- Molecule 2 is a protein called R11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	A	298	4356	1395	2143	383	434	1	0	0	0
2	C	294	4321	1385	2128	379	428	1	0	0	0
2	G	294	4337	1390	2137	380	429	1	0	1	0
2	E	293	4350	1393	2142	383	431	1	0	2	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 9	C 2	H 5	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 9	C 2	H 5	O 2	0	0
3	C	1	Total 9	C 2	H 5	O 2	0	0
3	C	1	Total 9	C 2	H 5	O 2	0	0
3	G	1	Total 9	C 2	H 5	O 2	0	0
3	G	1	Total 9	C 2	H 5	O 2	0	0
3	E	1	Total 9	C 2	H 5	O 2	0	0
3	H	1	Total 10	C 2	H 6	O 2	0	0
3	F	1	Total 9	C 2	H 5	O 2	0	0

- Molecule 4 is water.

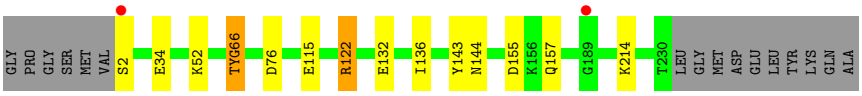
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	285	285	285	0	0
			Total	O		
4	A	245	245	245	0	0
			Total	O		
4	C	222	222	222	0	0
			Total	O		
4	G	291	291	291	0	0
			Total	O		
4	E	259	259	259	0	0
			Total	O		
4	D	250	250	250	0	0
			Total	O		
4	H	272	272	272	0	0
			Total	O		
4	F	271	271	271	0	0

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: Green fluorescent protein

Chain B:



• Molecule 1: Green fluorescent protein

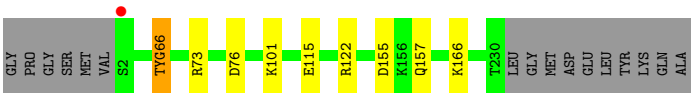
Chain D:

• Molecule 1: Green fluorescent protein

Chain H:

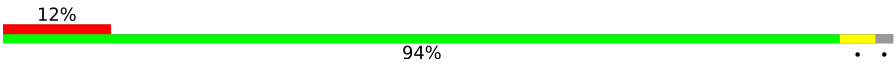
• Molecule 1: Green fluorescent protein

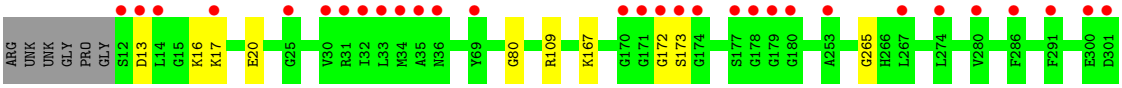
Chain F:

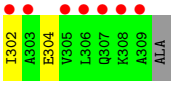


• Molecule 2: R11

Chain A:

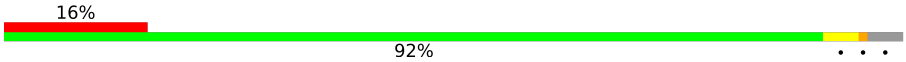


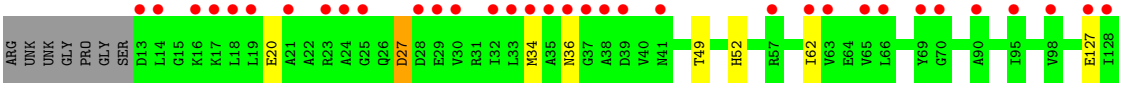


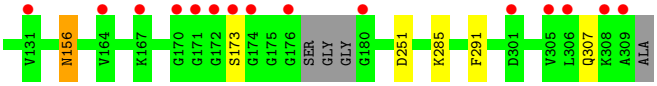


• Molecule 2: R11

Chain C:

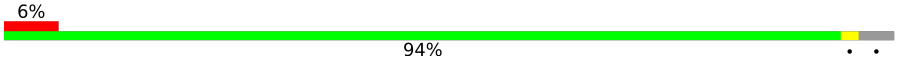


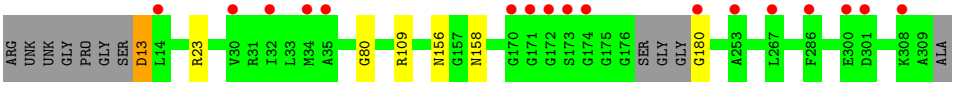




• Molecule 2: R11

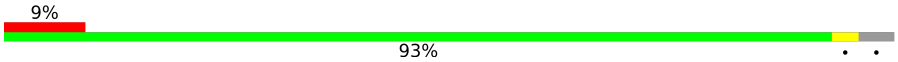
Chain G:

