



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 04:30 pm GMT

PDB ID : 2GON
Title : Xray Structure of Gag133-278
Authors : Kelly, B.N.
Deposited on : 2006-04-13
Resolution : 1.90 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

<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	:	trunk28620
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)	:	recalc28949

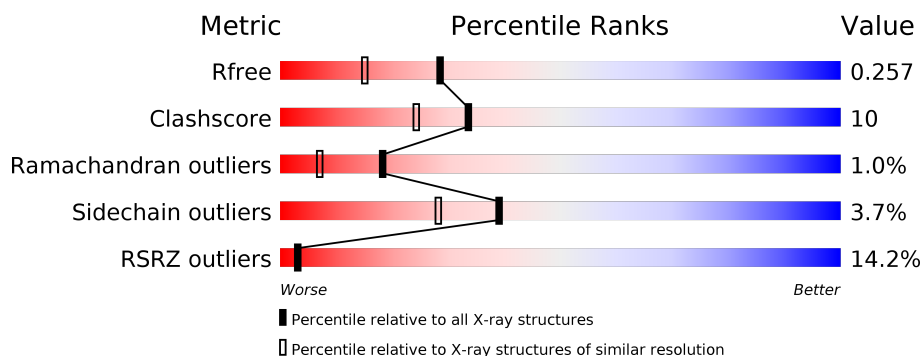
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	146	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	146	<div> <div>15%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	146	<div> <div>12%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>••</div> <div>5%</div> </div> </div>
1	D	146	<div> <div>12%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4484 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 Capsid protein p24 (CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	Se	0	2	0
			1007	637	176	186	8			
1	B	137	Total	C	N	O	Se	0	5	0
			1091	692	187	199	13			
1	C	138	Total	C	N	O	Se	0	4	0
			1101	697	191	202	11			
1	D	129	Total	C	N	O	Se	0	5	0
			1034	655	177	191	11			

There are 36 discrepancies between the modelled and reference sequences:

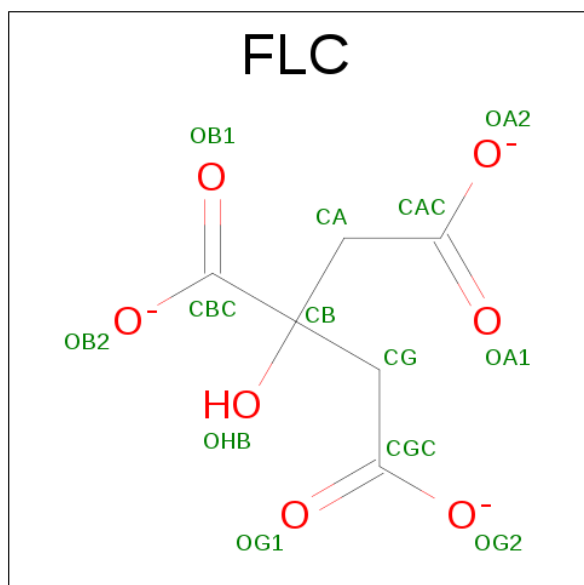
Chain	Residue	Modelled	Actual	Comment	Reference
A	142	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	171	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	187	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	198	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	200	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	224	GLU	ALA	ENGINEERED	UNP P12497
A	228	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	250	MSE	MET	MODIFIED RESIDUE	UNP P12497
A	276	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	142	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	171	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	187	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	198	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	200	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	224	GLU	ALA	ENGINEERED	UNP P12497
B	228	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	250	MSE	MET	MODIFIED RESIDUE	UNP P12497
B	276	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	142	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	171	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	187	MSE	MET	MODIFIED RESIDUE	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
C	198	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	200	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	224	GLU	ALA	ENGINEERED	UNP P12497
C	228	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	250	MSE	MET	MODIFIED RESIDUE	UNP P12497
C	276	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	142	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	171	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	187	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	198	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	200	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	224	GLU	ALA	ENGINEERED	UNP P12497
D	228	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	250	MSE	MET	MODIFIED RESIDUE	UNP P12497
D	276	MSE	MET	MODIFIED RESIDUE	UNP P12497

