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wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 03:31 PM EDT

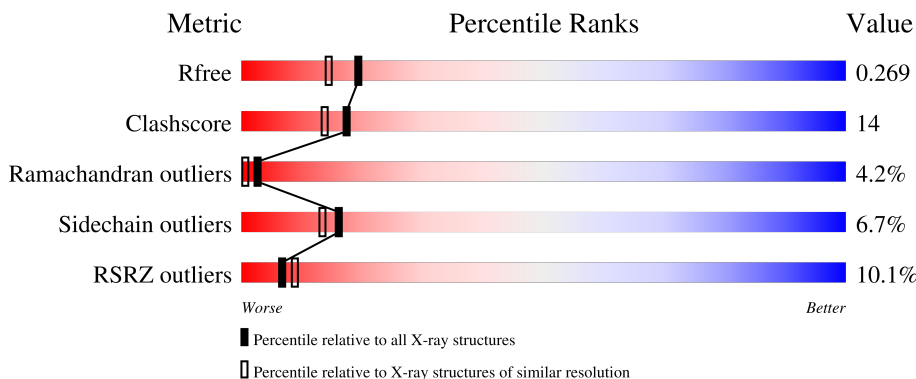|		
PDB ID	:	2G3O
Title	:	The 2.1A crystal structure of copGFP
Authors	:	Wilmann, P.G.
Deposited on	:	2006-02-20
Resolution	:	2.10 Å(reported)

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 2.10 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	Percentile Ranks	Value
Rfree		0.269
Clashscore		14
Ramachandran outliers		4.2%
Sidechain outliers		6.7%
RSRZ outliers		10.1%

Worse ... Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
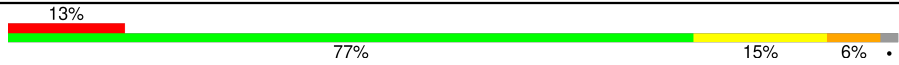
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	220	4% / 73% / 18% / 5% ··
1	B	220	7% / 75% / 16% / 5% ··
1	C	220	11% / 73% / 20% / ···
1	D	220	13% / 76% / 18% / ···
1	E	220	12% / 75% / 17% / 5% ·

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Mol	Chain	Length	Quality of chain
1	F	220	13% / 77% / 15% / 6% / ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9837 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called green fluorescent protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1621	1043	278	292	8			
1	B	213	Total	C	N	O	S	0	0	0
			1609	1034	278	289	8			
1	C	216	Total	C	N	O	S	0	0	0
			1605	1031	269	298	7			
1	D	216	Total	C	N	O	S	0	0	0
			1590	1023	265	295	7			
1	E	216	Total	C	N	O	S	0	0	0
			1603	1031	271	294	7			
1	F	216	Total	C	N	O	S	0	0	0
			1595	1026	267	295	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
A	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12
A	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
B	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
B	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12
B	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
C	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
C	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12
C	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
D	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
D	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12
D	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
E	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
E	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12
E	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
F	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12
F	57	CR2	TYR	CHROMOPHORE	UNP Q6WV12

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Chain	Residue	Modelled	Actual	Comment	Reference
F	57	CR2	GLY	CHROMOPHORE	UNP Q6WV12

