



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 09:46 AM EDT

PDB ID : 3GJ1
Title : Non photoactivated state of PA-GFP
Authors : Henderson, J.N.; Gepshtein, R.; Heenan, J.R.; Kallio, K.; Huppert, D.; Remington, S.J.
Deposited on : unknown
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

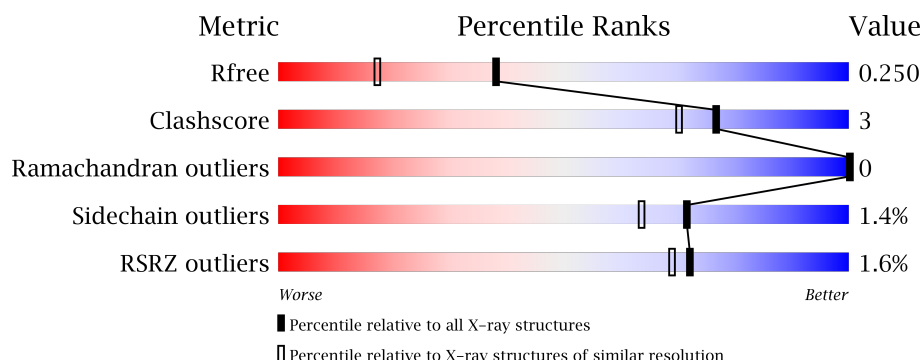
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	229	
1	B	229	
1	C	229	
1	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	231	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7792 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
1	A	227	Total	C	N	O	S	0	4	0
			1785	1139	301	340	5			
1	B	227	Total	C	N	O	S	0	13	0
			1857	1184	310	358	5			
1	C	223	Total	C	N	O	S	0	7	0
			1753	1117	292	339	5			
1	D	226	Total	C	N	O	S	0	3	0
			1751	1113	291	342	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P42212
A	?	-	SER	CHROMOPHORE	UNP P42212
A	80	ARG	GLN	ENGINEERED	UNP P42212
A	99	SER	PHE	ENGINEERED	UNP P42212
A	153	THR	MET	ENGINEERED	UNP P42212
A	163	ALA	VAL	ENGINEERED	UNP P42212
A	203	HIS	THR	ENGINEERED	UNP P42212
B	0	SER	-	EXPRESSION TAG	UNP P42212
B	?	-	SER	CHROMOPHORE	UNP P42212
B	80	ARG	GLN	ENGINEERED	UNP P42212
B	99	SER	PHE	ENGINEERED	UNP P42212
B	153	THR	MET	ENGINEERED	UNP P42212
B	163	ALA	VAL	ENGINEERED	UNP P42212
B	203	HIS	THR	ENGINEERED	UNP P42212
C	0	SER	-	EXPRESSION TAG	UNP P42212
C	?	-	SER	CHROMOPHORE	UNP P42212
C	80	ARG	GLN	ENGINEERED	UNP P42212
C	99	SER	PHE	ENGINEERED	UNP P42212
C	153	THR	MET	ENGINEERED	UNP P42212
C	163	ALA	VAL	ENGINEERED	UNP P42212
C	203	HIS	THR	ENGINEERED	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	EXPRESSION TAG	UNP P42212
D	?	-	SER	CHROMOPHORE	UNP P42212
D	80	ARG	GLN	ENGINEERED	UNP P42212
D	99	SER	PHE	ENGINEERED	UNP P42212
D	153	THR	MET	ENGINEERED	UNP P42212
D	163	ALA	VAL	ENGINEERED	UNP P42212
D	203	HIS	THR	ENGINEERED	UNP P42212

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	1
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	159	Total O 159 159	0	4
4	B	189	Total O 189 189	0	6
4	C	121	Total O 121 121	0	6
4	D	147	Total O 147 147	0	3

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: Green fluorescent protein

Chain A: 




