W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 05:35 pm BST

PDB ID	:	2PCP
Title	:	ANTIBODY FAB COMPLEXED WITH PHENCYCLIDINE
Authors	:	Lim, K.; Owens, S.M.; Arnold, L.; Sacchettini, J.C.; Linthicum, D.S.
Deposited on	:	1998-06-02
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

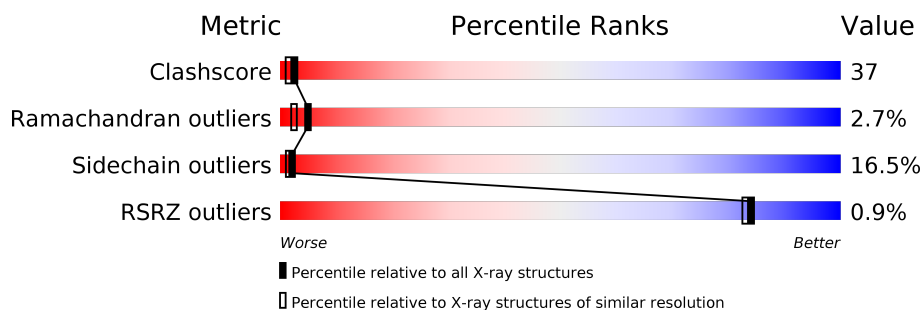|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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
Clashscore		37
Ramachandran outliers		2.7%
Sidechain outliers		16.5%
RSRZ outliers		0.9%

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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	216	38% 56% 6% •
1	C	216	38% 54% 7% •
2	B	215	31% 53% 15% •
2	D	215	43% 49% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7342 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 IMMUNOGLOBULIN.

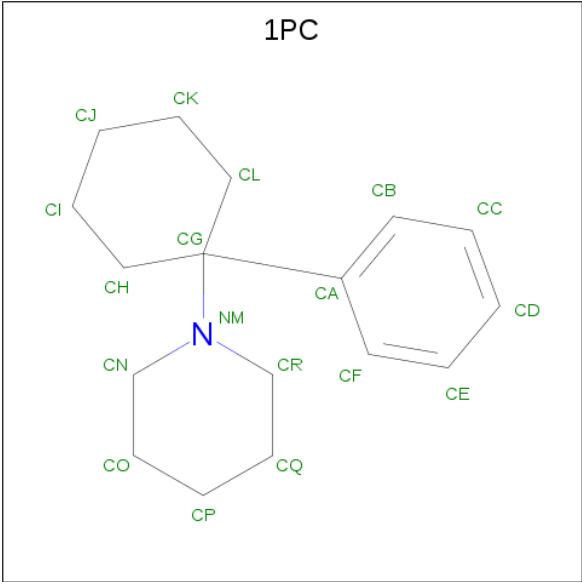| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total 1678	C 1051	N 283	O 338	S 6	0	0	0
1	C	216	Total 1678	C 1051	N 283	O 338	S 6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27A	THR	SER	CONFLICT	PIR PC4203
A	27E	SER	THR	CONFLICT	PIR PC4203
A	52	THR	SER	CONFLICT	PIR PC4203
A	92	THR	SER	CONFLICT	PIR PC4203
A	94	ALA	VAL	CONFLICT	PIR PC4203
A	96	TYR	ARG	CONFLICT	PIR PC4203
C	27A	THR	SER	CONFLICT	PIR PC4203
C	27E	SER	THR	CONFLICT	PIR PC4203
C	52	THR	SER	CONFLICT	PIR PC4203
C	92	THR	SER	CONFLICT	PIR PC4203
C	94	ALA	VAL	CONFLICT	PIR PC4203
C	96	TYR	ARG	CONFLICT	PIR PC4203

- Molecule 2 is a protein called IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total 1636	C 1033	N 268	O 328	S 7	0	0	0
2	D	215	Total 1636	C 1033	N 268	O 328	S 7	0	0	0

- Molecule 3 is 1-(PHENYL-1-CYCLOHEXYL)PIPERIDINE (three-letter code: 1PC) (formula: $C_{17}H_{25}N$).

