wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 12:24 AM EDT

PDB ID	:	5NI3
Title	:	sfGFP 204-204 mutant dimer
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Deposited on	:	2017-03-23
Resolution	:	1.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

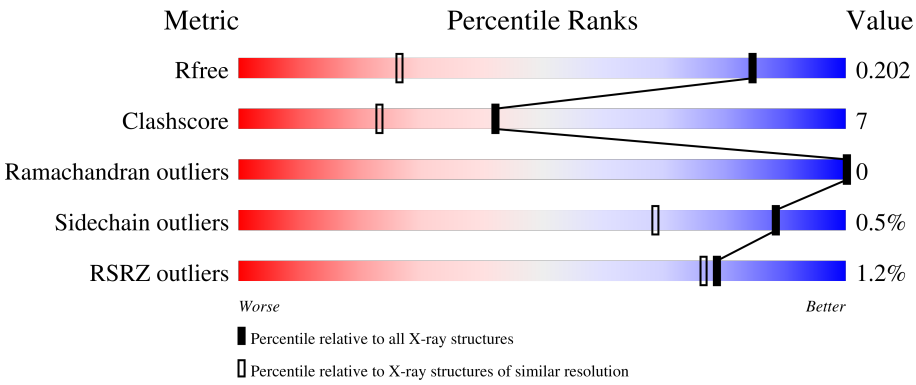
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

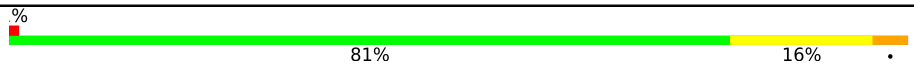
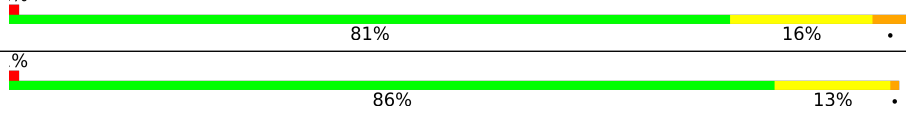
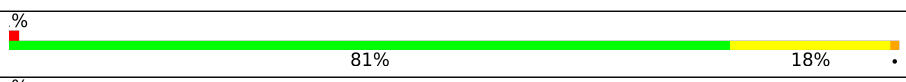
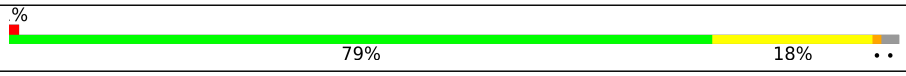
The reported resolution of this entry is 1.28 Å.

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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	225	
2	B	229	
3	C	229	
3	D	229	

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
5	DB5	A	303	-	-	X	-
6	GOL	B	303	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8346 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1811	1153	308	345	5	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	SER	conflict	UNP A0A059PIQ0
A	66	CRO	THR	chromophore	UNP A0A059PIQ0
A	66	CRO	TYR	chromophore	UNP A0A059PIQ0
A	66	CRO	GLY	chromophore	UNP A0A059PIQ0
A	72	SER	ALA	conflict	UNP A0A059PIQ0
A	80	ARG	GLN	conflict	UNP A0A059PIQ0
A	204	PHE	GLN	engineered mutation	UNP A0A059PIQ0
A	206	VAL	ALA	conflict	UNP A0A059PIQ0

- Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	229	1840	1170	314	350	6	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ARG	SER	conflict	UNP A0A059PIQ0
B	66	CRO	THR	chromophore	UNP A0A059PIQ0
B	66	CRO	TYR	chromophore	UNP A0A059PIQ0
B	66	CRO	GLY	chromophore	UNP A0A059PIQ0
B	72	SER	ALA	conflict	UNP A0A059PIQ0
B	80	ARG	GLN	conflict	UNP A0A059PIQ0
B	204	PHE	GLN	engineered mutation	UNP A0A059PIQ0
B	206	VAL	ALA	conflict	UNP A0A059PIQ0

- Molecule 3 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	229	1835	1164	316	349	6	0	2	0
3	D	225	1816	1153	310	348	5	0	4	0