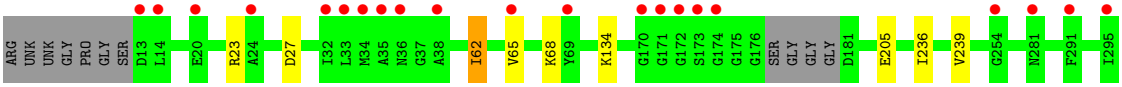


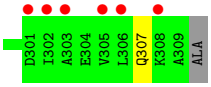


• Molecule 2: R11

Chain E:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.88Å 89.89Å 90.04Å 95.84° 116.53° 92.35°	Depositor
Resolution (Å)	44.68 – 1.57 44.68 – 1.57	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.68-1.57) 95.2 (44.68-1.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.158 , 0.203 0.160 , 0.204	Depositor DCC
R_{free} test set	15137 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33807	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 80.77 % 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 4.1464e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.30	0/1849	0.51	0/2499
1	D	0.29	0/1842	0.50	0/2489
1	F	0.29	0/1849	0.50	0/2499
1	H	0.30	0/1842	0.51	0/2489
2	A	0.25	0/2253	0.45	0/3066
2	C	0.26	0/2232	0.43	0/3037
2	E	0.26	0/2247	0.44	0/3057
2	G	0.26	0/2239	0.44	0/3047
All	All	0.28	0/16353	0.47	0/22183

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1824	1737	1761	9	0
1	D	1824	1737	1767	4	0
1	F	1824	1738	1761	6	0
1	H	1824	1738	1767	7	0
2	A	2213	2143	2157	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2193	2128	2140	9	0
2	E	2208	2142	2152	3	0
2	G	2200	2137	2148	6	0
3	A	12	16	18	0	0
3	B	4	6	6	3	0
3	C	8	10	12	0	0
3	E	4	5	6	1	0
3	F	4	5	6	1	0
3	G	8	10	12	0	0
3	H	4	6	6	1	0
4	A	245	0	0	2	0
4	B	285	0	0	4	0
4	C	222	0	0	5	0
4	D	250	0	0	2	0
4	E	259	0	0	2	0
4	F	271	0	0	2	0
4	G	291	0	0	6	0
4	H	272	0	0	1	0
All	All	18249	15558	15719	50	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 2.