1PC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 18	C 17	N 1	0	0
3	C	1	Total 18	C 17	N 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total 173	O 173	0	0
4	B	163	Total 163	O 163	0	0
4	C	150	Total 150	O 150	0	0
4	D	192	Total 192	O 192	0	0

3 Residue-property plots ⓘ

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. Residu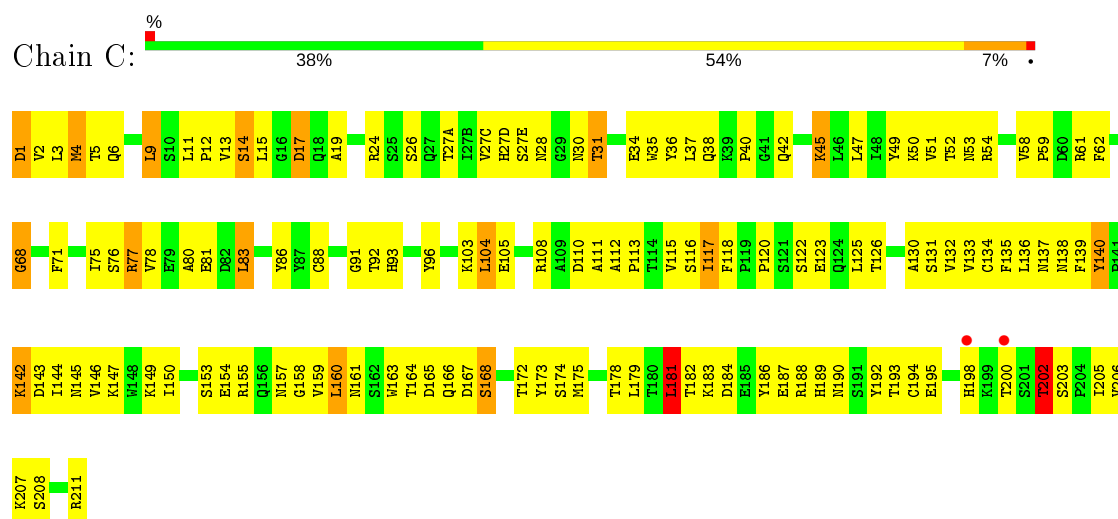es are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
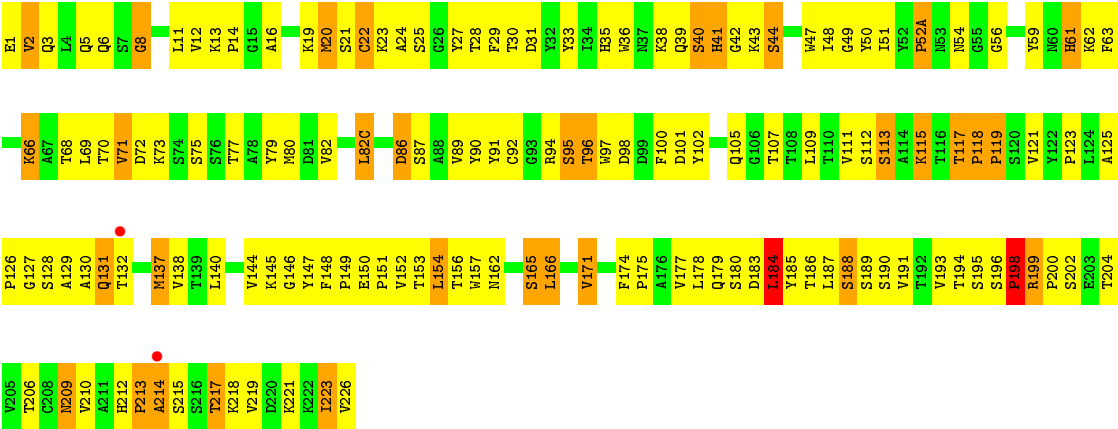
- Molecule 1: IMMUNOGLOBULIN
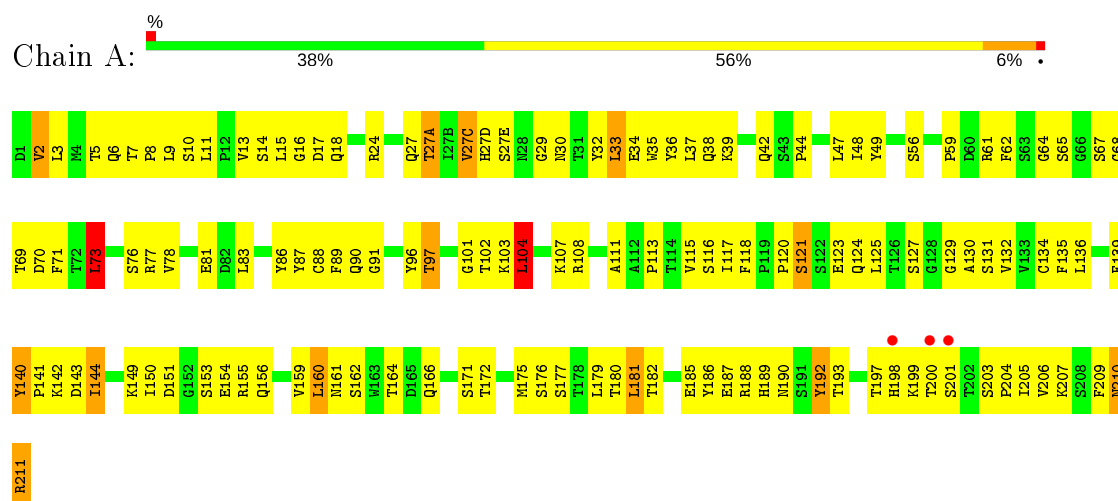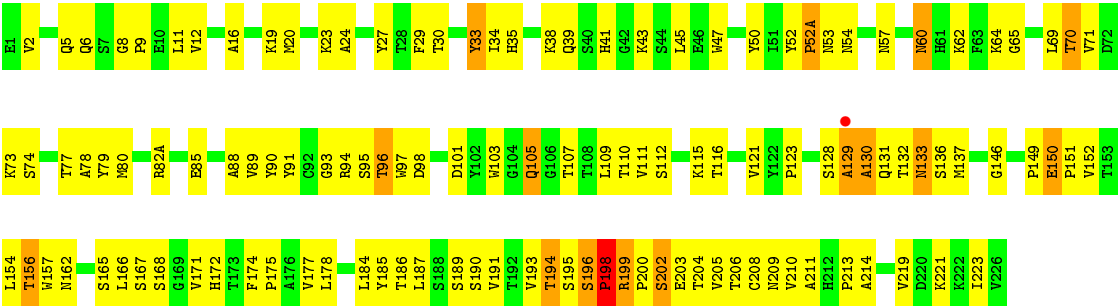