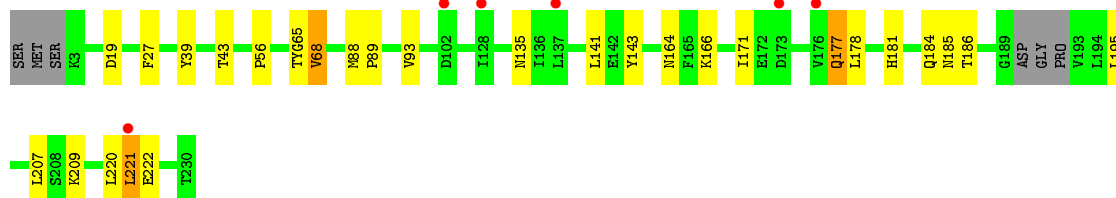
- Molecule 1: Green fluorescent protein

Chain B: 




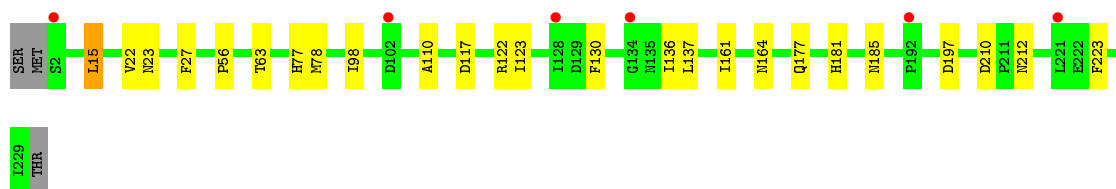
- Molecule 1: Green fluorescent protein

Chain C: 



- Molecule 1: Green fluorescent protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.52Å 86.72Å 144.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.37 – 1.80 46.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.37-1.80) 93.3 (46.35-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.252 0.207 , 0.250	Depositor DCC
R_{free} test set	4596 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7792	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CRO, SO4