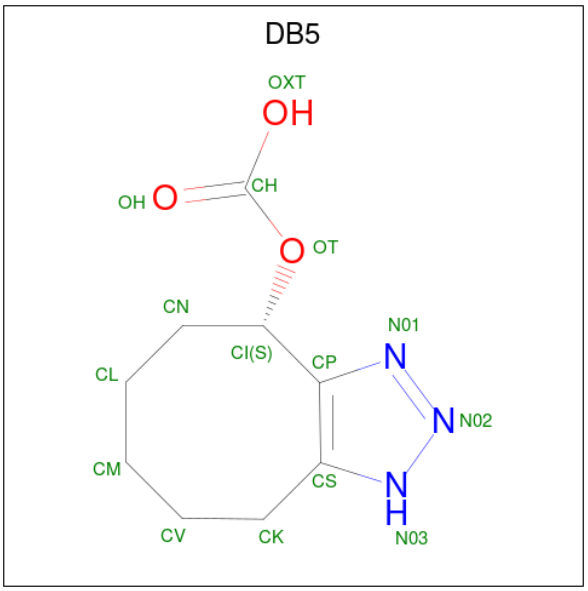
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	ARG	SER	conflict	UNP A0A059PIQ0
C	66	CRO	THR	chromophore	UNP A0A059PIQ0
C	66	CRO	TYR	chromophore	UNP A0A059PIQ0
C	66	CRO	GLY	chromophore	UNP A0A059PIQ0
C	72	SER	ALA	conflict	UNP A0A059PIQ0
C	80	ARG	GLN	conflict	UNP A0A059PIQ0
C	204	LYS	GLN	conflict	UNP A0A059PIQ0
C	206	VAL	ALA	conflict	UNP A0A059PIQ0
D	30	ARG	SER	conflict	UNP A0A059PIQ0
D	66	CRO	THR	chromophore	UNP A0A059PIQ0
D	66	CRO	TYR	chromophore	UNP A0A059PIQ0
D	66	CRO	GLY	chromophore	UNP A0A059PIQ0
D	72	SER	ALA	conflict	UNP A0A059PIQ0
D	80	ARG	GLN	conflict	UNP A0A059PIQ0
D	204	LYS	GLN	conflict	UNP A0A059PIQ0
D	206	VAL	ALA	conflict	UNP A0A059PIQ0

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

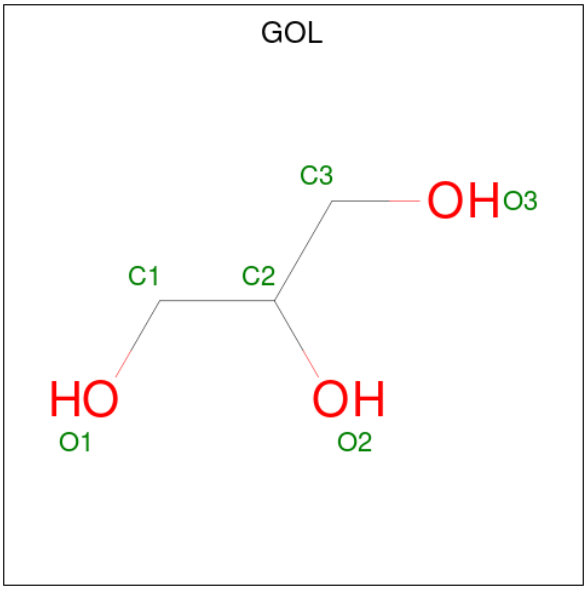
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
4	B	1	1	1	0	0
4	C	3	3	3	0	0
4	D	4	4	4	0	0

- Molecule 5 is [(4 {S})-4,5,6,7,8,9-hexahydro-1 {H}-cycloocta[d][1,2,3]triazol-4-yl] hydrogen carbonate (three-letter code: DB5) (formula: $C_9H_{13}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	9	3	2	0	0
5	B	1	14	9	3	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	C	1	1	1	0	0

- Molecule 8 is water.

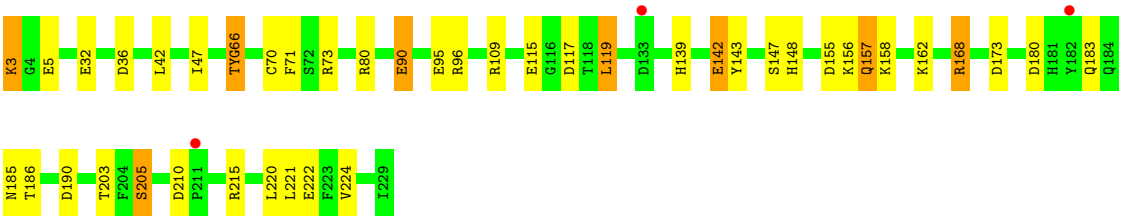
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	259	259	259	0	0
			Total	O		
8	B	256	256	256	0	0
			Total	O		
8	C	242	242	242	0	0
			Total	O		
8	D	218	218	218	0	0

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.