- Molecule 1: IMMUNOGLOBULIN

- Molecule 2: IMMUNOGLOBULIN

E1 V2 Q3 L4 Q5 Q6 S7 G8 L11 V12 K13 P14 G15 A16 K19 M20 S21 C22 K23 A24 S25 G26 Y27 T28 F29 T30 D31 Y32 Y33 I34 H35 W36 N37 K38 Q39 S40 H41 G42 K43 S44 W47 I48 G49 Y50 I51 Y52 P52A N53 N54 G55 G56 Y59 N60 H61 K62 F63

K66 A67 T68 L69 T70 V71 D72 K73 S74 S75 S76 T77 A78 Y79 M80 D81 V82 L82C D86 S87 A88 V89 Y90 Y91 C92 G93 R94 S95 T96 W97 D98 D99 F100 D101 Y102 Q105 G106 T107 T108 L109 T110 V111 S112 S113 A114 K115 T116 T117 P118 P119 S120 V121 Y122 P123 L124 A125

P126 G127 S128 A129 A130 Q131 T132 M137 V138 T139 L140 V144 K145 G146 Y147 F148 P149 E150 P151 V152 T153 L154 T156 W157 N162 S165 L166 V171 F174 P175 A176 V177 L178 Q179 S180 D183 L184 Y185 T186 L187 S188 S189 S190 V191 T192 V193 T194 S195 S196 P198 R199 P200 S202 E203 T204

V205 T206 C208 N209 V210 A211 H212 P213 A214 S215 S216 T217 K218 V219 D220 K221 K222 I223 V226

• Molecule 2: IMMUNOGLOBULIN

Chain D:

E1 V2 Q5 Q6 S7 G8 P9 E10 L11 V12 A16 K19 M20 K23 A24 Y27 T28 F29 T30 Y33 I34 H35 K38 Q39 S40 H41 G42 K43 S44 L45 E46 W47 Y50 I51 Y52 P52A N53 N54 N57 N60 H61 K62 F63 K64 G65 L69 T70 V71 D72

K73 S74 T77 A78 Y79 M80 R82A E85 A88 V89 Y90 Y91 C92 G93 R94 S95 T96 W97 D98 D101 Y102 W103 G104 Q105 G106 T107 T108 L109 T110 V111 S112 K115 T116 V121 Y122 P123 S128 A129 A130 Q131 T132 N133 S136 M137 G146 P149 E150 P151 V152 T153

L154 T156 W157 N162 S165 L166 S167 S168 G169 V171 H172 T173 F174 P175 A176 V177 L178 L184 Y185 T186 L187 S188 S189 S190 V191 T192 V193 T194 S195 S196 P198 R199 P200 S202 E203 T204 V205 T206 C208 N209 V210 A211 H212 P213 A214 V219 D220 K221 K222 I223 V226

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.46Å 67.72Å 68.04Å 62.11° 84.66° 83.17°	Depositor
Resolution (Å)	6.00 – 2.20 29.82 – 2.07	Depositor EDS
% Data completeness (in resolution range)	78.7 (6.00-2.20) 72.6 (29.82-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 2.08Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.290 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 107.9	EDS
L-test for twinning [2]	$<|L|>$ = 0.49, $<L^2>$ = 0.32	Xtriage
Estimated twinning fraction	0.109 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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.