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	1.11	1/1817 (0.1%)	0.99	7/2463 (0.3%)
1	B	1.09	4/1916 (0.2%)	0.99	2/2592 (0.1%)
1	C	1.02	1/1792 (0.1%)	0.92	1/2428 (0.0%)
1	D	1.03	0/1780	0.94	4/2421 (0.2%)
All	All	1.06	6/7305 (0.1%)	0.96	14/9904 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	LYS	CB-CG	7.18	1.72	1.52
1	B	87	ALA	CA-CB	6.81	1.66	1.52
1	C	39	TYR	CD1-CE1	6.12	1.48	1.39
1	B	90	GLU	CD-OE1	5.88	1.32	1.25
1	B	90	GLU	CG-CD	5.63	1.60	1.51
1	B	92	TYR	CD1-CE1	5.19	1.47	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	D	117	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	117	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	141	LEU	CB-CG-CD1	-5.98	100.84	111.00
1	C	19	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	109	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	109	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	82	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	15	LEU	CA-CB-CG	5.50	127.96	115.30
1	D	210	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	21	ASP	CB-CG-OD2	-5.26	113.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	168[A]	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	168[B]	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1785	0	1680	7	0
1	B	1857	0	1787	6	0
1	C	1753	0	1632	25	0
1	D	1751	0	1599	11	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	159	0	0	1	0
4	B	189	0	0	0	0
4	C	121	0	0	1	0
4	D	147	0	0	1	0
All	All	7792	0	6698	48	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 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:CRO:C3	1:C:68:VAL:N	1.73	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43[B]:THR:HG22	1:C:221[B]:LEU:HG	1.30	1.09
1:C:65:CRO:C3	1:C:68:VAL:CA	2.40	0.98
3:D:233:CL:CL	4:D:441:HOH:O	2.29	0.88
1:C:43[B]:THR:HG22	1:C:221[B]:LEU:CG	2.05	0.87
1:C:65:CRO:CA3	1:C:68:VAL:N	2.43	0.81
1:C:43[B]:THR:CG2	1:C:221[B]:LEU:HG	2.16	0.74
1:D:161:ILE:HG13	1:D:185:ASN:HB2	1.74	0.69
1:C:65:CRO:C3	1:C:68:VAL:HA	2.23	0.66
1:C:221[A]:LEU:HD23	1:D:223:PHE:HE2	1.62	0.64
1:C:221[A]:LEU:HD23	1:D:223:PHE:CE2	2.33	0.64
1:C:171:ILE:HD11	1:C:177:GLN:HB2	1.82	0.62
1:A:158:LYS:O	1:A:186:THR:HG23	2.00	0.60
1:B:73:ARG:HB3	1:B:225[B]:THR:HG22	1.86	0.57
1:A:36:ASP:OD1	4:A:277:HOH:O	2.18	0.54
1:D:23:ASN:ND2	1:D:137:LEU:HD11	2.23	0.53
1:D:110:ALA:HA	1:D:122:ARG:O	2.10	0.51
1:C:135:ASN:HD22	1:C:177:GLN:HG3	1.76	0.50
1:D:63:THR:CG2	1:D:123:ILE:HG21	2.42	0.50
1:C:93:VAL:O	1:C:185:ASN:HA	2.14	0.48
1:C:88:MET:HB3	1:C:89:PRO:HA	1.96	0.47
1:A:147[B]:SER:OG	1:A:204:GLN:HG2	2.14	0.47
1:C:164:ASN:HA	1:C:181:HIS:O	2.15	0.47
1:C:65:CRO:OG1	1:C:222:GLU:OE1	2.22	0.46
1:D:98:ILE:HG12	1:D:181:HIS:CD2	2.52	0.45
1:D:22:VAL:HG23	1:D:27:PHE:HE2	1.82	0.45
1:A:221[B]:LEU:HG	1:A:222:GLU:N	2.26	0.45
1:C:195:LEU:HD23	1:C:195:LEU:N	2.31	0.45
1:A:63:THR:CG2	1:A:123:ILE:HG21	2.46	0.45
1:A:53:LEU:HD21	1:A:60:LEU:HD12	1.99	0.44
1:B:63:THR:CG2	1:B:123:ILE:HG21	2.48	0.44
1:D:56:PRO:HD3	1:D:136:ILE:O	2.17	0.44
1:C:166:LYS:HD3	1:C:178:LEU:HD13	1.99	0.43
1:C:27:PHE:N	1:C:27:PHE:CD2	2.86	0.43
1:B:151:TYR:CD1	1:B:200:TYR:HB3	2.53	0.43
1:A:53:LEU:HD22	1:A:57:TRP:CD2	2.53	0.43
1:D:23:ASN:HD21	1:D:130:PHE:HB2	1.83	0.43
1:C:207:LEU:CD2	1:C:220:LEU:HD13	2.50	0.42
1:C:68:VAL:N	4:C:528:HOH:O	2.52	0.42
1:D:77:HIS:CD2	1:D:78:MET:HG3	2.55	0.42
1:C:171:ILE:HD11	1:C:177:GLN:HG3	2.02	0.41
1:C:56:PRO:HG2	1:C:141:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:C	1:B:125:LEU:HD23	2.41	0.41
1:C:135:ASN:HD22	1:C:177:GLN:CG	2.34	0.41
1:C:143:TYR:CZ	1:C:209:LYS:HE2	2.56	0.41
1:B:17:GLU:HB2	1:B:122[B]:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
1	B	235/229 (103%)	233 (99%)	2 (1%)	0	100	100
1	C	223/229 (97%)	218 (98%)	5 (2%)	0	100	100
1	D	224/229 (98%)	220 (98%)	4 (2%)	0	100	100
All	All	908/916 (99%)	894 (98%)	14 (2%)	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	184/199 (92%)	183 (100%)	1 (0%)	91	90
1	B	200/199 (100%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	181/199 (91%)	175 (97%)	6 (3%)	43	26
1	D	178/199 (89%)	174 (98%)	4 (2%)	57	44
All	All	743/796 (93%)	732 (98%)	11 (2%)	71	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	GLU
1	C	68	VAL
1	C	177	GLN
1	C	184	GLN
1	C	186	THR
1	C	221[A]	LEU
1	C	221[B]	LEU
1	D	15	LEU
1	D	164	ASN
1	D	177	GLN
1	D	212	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	B	157	GLN
1	B	184	GLN
1	C	135	ASN
1	C	177	GLN
1	D	23	ASN
1	D	149	ASN
1	D	164	ASN
1	D	177	GLN
1	D	212	ASN