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

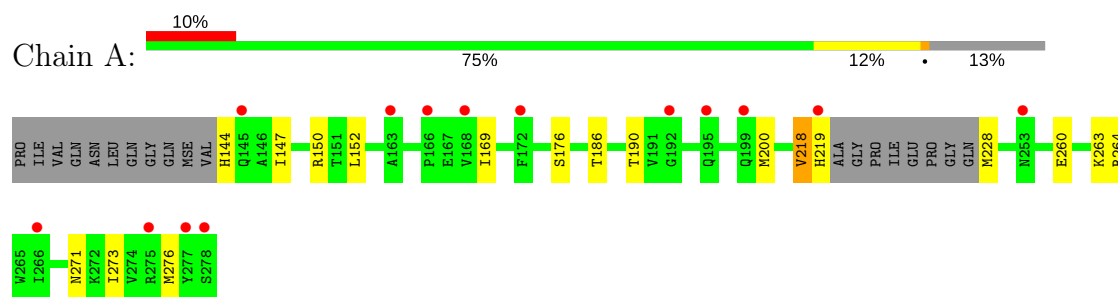
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	53	Total 53	O 53	0	0
3	C	52	Total 52	O 52	0	0
3	D	57	Total 57	O 57	0	0

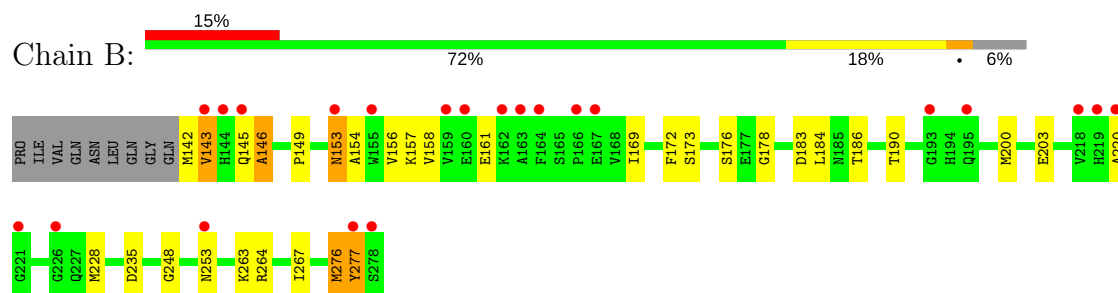
3 Residue-property plots [i](#)

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

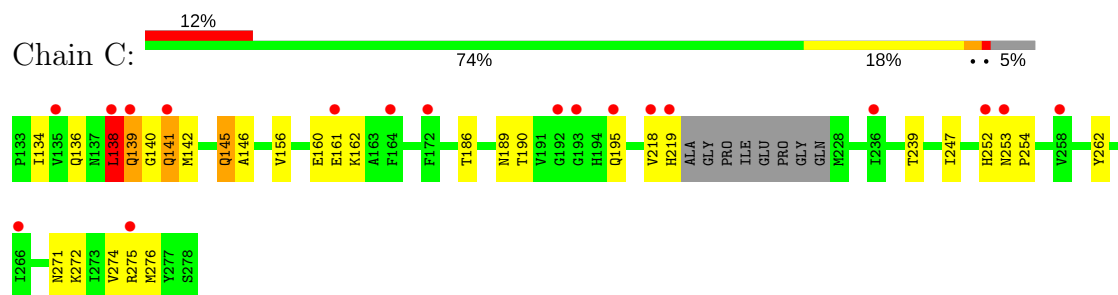
- Molecule 1: Capsid protein p24 (CA)



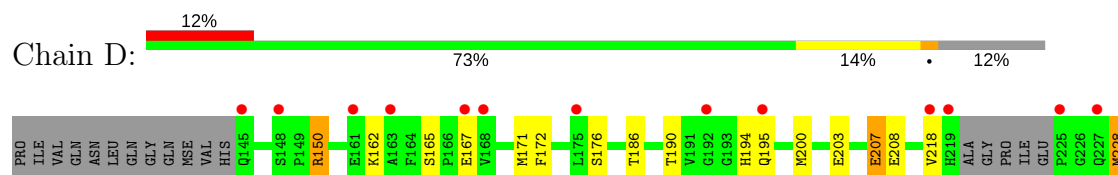
- Molecule 1: Capsid protein p24 (CA)



- Molecule 1: Capsid protein p24 (CA)



- Molecule 1: Capsid protein p24 (CA)