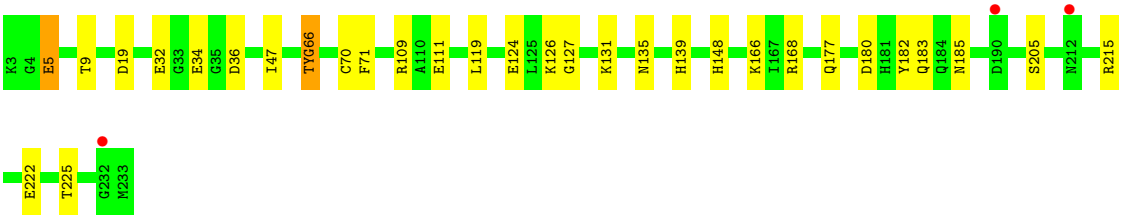
• Molecule 1: Green fluorescent protein

Chain A:



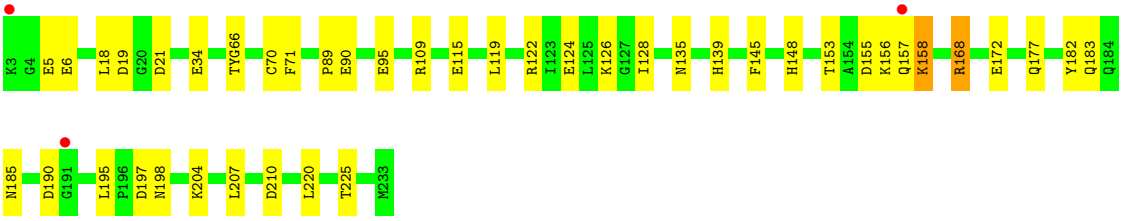
• Molecule 2: Green fluorescent protein

Chain B:



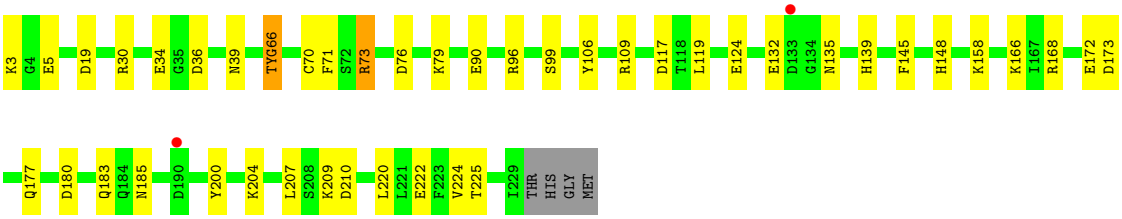
• Molecule 3: Green fluorescent protein

Chain C:



• Molecule 3: Green fluorescent protein

Chain D:


K3
G4
E5
D19
R30
E34
G35
D36
N39
TYG66
C70
F71
S72
R73
D76
K79
E90
R96
S99
Y106
R109
D117
T118
L119
E124
E132
D133
G134
N135
H139
F145
H148
K158
K166
I167
R168
E172
D173
Q177
D180
Q183
Q184
N185
D190
Y200
K204
L207
S208
K209
D210
L220
L221
E222
F223
V224
T225
I229
THR
HIS
GLY
MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.70Å 98.02Å 102.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.17 – 1.28 57.17 – 1.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.17-1.28) 99.9 (57.17-1.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.28Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.174 , 0.191 0.183 , 0.202	Depositor DCC
R_{free} test set	12228 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8346	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: GOL, CL, DB5, CRO, NA

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	1.32	10/1837 (0.5%)	1.19	17/2482 (0.7%)
2	B	1.21	6/1867 (0.3%)	1.05	6/2522 (0.2%)
3	C	1.31	12/1858 (0.6%)	1.17	10/2507 (0.4%)
3	D	1.26	9/1841 (0.5%)	1.16	14/2486 (0.6%)
All	All	1.28	37/7403 (0.5%)	1.15	47/9997 (0.5%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	GLU	CD-OE1	10.75	1.37	1.25
1	A	32	GLU	CD-OE2	9.39	1.35	1.25
2	B	222	GLU	CD-OE1	9.01	1.35	1.25
3	C	124	GLU	CD-OE1	8.39	1.34	1.25
1	A	90	GLU	CD-OE1	8.13	1.34	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	109	ARG	NE-CZ-NH1	-12.04	114.28	120.30
1	A	80	ARG	NE-CZ-NH2	10.87	125.73	120.30
3	C	168	ARG	NE-CZ-NH2	-9.52	115.54	120.30
3	D	204	LYS	CD-CE-NZ	8.89	132.14	111.70
1	A	80	ARG	NE-CZ-NH1	-8.53	116.04	120.30