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
1	CRO	A	65	1	22,22,24	3.21	5 (22%)	27,30,34	3.69	11 (40%)
1	CRO	B	65	1	22,22,24	3.14	4 (18%)	27,30,34	3.45	11 (40%)
1	CRO	C	65	-	22,22,24	3.13	6 (27%)	27,30,34	3.91	11 (40%)
1	CRO	D	65	1	22,22,24	3.97	5 (22%)	27,30,34	3.53	8 (29%)

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	A	65	1	-	0/9/29/32	0/2/2/2
1	CRO	B	65	1	-	0/9/29/32	0/2/2/2
1	CRO	C	65	-	-	0/9/29/32	0/2/2/2
1	CRO	D	65	1	-	0/9/29/32	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	65	CRO	CA2-C2	-6.59	1.41	1.48
1	B	65	CRO	CA2-C2	-5.51	1.43	1.48
1	A	65	CRO	C2-N3	-3.64	1.30	1.39
1	C	65	CRO	C2-N3	-3.58	1.31	1.39
1	B	65	CRO	C2-N3	-3.22	1.31	1.39
1	C	65	CRO	CA2-C2	-3.14	1.45	1.48
1	D	65	CRO	C2-N3	-2.67	1.33	1.39
1	A	65	CRO	CA2-C2	-2.21	1.46	1.48
1	A	65	CRO	O2-C2	2.14	1.27	1.23
1	D	65	CRO	O2-C2	2.42	1.28	1.23
1	C	65	CRO	CD2-CE2	2.56	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	CRO	O2-C2	2.87	1.29	1.23
1	C	65	CRO	C1-N2	3.90	1.38	1.32
1	D	65	CRO	C1-N2	4.23	1.38	1.32
1	B	65	CRO	C1-N2	5.21	1.40	1.32
1	A	65	CRO	C1-N2	5.23	1.40	1.32
1	B	65	CRO	CB2-CA2	11.58	1.45	1.35
1	C	65	CRO	CB2-CA2	12.29	1.46	1.35
1	A	65	CRO	CB2-CA2	12.62	1.46	1.35
1	D	65	CRO	CB2-CA2	16.08	1.49	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	CRO	O2-C2-CA2	-12.13	124.43	130.97
1	C	65	CRO	O2-C2-CA2	-11.38	124.83	130.97
1	D	65	CRO	O2-C2-CA2	-10.15	125.50	130.97
1	B	65	CRO	O2-C2-CA2	-9.94	125.61	130.97
1	C	65	CRO	CA1-C1-N3	-5.55	118.09	124.75
1	A	65	CRO	CD2-CE2-CZ	-5.08	114.11	119.88
1	B	65	CRO	CA2-N2-C1	-4.15	102.50	105.75
1	A	65	CRO	O3-C3-CA3	-3.32	115.40	126.38
1	A	65	CRO	CE1-CD1-CG2	-3.26	117.00	121.28
1	B	65	CRO	CA1-C1-N3	-3.20	120.91	124.75
1	A	65	CRO	CA2-N2-C1	-3.03	103.38	105.75
1	B	65	CRO	C1-CA1-N1	-3.01	97.67	108.88
1	B	65	CRO	CE1-CD1-CG2	-2.77	117.64	121.28
1	C	65	CRO	C2-CA2-N2	-2.50	107.10	108.93
1	D	65	CRO	O3-C3-CA3	-2.42	118.38	126.38
1	A	65	CRO	C1-CA1-N1	-2.35	100.14	108.88
1	D	65	CRO	CA1-C1-N3	-2.26	122.03	124.75
1	B	65	CRO	O3-C3-CA3	-2.24	118.97	126.38
1	C	65	CRO	CA2-N2-C1	-2.20	104.03	105.75
1	B	65	CRO	CG2-CB2-CA2	-2.15	127.70	130.19
1	B	65	CRO	CD2-CG2-CB2	-2.14	113.87	121.23
1	C	65	CRO	C1-CA1-N1	-2.12	100.98	108.88
1	B	65	CRO	CD2-CE2-CZ	-2.09	117.50	119.88
1	D	65	CRO	CA1-C1-N2	2.01	127.62	123.56
1	D	65	CRO	CB2-CA2-C2	2.30	125.22	122.32
1	A	65	CRO	CA3-N3-C1	2.31	129.90	127.20
1	C	65	CRO	N3-C1-N2	2.42	113.13	111.45
1	C	65	CRO	CA1-C1-N2	2.53	128.67	123.56
1	A	65	CRO	CD2-CG2-CD1	2.55	121.46	117.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	CRO	CD2-CG2-CD1	2.59	121.52	117.63
1	C	65	CRO	CB2-CA2-C2	2.70	125.72	122.32
1	A	65	CRO	CE2-CZ-CE1	2.70	124.61	119.74
1	C	65	CRO	CG2-CB2-CA2	3.15	133.86	130.19
1	D	65	CRO	CB1-CA1-C1	3.37	118.77	110.23
1	D	65	CRO	CA3-N3-C1	3.40	131.18	127.20
1	A	65	CRO	CB1-CA1-C1	3.58	119.29	110.23
1	C	65	CRO	CB1-CA1-C1	4.89	122.61	110.23
1	A	65	CRO	CA2-C2-N3	10.35	107.92	103.30
1	B	65	CRO	CA2-C2-N3	11.58	108.47	103.30
1	D	65	CRO	CA2-C2-N3	12.78	109.00	103.30
1	C	65	CRO	CA2-C2-N3	13.13	109.16	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	65	CRO	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
2	SO4	A	231	-	4,4,4	0.44	0	6,6,6	0.64	0
2	SO4	B	231	-	4,4,4	0.21	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	231	-	4,4,4	0.42	0	6,6,6	0.41	0
2	SO4	D	231	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	D	232[B]	-	4,4,4	0.11	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	231	-	-	0/0/0/0	0/0/0/0
2	SO4	B	231	-	-	0/0/0/0	0/0/0/0
2	SO4	C	231	-	-	0/0/0/0	0/0/0/0
2	SO4	D	231	-	-	0/0/0/0	0/0/0/0
2	SO4	D	232[B]	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	65:CRO	C3	68:VAL	N	1.73
1	D	64:PHE	C	65:CRO	N1	1.61
1	C	64:PHE	C	65:CRO	N1	1.60