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total 47	O 47	0	0
2	B	47	Total 47	O 47	0	0
2	C	29	Total 29	O 29	0	0
2	D	40	Total 40	O 40	0	0
2	E	16	Total 16	O 16	0	0
2	F	35	Total 35	O 35	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: green fluorescent protein 2
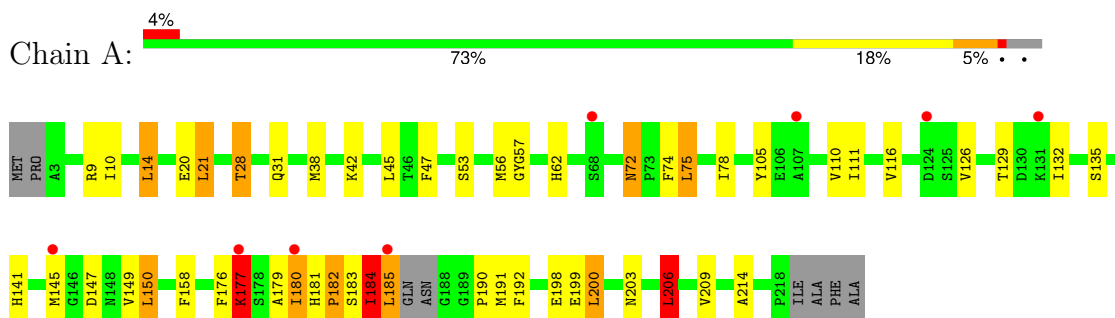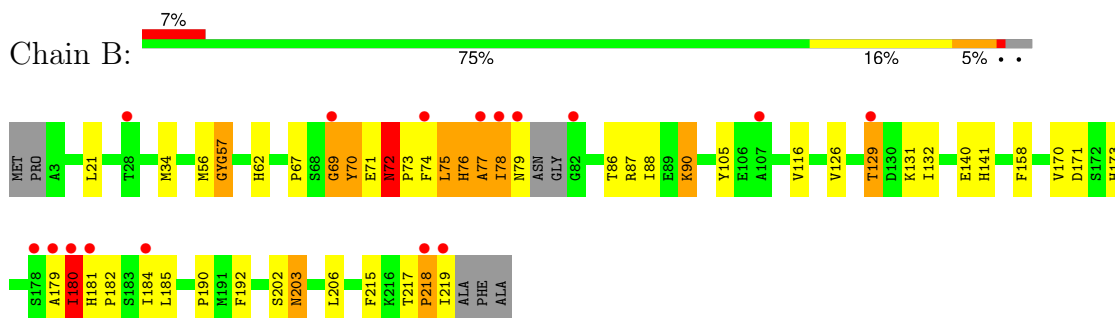
Chain A:

- Molecule 1: green fluorescent protein 2

Chain B:

- Molecule 1: green fluorescent protein 2

Chain C:

- Molecule 1: green fluorescent protein 2

Chain D:

• Molecule 1: green fluorescent protein 2

Chain E:

• Molecule 1: green fluorescent protein 2

Chain F:
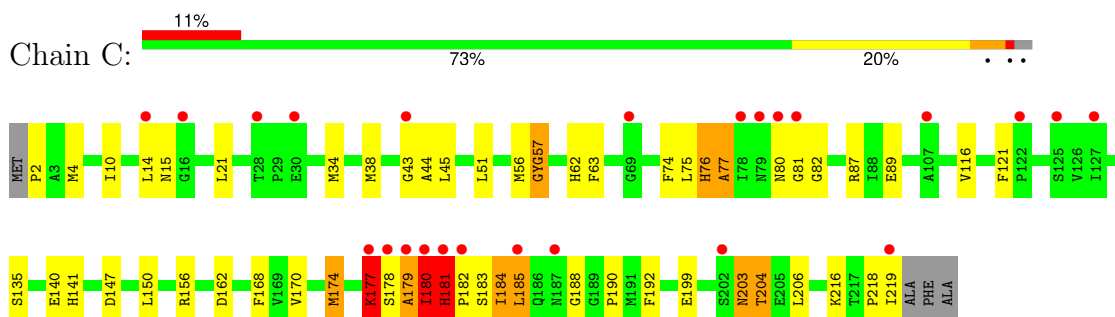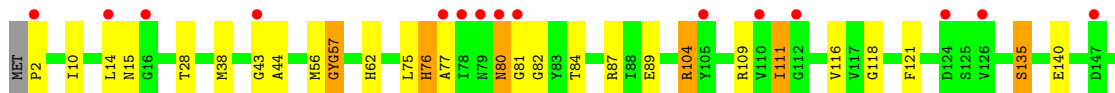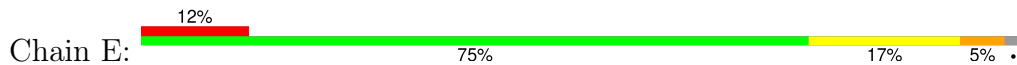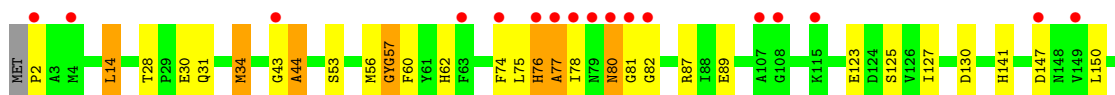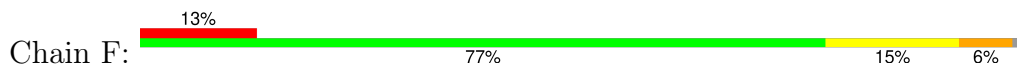
4 Data and refinement statistics ⓘ