All (50) 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:F:166:LYS:NZ	4:F:401:HOH:O	2.11	0.81
2:G:80:GLY:O	4:G:501:HOH:O	1.98	0.81
2:A:80:GLY:O	4:A:501:HOH:O	1.97	0.80
1:B:115:GLU:OE2	1:B:122:ARG:NH2	2.14	0.79
2:A:109:ARG:O	4:A:501:HOH:O	2.02	0.78
1:H:115:GLU:OE2	1:H:122:ARG:NH2	2.18	0.77
2:C:49:THR:OG1	4:C:501:HOH:O	2.05	0.74
2:G:109:ARG:O	4:G:501:HOH:O	2.06	0.74
1:H:34:GLU:OE2	4:H:401:HOH:O	2.08	0.71
2:C:251:ASP:N	4:C:502:HOH:O	2.24	0.70
1:B:34:GLU:OE2	4:B:401:HOH:O	2.09	0.69
1:D:115:GLU:OE2	1:D:122:ARG:NH2	2.26	0.69
2:C:156:ASN:OD1	1:D:73:ARG:NH1	2.27	0.68
2:G:158:ASN:OD1	4:G:502:HOH:O	2.10	0.68
1:F:115:GLU:OE2	1:F:122:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:307:GLN:OE1	4:E:501:HOH:O	2.14	0.65
1:F:73:ARG:NH1	4:F:403:HOH:O	2.29	0.64
2:G:180:GLY:N	4:G:506:HOH:O	2.34	0.60
1:D:36:ASP:OD1	4:D:301:HOH:O	2.16	0.60
1:B:144:ASN:HA	3:B:301:EDO:H12	1.83	0.60
3:B:301:EDO:O1	4:B:402:HOH:O	2.16	0.59
2:C:52:HIS:N	4:C:501:HOH:O	2.37	0.58
1:D:73:ARG:NH2	4:D:306:HOH:O	2.36	0.57
2:C:127:GLU:N	2:C:127:GLU:OE1	2.40	0.54
2:G:13:ASP:N	4:G:511:HOH:O	2.40	0.54
2:G:156:ASN:ND2	4:G:510:HOH:O	2.40	0.53
2:C:27:ASP:OD1	2:C:27:ASP:N	2.39	0.52
1:B:2:SER:N	4:B:412:HOH:O	2.44	0.50
1:B:132:GLU:OE2	4:B:403:HOH:O	2.19	0.49
2:C:307:GLN:NE2	4:C:513:HOH:O	2.46	0.49
2:C:251:ASP:O	4:C:502:HOH:O	2.19	0.48
2:E:62:ILE:HA	2:E:65:VAL:HG12	1.96	0.47
1:H:101:LYS:HB2	3:H:301:EDO:H12	1.96	0.47
2:C:291:PHE:CE1	2:C:307:GLN:HG3	2.52	0.44
1:F:155:ASP:OD1	1:F:157:GLN:NE2	2.50	0.44
1:H:66:CRO:HD2	1:H:66:CRO:N2	2.34	0.43
1:F:101:LYS:HB2	3:F:301:EDO:H21	2.00	0.42
2:A:167:LYS:HA	2:A:172:GLY:HA2	2.02	0.41
1:H:163:VAL:HB	1:H:183:GLN:HB3	2.02	0.41
1:F:66:CRO:HD2	1:F:66:CRO:N2	2.36	0.41
3:E:401:EDO:O2	4:E:502:HOH:O	2.21	0.41
2:A:16:LYS:O	2:A:20:GLU:HG2	2.21	0.41
1:B:155:ASP:OD1	1:B:157:GLN:NE2	2.54	0.41
1:B:143:TYR:O	3:B:301:EDO:H12	2.21	0.40
1:H:76:ASP:HA	1:H:79:LYS:HE2	2.03	0.40
1:B:66:CRO:HD2	1:B:66:CRO:N2	2.37	0.40
1:B:136:ILE:HD12	1:B:136:ILE:N	2.37	0.40
2:A:265:GLY:HA2	2:A:302:ILE:HD12	2.03	0.40
2:E:236:ILE:HA	2:E:239:VAL:HG12	2.04	0.40
1:H:132:GLU:OE2	1:H:132:GLU:N	2.51	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	B	224/243 (92%)	222 (99%)	2 (1%)	0	100	100
1	D	223/243 (92%)	221 (99%)	2 (1%)	0	100	100
1	F	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
1	H	223/243 (92%)	220 (99%)	3 (1%)	0	100	100
2	A	296/305 (97%)	291 (98%)	4 (1%)	1 (0%)	41	21
2	C	290/305 (95%)	282 (97%)	7 (2%)	1 (0%)	41	21
2	E	291/305 (95%)	288 (99%)	3 (1%)	0	100	100
2	G	291/305 (95%)	287 (99%)	4 (1%)	0	100	100
All	All	2062/2192 (94%)	2032 (98%)	28 (1%)	2 (0%)	51	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	173	SER
2	A	173	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	B	200/210 (95%)	196 (98%)	4 (2%)	55	29
1	D	199/210 (95%)	197 (99%)	2 (1%)	76	59
1	F	200/210 (95%)	199 (100%)	1 (0%)	88	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	199/210 (95%)	198 (100%)	1 (0%)	88	80
2	A	220/222 (99%)	217 (99%)	3 (1%)	67	45
2	C	218/222 (98%)	211 (97%)	7 (3%)	39	13
2	E	220/222 (99%)	214 (97%)	6 (3%)	44	18
2	G	219/222 (99%)	217 (99%)	2 (1%)	78	64
All	All	1675/1728 (97%)	1649 (98%)	26 (2%)	62	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	LYS