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: 1PC

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	0.71	0/1717	0.99	7/2330 (0.3%)
1	C	0.74	0/1717	1.00	1/2330 (0.0%)
2	B	0.76	0/1681	1.00	4/2295 (0.2%)
2	D	0.72	0/1681	1.07	8/2295 (0.3%)
All	All	0.73	0/6796	1.01	20/9250 (0.2%)

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	2
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	129	ALA	N-CA-C	-9.62	85.02	111.00
1	A	160	LEU	CA-CB-CG	7.05	131.51	115.30
2	D	130	ALA	N-CA-C	6.69	129.06	111.00
1	A	104	LEU	CA-CB-CG	6.53	130.32	115.30
1	C	181	LEU	CA-CB-CG	6.47	130.18	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	A	192	TYR	Sidechain
2	B	50	TYR	Sidechain
1	C	140	TYR	Sidechain
2	D	50	TYR	Sidechain

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	1678	0	1621	123	0
1	C	1678	0	1621	120	0
2	B	1636	0	1578	165	0
2	D	1636	0	1578	111	0
3	B	18	0	25	5	0
3	C	18	0	25	8	0
4	A	173	0	0	4	0
4	B	163	0	0	6	0
4	C	150	0	0	4	0
4	D	192	0	0	8	0
All	All	7342	0	6448	482	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 37.

The worst 5 of 482 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:4:MET:HA	1:C:4:MET:HE2	1.29	1.13
1:A:190:ASN:HB2	1:C:203:SER:HB2	1.31	1.10
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.36	1.07
2:B:199:ARG:HD2	2:B:200:PRO:HA	1.36	1.05
2:D:171:VAL:HG12	2:D:191:VAL:HG23	1.37	1.03

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	214/216 (99%)	193 (90%)	19 (9%)	2 (1%)	17	16
1	C	214/216 (99%)	190 (89%)	21 (10%)	3 (1%)	11	8
2	B	213/215 (99%)	181 (85%)	20 (9%)	12 (6%)	2	0
2	D	213/215 (99%)	181 (85%)	26 (12%)	6 (3%)	5	2
All	All	854/862 (99%)	745 (87%)	86 (10%)	23 (3%)	5	2

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
2	B	131	GLN
2	B	198	PRO
2	B	214	ALA
1	C	68	GLY

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	192/192 (100%)	171 (89%)	21 (11%)	6	5
1	C	192/192 (100%)	158 (82%)	34 (18%)	2	1
2	B	186/186 (100%)	144 (77%)	42 (23%)	1	0
2	D	186/186 (100%)	158 (85%)	28 (15%)	3	2
All	All	756/756 (100%)	631 (84%)	125 (16%)	2	1

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	199	ARG
1	C	17	ASP
2	D	136	SER
2	B	209	ASN
1	C	1	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	ASN
1	C	157	ASN
2	D	172	HIS
1	C	137	ASN
1	C	156	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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
3	1PC	B	227	-	19,20,20	3.37	8 (42%)	24,27,27	1.55	3 (12%)
3	1PC	C	212	-	19,20,20	3.29	7 (36%)	24,27,27	1.37	3 (12%)

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	1PC	B	227	-	-	2/12/30/30	0/3/3/3
3	1PC	C	212	-	-	0/12/30/30	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	212	1PC	CH-CG	8.83	1.62	1.54
3	C	212	1PC	CL-CG	7.81	1.61	1.54
3	B	227	1PC	CH-CG	7.00	1.60	1.54
3	B	227	1PC	CG-CA	6.32	1.60	1.52
3	B	227	1PC	CN-NM	6.20	1.56	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	227	1PC	CL-CG-CH	-5.44	99.57	108.44
3	C	212	1PC	CL-CG-CH	-3.27	103.11	108.44
3	B	227	1PC	CI-CH-CG	-3.20	107.73	113.15
3	C	212	1PC	CI-CH-CG	-2.92	108.21	113.15
3	B	227	1PC	CL-CG-NM	-2.50	104.56	109.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	227	1PC	CL-CG-NM-CR
3	B	227	1PC	CL-CG-NM-CN

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	227	1PC	5	0
3	C	212	1PC	8	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	216/216 (100%)	-0.47	3 (1%)	75	73	7, 19, 34, 75	0
1	C	216/216 (100%)	-0.44	2 (0%)	84	83	4, 22, 35, 57	0
2	B	215/215 (100%)	-0.34	2 (0%)	84	83	5, 23, 39, 56	0
2	D	215/215 (100%)	-0.31	1 (0%)	91	90	6, 24, 41, 61	0
All	All	862/862 (100%)	-0.39	8 (0%)	84	83	4, 22, 38, 75	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	THR	6.9
2	D	129	ALA	5.5
1	A	200	THR	4.7
1	A	201	SER	3.8
1	C	200	THR	3.3

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. 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	1PC	C	212	18/18	0.84	0.19	3,19,31,31	0
3	1PC	B	227	18/18	0.89	0.14	4,17,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.