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	A	1811	0	1778	28	0
2	B	1840	0	1804	20	0
3	C	1835	0	1801	27	9
3	D	1816	0	1781	26	9
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
5	A	14	0	0	7	0
5	B	14	0	0	3	0
6	B	18	0	20	4	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	C	1	0	0	0	0
8	A	259	0	0	7	0
8	B	256	0	0	3	0
8	C	242	0	0	5	0
8	D	218	0	0	5	0
All	All	8346	0	7200	101	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 101 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)
3:C:71:PHE:CE2	3:C:119:LEU:HD23	1.73	1.21
3:C:157:GLN:OE1	8:C:402:HOH:O	1.57	1.18
3:D:132:GLU:OE2	8:D:401:HOH:O	1.66	1.13
1:A:142:GLU:OE1	8:A:405:HOH:O	1.69	1.09
3:C:115:GLU:OE1	3:C:122:ARG:NH2	1.94	1.00

The worst 5 of 9 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)
3:C:157:GLN:NE2	3:D:209:LYS:C[2_454]	0.64	1.56
3:C:157:GLN:CD	3:D:209:LYS:O[2_454]	0.67	1.53
3:C:157:GLN:NE2	3:D:209:LYS:CA[2_454]	1.09	1.11
3:C:157:GLN:OE1	3:D:209:LYS:O[2_454]	1.12	1.08
3:C:157:GLN:NE2	3:D:209:LYS:O[2_454]	1.35	0.85

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	223/225 (99%)	220 (99%)	3 (1%)	0	100	100
2	B	227/229 (99%)	224 (99%)	3 (1%)	0	100	100
3	C	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
3	D	224/229 (98%)	221 (99%)	3 (1%)	0	100	100
All	All	900/912 (99%)	888 (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	199/196 (102%)	197 (99%)	2 (1%)	76	46
2	B	202/199 (102%)	201 (100%)	1 (0%)	88	68
3	C	201/199 (101%)	200 (100%)	1 (0%)	88	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	200/199 (100%)	200 (100%)	0	100	100
All	All	802/793 (101%)	798 (100%)	4 (0%)	88	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	157	GLN
2	B	126	LYS
3	C	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	157	GLN
3	D	39	ASN
3	C	185	ASN
3	D	139	HIS
2	B	146	ASN

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	$\#\|Z\| > 2$
2	CRO	B	66	2	23,23,24	2.86	6 (26%)	30,32,34	3.21	10 (33%)
3	CRO	D	66	3	23,23,24	2.76	6 (26%)	30,32,34	3.40	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CRO	A	66	1	23,23,24	2.86	7 (30%)	30,32,34	2.12	5 (16%)
3	CRO	C	66	3	23,23,24	3.30	8 (34%)	30,32,34	2.52	7 (23%)

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
3	CRO	D	66	3	-	0/12/31/32	0/2/2/2
1	CRO	A	66	1	-	0/12/31/32	0/2/2/2
3	CRO	C	66	3	-	0/12/31/32	0/2/2/2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	66	CRO	CB2-CA2	11.70	1.44	1.35
1	A	66	CRO	CB2-CA2	10.80	1.44	1.35
3	D	66	CRO	CB2-CA2	10.35	1.43	1.35
2	B	66	CRO	CB2-CA2	9.48	1.43	1.35
2	B	66	CRO	CA2-C2	-6.70	1.42	1.48