1	B	76	ASP
1	B	122	ARG
1	B	214	LYS
2	A	13	ASP
2	A	17	LYS
2	A	304	GLU
2	C	20	GLU
2	C	27	ASP
2	C	34	MET
2	C	36	ASN
2	C	62	ILE
2	C	156	ASN
2	C	285	LYS
2	G	13	ASP
2	G	23	ARG
2	E	23	ARG
2	E	27	ASP
2	E	62	ILE
2	E	68	LYS
2	E	134	LYS
2	E	205	GLU
1	D	52	LYS
1	D	122	ARG
1	H	52	LYS
1	F	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	200	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	CRO	H	66	1	23,23,24	1.73	5 (21%)	30,32,34	2.61	10 (33%)
1	CRO	F	66	1	23,23,24	1.78	5 (21%)	30,32,34	2.96	9 (30%)
1	CRO	D	66	1	23,23,24	1.87	5 (21%)	30,32,34	2.87	9 (30%)
1	CRO	B	66	1	23,23,24	1.92	4 (17%)	30,32,34	2.77	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
1	CRO	H	66	1	-	0/12/31/32	0/2/2/2
1	CRO	F	66	1	-	0/12/31/32	0/2/2/2
1	CRO	D	66	1	-	0/12/31/32	0/2/2/2
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	C1-N2	5.93	1.40	1.32
1	D	66	CRO	C1-N2	5.44	1.40	1.32
1	F	66	CRO	C1-N2	5.30	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	66	CRO	C1-N2	5.18	1.39	1.32
1	B	66	CRO	CA2-C2	3.81	1.52	1.48
1	D	66	CRO	CA2-C2	3.57	1.52	1.48
1	B	66	CRO	C1-N3	3.41	1.42	1.37
1	F	66	CRO	CA2-C2	3.38	1.51	1.48
1	D	66	CRO	C1-N3	3.33	1.42	1.37
1	H	66	CRO	CA2-C2	3.25	1.51	1.48
1	F	66	CRO	C1-N3	3.11	1.42	1.37
1	H	66	CRO	C1-N3	3.10	1.42	1.37
1	B	66	CRO	CG2-CB2	2.88	1.52	1.46
1	D	66	CRO	CG2-CB2	2.85	1.52	1.46
1	F	66	CRO	CG2-CB2	2.78	1.52	1.46
1	H	66	CRO	CG2-CB2	2.44	1.51	1.46
1	H	66	CRO	CA3-N3	-2.19	1.42	1.47
1	F	66	CRO	CA3-N3	-2.09	1.43	1.47
1	D	66	CRO	CA3-N3	-2.07	1.43	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	CRO	CA2-C2-N3	9.14	107.69	103.37
1	F	66	CRO	CA2-C2-N3	8.76	107.51	103.37
1	B	66	CRO	CA2-C2-N3	8.66	107.47	103.37
1	F	66	CRO	O2-C2-CA2	-8.15	126.39	130.96
1	H	66	CRO	CA2-C2-N3	7.45	106.90	103.37
1	B	66	CRO	O2-C2-CA2	-7.40	126.80	130.96
1	D	66	CRO	O2-C2-CA2	-7.09	126.98	130.96
1	H	66	CRO	O2-C2-CA2	-6.43	127.35	130.96
1	F	66	CRO	C2-N3-C1	-5.89	104.99	107.97
1	D	66	CRO	C2-N3-C1	-5.65	105.11	107.97
1	B	66	CRO	C2-N3-C1	-5.32	105.27	107.97
1	H	66	CRO	C2-N3-C1	-4.71	105.58	107.97
1	D	66	CRO	CA2-N2-C1	4.07	108.78	105.77
1	F	66	CRO	CA2-N2-C1	3.96	108.69	105.77
1	D	66	CRO	C2-CA2-N2	-3.93	106.18	108.93
1	H	66	CRO	CG2-CB2-CA2	-3.93	125.13	129.94
1	F	66	CRO	C2-CA2-N2	-3.70	106.34	108.93
1	B	66	CRO	CG2-CB2-CA2	-3.51	125.64	129.94
1	H	66	CRO	CA1-C1-N3	-3.48	120.57	124.75
1	B	66	CRO	CA2-N2-C1	3.41	108.29	105.77
1	D	66	CRO	CG2-CB2-CA2	-3.41	125.77	129.94
1	F	66	CRO	CG2-CB2-CA2	-3.35	125.84	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CRO	C2-CA2-N2	-3.23	106.67	108.93
1	H	66	CRO	O3-C3-CA3	-3.20	116.74	126.39
1	H	66	CRO	CA2-N2-C1	3.14	108.08	105.77
1	D	66	CRO	O3-C3-CA3	-3.11	116.99	126.39
1	F	66	CRO	CA1-C1-N3	-2.99	121.16	124.75
1	F	66	CRO	O3-C3-CA3	-2.99	117.36	126.39
1	H	66	CRO	C1-CA1-N1	-2.90	105.26	109.96
1	H	66	CRO	C2-CA2-N2	-2.81	106.96	108.93
1	F	66	CRO	C1-CA1-N1	-2.80	105.42	109.96
1	B	66	CRO	CA1-C1-N3	-2.79	121.41	124.75
1	B	66	CRO	C1-CA1-N1	-2.56	105.81	109.96
1	B	66	CRO	O3-C3-CA3	-2.47	118.94	126.39
1	D	66	CRO	CA1-C1-N3	-2.41	121.85	124.75
1	D	66	CRO	C1-CA1-N1	-2.28	106.27	109.96
1	H	66	CRO	CA1-C1-N2	2.19	126.95	123.89