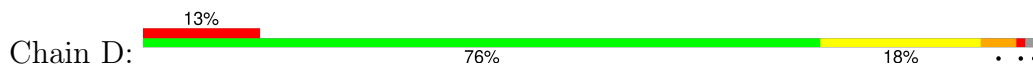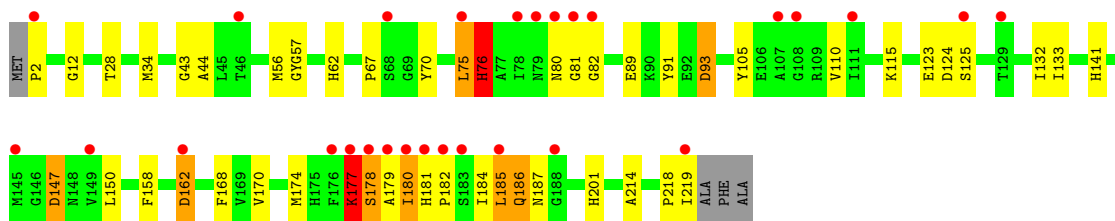| Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	145.95Å 145.95Å 53.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.71 – 2.10	Depositor
	35.71 – 2.10	EDS
% Data completeness	99.5 (35.71-2.10)	Depositor
(in resolution range)	99.5 (35.71-2.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.272	Depositor
	0.229 , 0.269	DCC
R_{free} test set	3752 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.6	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.136 for -h,-k,l 0.179 for h,-h-k,-l 0.096 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9837	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

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5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	2/1645 (0.1%)	0.69	3/2225 (0.1%)
1	B	0.48	0/1632	0.69	1/2210 (0.0%)
1	C	0.41	0/1630	0.68	3/2215 (0.1%)
1	D	0.55	3/1614 (0.2%)	0.71	4/2195 (0.2%)
1	E	0.41	0/1627	0.65	2/2210 (0.1%)
1	F	0.49	0/1619	0.65	1/2200 (0.0%)
All	All	0.48	5/9767 (0.1%)	0.68	14/13255 (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	B	0	1
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	LYS	CE-NZ	8.92	1.71	1.49
1	D	93	ASP	CG-OD2	7.02	1.41	1.25
1	A	185	LEU	C-O	6.09	1.34	1.23
1	D	93	ASP	CG-OD1	5.53	1.38	1.25
1	D	115	LYS	CE-NZ	5.03	1.61	1.49

The worst 5 of 14 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	LEU	CA-CB-CG	7.86	133.38	115.30
1	D	93	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	2	PRO	N-CA-CB	6.02	110.52	103.30
1	A	200	LEU	CA-CB-CG	5.94	128.96	115.30
1	C	2	PRO	N-CA-CB	5.92	110.40	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	180	ILE	Peptide
1	E	180	ILE	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	1621	0	1512	34	0
1	B	1609	0	1480	49	0
1	C	1605	0	1420	48	0
1	D	1590	0	1401	41	0
1	E	1603	0	1430	41	0
1	F	1595	0	1411	41	0
2	A	47	0	0	2	0
2	B	47	0	0	2	0
2	C	29	0	0	1	0
2	D	40	0	0	6	0
2	E	16	0	0	1	0
2	F	35	0	0	3	0
All	All	9837	0	8654	253	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 14.

The worst 5 of 253 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:A:177:LYS:NZ	1:A:177:LYS:CE	1.71	1.54
1:B:78:ILE:CB	1:B:79:ASN:HA	1.70	1.19
1:B:181:HIS:HB2	1:B:185:LEU:HG	1.28	1.16
1:F:80:ASN:HB3	1:F:81:GLY:HA2	1.21	1.12
1:D:185:LEU:HA	1:D:187:ASN:H	1.17	1.10

There are no symmetry-related clashes.