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	CRO	CA2-C2-N3	12.74	109.39	103.37
3	D	66	CRO	CA2-C2-N3	11.69	108.90	103.37
3	D	66	CRO	O2-C2-CA2	-10.96	124.81	130.96
1	A	66	CRO	CA2-C2-N3	8.45	107.37	103.37
3	C	66	CRO	CA2-C2-N3	8.07	107.19	103.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	66	CRO	1	0
3	D	66	CRO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	GOL	C	301	-	5,5,5	0.74	0	5,5,5	1.25	0
6	GOL	B	302	6	5,5,5	2.43	1 (20%)	5,5,5	1.33	0
6	GOL	D	301	-	5,5,5	0.55	0	5,5,5	0.90	0
5	DB5	B	305	3,2	14,15,16	3.73	7 (50%)	7,19,21	3.01	2 (28%)
5	DB5	A	303	3,1	14,15,16	2.70	5 (35%)	7,19,21	3.68	4 (57%)
6	GOL	B	303	6	5,5,5	2.71	2 (40%)	5,5,5	0.93	0
6	GOL	B	301	-	5,5,5	0.61	0	5,5,5	0.93	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
6	GOL	C	301	-	-	1/4/4/4	-
6	GOL	B	302	6	-	0/4/4/4	-
6	GOL	D	301	-	-	2/4/4/4	-
5	DB5	B	305	3,2	-	1/1/15/16	0/2/2/2
5	DB5	A	303	3,1	-	1/1/15/16	1/2/2/2
6	GOL	B	303	6	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	301	-	-	3/4/4/4	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	305	DB5	OT-CH	7.82	1.50	1.33
5	B	305	DB5	OT-CI	-5.91	1.36	1.44
5	A	303	DB5	CP-N01	5.69	1.41	1.34
5	B	305	DB5	CP-CS	-5.68	1.34	1.43
5	A	303	DB5	OT-CH	5.53	1.45	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	303	DB5	OT-CH-OH	-7.58	115.92	125.57
5	B	305	DB5	CV-CK-CS	-6.02	104.06	114.12
5	B	305	DB5	OT-CH-OH	-4.80	119.46	125.57
5	A	303	DB5	CI-OT-CH	-3.97	111.80	117.47
5	A	303	DB5	CM-CV-CK	-3.62	109.41	115.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	DB5	OH-CH-OT-CI
5	B	305	DB5	OH-CH-OT-CI
6	D	301	GOL	O1-C1-C2-C3
6	B	301	GOL	O1-C1-C2-C3
6	B	301	GOL	O1-C1-C2-O2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	DB5	CI-CK-CL-CM-CN-CP-CS-CV

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	302	GOL	2	0
5	B	305	DB5	3	0
5	A	303	DB5	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	GOL	2	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	A	224/225 (99%)	-0.03	3 (1%)	77	74	12, 21, 35, 48	0
2	B	228/229 (99%)	-0.11	3 (1%)	77	74	13, 22, 39, 52	0
3	C	228/229 (99%)	-0.11	3 (1%)	77	74	14, 23, 35, 48	0
3	D	224/229 (97%)	-0.06	2 (0%)	84	82	14, 23, 43, 56	0
All	All	904/912 (99%)	-0.08	11 (1%)	79	76	12, 22, 38, 56	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	232	GLY	5.4
3	D	190	ASP	2.8
3	C	191	GLY	2.8
1	A	182	TYR	2.7
2	B	212	ASN	2.7

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	A	66	22/23	0.97	0.05	13,14,16,18	0
2	CRO	B	66	22/23	0.97	0.05	13,14,17,18	0
3	CRO	C	66	22/23	0.97	0.05	15,16,18,19	0
3	CRO	D	66	22/23	0.97	0.05	14,16,18,18	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
6	GOL	B	301	6/6	0.77	0.27	29,40,45,47	0
6	GOL	B	303	6/6	0.78	0.51	47,62,68,77	0
6	GOL	C	301	6/6	0.79	0.31	33,41,42,43	0
5	DB5	A	303	14/15	0.80	0.25	32,44,49,49	0
7	CL	C	305	1/1	0.81	0.18	45,45,45,45	0
6	GOL	B	302	6/6	0.82	0.50	47,62,67,69	0
5	DB5	B	305	14/15	0.84	0.25	34,42,44,45	0
6	GOL	D	301	6/6	0.84	0.26	32,42,46,50	0
4	NA	A	301	1/1	0.84	0.24	39,39,39,39	0
4	NA	D	304	1/1	0.85	0.28	38,38,38,38	0
4	NA	B	304	1/1	0.86	0.32	45,45,45,45	0
4	NA	D	303	1/1	0.87	0.23	32,32,32,32	0
4	NA	D	302	1/1	0.88	0.14	32,32,32,32	0
4	NA	C	303	1/1	0.89	0.20	37,37,37,37	0
4	NA	A	302	1/1	0.89	0.09	38,38,38,38	0
4	NA	C	304	1/1	0.90	0.09	40,40,40,40	0
4	NA	D	305	1/1	0.91	0.18	45,45,45,45	0
4	NA	C	302	1/1	0.94	0.06	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.