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
1	H	66	CRO	1	0
1	F	66	CRO	1	0
1	B	66	CRO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	C	402	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.21	0
3	EDO	G	401	-	3,3,3	0.41	0	2,2,2	0.37	0
3	EDO	B	301	-	3,3,3	0.36	0	2,2,2	0.55	0
3	EDO	C	401	-	3,3,3	0.36	0	2,2,2	0.44	0
3	EDO	A	401	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	H	301	-	3,3,3	0.53	0	2,2,2	0.17	0
3	EDO	F	301	-	3,3,3	0.49	0	2,2,2	0.09	0
3	EDO	A	402	-	3,3,3	0.45	0	2,2,2	0.27	0
3	EDO	E	401	-	3,3,3	0.37	0	2,2,2	0.34	0
3	EDO	G	402	-	3,3,3	0.49	0	2,2,2	0.14	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	EDO	C	402	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	G	401	-	-	0/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	C	401	-	-	1/1/1/1	-
3	EDO	A	401	-	-	0/1/1/1	-
3	EDO	H	301	-	-	1/1/1/1	-
3	EDO	F	301	-	-	1/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	E	401	-	-	0/1/1/1	-
3	EDO	G	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	EDO	O1-C1-C2-O2
3	G	402	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	401	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	F	301	EDO	O1-C1-C2-O2
3	A	402	EDO	O1-C1-C2-O2
3	H	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	EDO	3	0
3	H	301	EDO	1	0
3	F	301	EDO	1	0
3	E	401	EDO	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	226/243 (93%)	-0.10	2 (0%)	84	85	12, 21, 45, 83	0
1	D	226/243 (93%)	-0.06	1 (0%)	92	93	12, 22, 43, 89	0
1	F	226/243 (93%)	-0.05	1 (0%)	92	93	11, 20, 43, 100	0
1	H	226/243 (93%)	-0.09	1 (0%)	92	93	11, 19, 44, 82	0
2	A	298/305 (97%)	0.42	37 (12%)	4	3	11, 30, 67, 94	0
2	C	294/305 (96%)	0.64	49 (16%)	1	1	13, 31, 84, 111	0
2	E	293/305 (96%)	0.32	27 (9%)	9	8	11, 30, 61, 77	0
2	G	294/305 (96%)	0.13	17 (5%)	23	23	12, 27, 59, 121	0
All	All	2083/2192 (95%)	0.18	135 (6%)	18	19	11, 25, 61, 121	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	172	GLY	10.8
2	C	33	LEU	8.8
2	C	36	ASN	8.6
2	C	32	ILE	7.7
2	A	177	SER	7.5
2	C	171	GLY	6.6
2	A	178	GLY	6.3
2	C	37	GLY	5.6
2	A	14	LEU	5.4
2	C	62	ILE	5.1
2	A	307	GLN	5.0
2	C	69	TYR	5.0
2	A	174	GLY	4.9
2	C	24	ALA	4.7
2	E	14	LEU	4.7
1	F	2	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	E	69	TYR	4.6
2	C	28	ASP	4.5
2	C	35	ALA	4.5
2	E	32	ILE	4.4
2	A	306	LEU	4.4
1	H	2	SER	4.3
2	E	306	LEU	4.3
2	A	267	LEU	4.2
2	C	30	VAL	4.1
2	G	174	GLY	4.1
2	A	173	SER	4.1
2	C	308	LYS	4.0
2	C	173	SER	3.9
2	C	29	GLU	3.9
2	A	32	ILE	3.9
2	A	305	VAL	3.8