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/229 (98%)	-0.30	0 100 100	10, 19, 32, 43	0
1	B	226/229 (98%)	-0.23	2 (0%) 84 82	11, 18, 32, 42	0
1	C	222/229 (96%)	0.23	6 (2%) 55 50	15, 26, 40, 55	0
1	D	225/229 (98%)	0.05	6 (2%) 55 50	12, 24, 41, 49	0
All	All	899/916 (98%)	-0.07	14 (1%) 72 69	10, 21, 38, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	3.3
1	C	102	ASP	2.8
1	D	2	SER	2.8
1	D	221[A]	LEU	2.7
1	B	230	THR	2.6
1	D	128	ILE	2.6
1	C	221[A]	LEU	2.5
1	C	128	ILE	2.3
1	D	134	GLY	2.3
1	B	2	SER	2.1
1	C	137	LEU	2.1
1	C	176	VAL	2.1
1	D	192	PRO	2.0
1	D	102	ASP	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	CRO	B	65	21/23	0.97	0.08	-	9,15,18,22	0
1	CRO	A	65	21/23	0.97	0.09	-	9,11,17,20	0
1	CRO	D	65	21/23	0.96	0.09	-	11,18,21,22	0
1	CRO	C	65	21/23	0.94	0.10	-	13,19,25,28	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	231	5/5	0.93	0.15	3.19	13,14,20,24	5
2	SO4	D	231	5/5	0.97	0.09	0.93	13,22,25,26	5
2	SO4	C	231	5/5	0.97	0.10	0.93	15,15,22,22	5
2	SO4	D	232[B]	5/5	0.93	0.13	0.35	35,35,37,37	5
3	CL	B	233	1/1	0.99	0.08	-1.95	18,18,18,18	0
3	CL	A	232	1/1	0.98	0.07	-1.99	37,37,37,37	0
3	CL	C	232	1/1	0.97	0.10	-	26,26,26,26	0
3	CL	D	233	1/1	0.89	0.11	-	41,41,41,41	0
2	SO4	B	231	5/5	0.84	0.23	-	47,48,49,49	5
3	CL	B	232	1/1	0.99	0.08	-	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.