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	205/220 (93%)	193 (94%)	9 (4%)	3 (2%)	10	5
1	B	206/220 (94%)	186 (90%)	9 (4%)	11 (5%)	2	0
1	C	211/220 (96%)	189 (90%)	10 (5%)	12 (6%)	1	0
1	D	211/220 (96%)	192 (91%)	9 (4%)	10 (5%)	2	0
1	E	211/220 (96%)	191 (90%)	12 (6%)	8 (4%)	3	1
1	F	211/220 (96%)	192 (91%)	10 (5%)	9 (4%)	2	0
All	All	1255/1320 (95%)	1143 (91%)	59 (5%)	53 (4%)	3	0

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ILE
1	B	70	TYR
1	B	76	HIS
1	B	77	ALA
1	B	182	PRO

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	161/183 (88%)	145 (90%)	16 (10%)	8	5
1	B	156/183 (85%)	148 (95%)	8 (5%)	24	22
1	C	150/183 (82%)	141 (94%)	9 (6%)	19	16
1	D	147/183 (80%)	138 (94%)	9 (6%)	18	16
1	E	150/183 (82%)	141 (94%)	9 (6%)	19	16
1	F	148/183 (81%)	138 (93%)	10 (7%)	16	13
All	All	912/1098 (83%)	851 (93%)	61 (7%)	16	13

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	162	ASP
1	F	34	MET
1	D	76	HIS
1	F	31	GLN
1	F	174	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	76	HIS
1	F	62	HIS
1	F	141	HIS
1	E	141	HIS
1	C	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	F	57	1	20,20,21	2.73	6 (30%)	25,27,29	6.10	14 (56%)
1	CR2	B	57	1	20,20,21	2.67	5 (25%)	25,27,29	5.90	12 (48%)
1	CR2	A	57	1	20,20,21	2.66	5 (25%)	25,27,29	5.97	11 (44%)
1	CR2	D	57	1	20,20,21	2.72	6 (30%)	25,27,29	6.09	14 (56%)
1	CR2	C	57	1	20,20,21	2.76	6 (30%)	25,27,29	6.71	11 (44%)
1	CR2	E	57	1	20,20,21	2.64	6 (30%)	25,27,29	6.53	12 (48%)

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	F	57	1	-	0/6/25/26	0/2/2/2
1	CR2	B	57	1	-	0/6/25/26	0/2/2/2
1	CR2	A	57	1	-	0/6/25/26	0/2/2/2
1	CR2	D	57	1	-	0/6/25/26	0/2/2/2
1	CR2	C	57	1	-	0/6/25/26	0/2/2/2
1	CR2	E	57	1	-	0/6/25/26	0/2/2/2

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	CR2	CG2-CB2	-9.61	1.29	1.46
1	D	57	CR2	CG2-CB2	-9.58	1.29	1.46
1	F	57	CR2	CG2-CB2	-9.55	1.29	1.46
1	A	57	CR2	CG2-CB2	-9.39	1.29	1.46
1	B	57	CR2	CG2-CB2	-9.20	1.29	1.46

The worst 5 of 74 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	CR2	CG2-CB2-CA2	28.97	164.31	129.87
1	E	57	CR2	CG2-CB2-CA2	27.23	162.23	129.87
1	D	57	CR2	CG2-CB2-CA2	24.69	159.22	129.87
1	F	57	CR2	CG2-CB2-CA2	24.59	159.10	129.87
1	A	57	CR2	CG2-CB2-CA2	23.55	157.86	129.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	57	CR2	1	0
1	B	57	CR2	1	0
1	C	57	CR2	1	0
1	E	57	CR2	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

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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(Å²)	Q<0.9
1	A	211/220 (95%)	0.39	8 (3%)	40	46	35, 39, 43, 48	0
1	B	212/220 (96%)	0.53	16 (7%)	14	18	34, 39, 45, 57	0
1	C	215/220 (97%)	0.75	24 (11%)	5	6	35, 39, 42, 48	0
1	D	215/220 (97%)	0.76	28 (13%)	3	4	36, 39, 42, 48	0
1	E	215/220 (97%)	0.87	26 (12%)	4	5	35, 39, 41, 48	0
1	F	215/220 (97%)	0.71	28 (13%)	3	4	35, 39, 42, 48	0
All	All	1283/1320 (97%)	0.67	130 (10%)	7	9	34, 39, 42, 57	0

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	ALA	17.6
1	B	180	ILE	12.4
1	B	219	ILE	10.1
1	E	219	ILE	9.0
1	F	180	ILE	8.7

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

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(Å²)	Q<0.9
1	CR2	E	57	19/20	0.87	0.20	32,35,38,39	0
1	CR2	B	57	19/20	0.89	0.17	21,26,34,34	0
1	CR2	C	57	19/20	0.92	0.15	32,35,38,38	0
1	CR2	F	57	19/20	0.92	0.11	30,34,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CR2	D	57	19/20	0.93	0.10	30,33,37,37	0
1	CR2	A	57	19/20	0.94	0.12	22,25,33,33	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.