2	G	14	LEU	3.7
1	D	2	SER	3.7
2	G	253	ALA	3.7
2	G	300	GLU	3.6
2	A	35	ALA	3.5
2	E	38	ALA	3.5
2	C	164	VAL	3.5
2	G	180	GLY	3.5
2	E	305	VAL	3.5
2	G	35	ALA	3.4
2	C	34	MET	3.4
2	A	286	PHE	3.4
2	A	291	PHE	3.4
2	A	170	GLY	3.4
2	E	173	SER	3.4
2	A	300	GLU	3.3
2	G	173	SER	3.3
2	C	65	VAL	3.3
2	A	308	LYS	3.3
2	A	33	LEU	3.3
2	E	308	LYS	3.2
2	A	303	ALA	3.2
2	C	38	ALA	3.2
2	A	13	ASP	3.1
2	G	308	LYS	3.1
2	C	18	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	30	VAL	3.1
2	E	170	GLY	3.0
2	C	13	ASP	3.0
2	C	23	ARG	3.0
2	C	174	GLY	2.9
1	B	2	SER	2.9
2	A	180	GLY	2.9
2	C	14	LEU	2.9
2	E	35	ALA	2.9
2	G	32	ILE	2.8
2	C	176	GLY	2.8
2	C	167	LYS	2.8
2	G	286	PHE	2.8
2	E	171	GLY	2.8
2	C	305	VAL	2.8
2	C	309	ALA	2.8
2	E	24	ALA	2.8
2	G	171	GLY	2.7
2	C	16	LYS	2.7
2	G	34	MET	2.7
2	A	69	TYR	2.7
2	E	291	PHE	2.7
2	E	301	ASP	2.6
2	A	274	LEU	2.6
2	A	171	GLY	2.6
2	A	34	MET	2.6
2	G	301	ASP	2.6
2	G	267	LEU	2.6
2	E	302	ILE	2.6
2	G	170	GLY	2.5
1	B	189	GLY	2.5
2	E	34	MET	2.5
2	E	303	ALA	2.5
2	G	30	VAL	2.5
2	C	25	GLY	2.4
2	A	309	ALA	2.4
2	C	306	LEU	2.4
2	C	70	GLY	2.4
2	C	17	LYS	2.4
2	E	172	GLY	2.4
2	C	63	VAL	2.4
2	C	128	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	17	LYS	2.4
2	C	180	GLY	2.4
2	E	13	ASP	2.4
2	E	36	ASN	2.3
2	A	179	GLY	2.3
2	C	66	LEU	2.3
2	C	21	ALA	2.3
2	A	301	ASP	2.3
2	A	253	ALA	2.3
2	C	95	ILE	2.3
2	E	295	ILE	2.3
2	A	36	ASN	2.2
2	C	127	GLU	2.2
2	C	170	GLY	2.2
2	C	98	VAL	2.2
2	E	281	ASN	2.2
2	A	31	ARG	2.2
2	A	172	GLY	2.2
2	E	174	GLY	2.1
2	E	33	LEU	2.1
2	C	39	ASP	2.1
2	E	254	GLY	2.1
2	A	280	VAL	2.1
2	C	41	ASN	2.1
2	C	57	ARG	2.1
2	C	301	ASP	2.1
2	G	172	GLY	2.1
2	A	302	ILE	2.0
2	C	131	VAL	2.0
2	E	65	VAL	2.0
2	A	25	GLY	2.0
2	A	12	SER	2.0
2	C	90	ALA	2.0
2	C	19	LEU	2.0
2	E	20	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CRO	D	66	22/23	0.96	0.14	17,21,28,28	0
1	CRO	F	66	22/23	0.96	0.15	17,21,27,27	0
1	CRO	H	66	22/23	0.97	0.13	17,21,26,26	0
1	CRO	B	66	22/23	0.97	0.14	17,21,27,27	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	401	4/4	0.68	0.23	48,58,67,81	0
3	EDO	G	402	4/4	0.68	0.13	39,44,48,53	0
3	EDO	H	301	4/4	0.72	0.22	43,52,57,61	0
3	EDO	G	401	4/4	0.75	0.18	37,44,47,57	0
3	EDO	F	301	4/4	0.77	0.27	35,42,58,70	0
3	EDO	C	402	4/4	0.87	0.10	37,44,48,52	0
3	EDO	B	301	4/4	0.89	0.21	23,30,35,36	0
3	EDO	C	401	4/4	0.90	0.24	19,34,44,53	0
3	EDO	E	401	4/4	0.90	0.21	20,34,43,51	0
3	EDO	A	403	4/4	0.93	0.10	40,44,49,53	0
3	EDO	A	402	4/4	0.95	0.31	43,52,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.