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	106.26Å 134.51Å 42.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 1.90 19.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.80-1.90) 100.0 (19.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.257 0.206 , 0.257	Depositor DCC
R_{free} test set	2448 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4484	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 49.86 % 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 7.0234e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.08	1/1029 (0.1%)	0.89	2/1386 (0.1%)
1	B	1.03	1/1131 (0.1%)	0.90	2/1522 (0.1%)
1	C	1.00	1/1135 (0.1%)	0.92	1/1526 (0.1%)
1	D	1.01	2/1071 (0.2%)	0.88	1/1438 (0.1%)
All	All	1.03	5/4366 (0.1%)	0.90	6/5872 (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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CD-OE2	6.87	1.33	1.25
1	A	260	GLU	CD-OE2	5.90	1.32	1.25
1	D	208	GLU	CD-OE1	5.26	1.31	1.25
1	D	207	GLU	CD-OE1	-5.19	1.20	1.25
1	C	262	TYR	CD2-CE2	5.16	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	LEU	CA-CB-CG	6.55	130.37	115.30
1	D	264	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	B	264	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	B	235	ASP	CB-CG-OD2	5.51	123.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH2	-5.36	117.62	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	VAL	Peptide

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	1007	0	996	15	0
1	B	1091	0	1087	18	0
1	C	1101	0	1100	17	0
1	D	1034	0	1027	32	0
2	A	13	0	5	0	0
2	D	13	0	5	0	0
3	A	63	0	0	5	1
3	B	53	0	0	1	1
3	C	52	0	0	3	0
3	D	57	0	0	2	0
All	All	4484	0	4220	82	1

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 10.

The worst 5 of 82 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:228:MSE:CE	1:A:228:MSE:SE	2.15	1.45
1:A:144:HIS:HE1	3:A:330:HOH:O	1.06	1.34
1:D:200:MSE:CE	1:D:276[A]:MSE:HE3	1.74	1.18
1:A:200:MSE:HE1	1:A:276:MSE:SE	1.99	1.12
1:A:264:ARG:NH1	3:A:326:HOH:O	1.83	1.08

All (1) 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:A:299:HOH:O	3:B:299:HOH:O[1_554]	2.19	0.01

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	124/146 (85%)	120 (97%)	3 (2%)	1 (1%)	22	11
1	B	140/146 (96%)	130 (93%)	7 (5%)	3 (2%)	8	1
1	C	137/146 (94%)	131 (96%)	5 (4%)	1 (1%)	25	13
1	D	130/146 (89%)	127 (98%)	3 (2%)	0	100	100
All	All	531/584 (91%)	508 (96%)	18 (3%)	5 (1%)	18	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	VAL
1	C	161	GLU
1	B	146	ALA
1	A	147	ILE
1	B	220	ALA

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	110/116 (95%)	109 (99%)	1 (1%)	82	82
1	B	121/116 (104%)	114 (94%)	7 (6%)	23	12
1	C	123/116 (106%)	116 (94%)	7 (6%)	24	13
1	D	115/116 (99%)	111 (96%)	4 (4%)	41	30
All	All	469/464 (101%)	450 (96%)	19 (4%)	39	24

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	LEU
1	C	141	GLN
1	D	150	ARG
1	B	277	TYR
1	D	195	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	FLC	A	279	-	3,12,12	3.05	1 (33%)	3,17,17	2.91	1 (33%)
2	FLC	D	279	-	3,12,12	2.06	1 (33%)	3,17,17	1.99	1 (33%)

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	FLC	A	279	-	-	0/6/16/16	0/0/0/0
2	FLC	D	279	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	279	FLC	OHB-CB	3.28	1.48	1.43
2	A	279	FLC	OHB-CB	5.24	1.51	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	279	FLC	CB-CG-CGC	-4.85	107.37	114.95
2	D	279	FLC	CB-CG-CGC	-3.18	109.98	114.95

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](#)

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	120/146 (82%)	0.70	14 (11%) 5 5	15, 30, 56, 62	1 (0%)
1	B	129/146 (88%)	0.88	22 (17%) 2 2	17, 33, 68, 81	0
1	C	130/146 (89%)	0.84	18 (13%) 3 3	17, 33, 60, 66	0
1	D	122/146 (83%)	0.82	17 (13%) 3 3	18, 32, 57, 67	0
All	All	501/584 (85%)	0.81	71 (14%) 3 3	15, 33, 60, 81	1 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	VAL	12.6
1	B	163	ALA	8.5
1	C	138	LEU	6.7
1	D	218	VAL	6.7
1	C	219	HIS	6.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	FLC	A	279	13/13	0.96	0.10	-0.65	18,21,23,24	0
2	FLC	D	279	13/13	0.96	0.09	-0.69	18,22,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.