



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2018 – 06:38 PM EDT

PDB ID : 6C1R  
Title : Crystal structure of human C5a receptor in complex with an orthosteric antagonist PMX53 and an allosteric antagonist avacopan  
Authors : Liu, H.; Wang, L.; Wei, Z.; Zhang, C.  
Deposited on : 2018-01-05  
Resolution : 2.20 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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

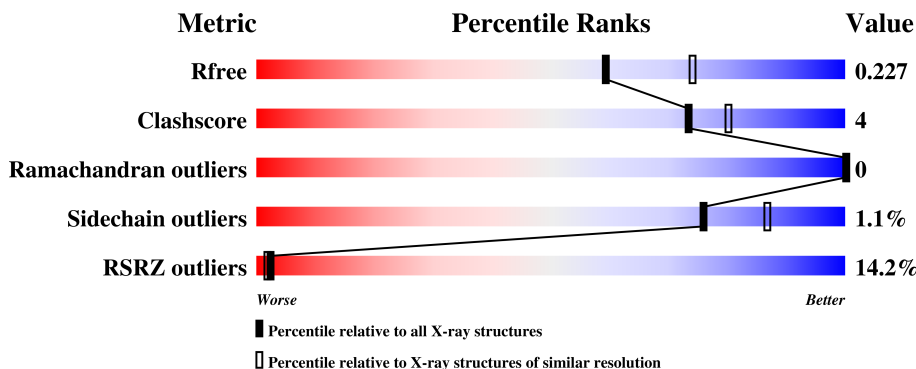
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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  $\geq 3$ , 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	B	422	<div> <div>13%</div> <div>81%</div> <div>7%</div> <div>12%</div> </div>
2	L	7	<div> <div>86%</div> <div>14%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3087 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 Soluble cytochrome b562, C5a anaphylatoxin chemotactic receptor 1 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	371	Total	C	N	O	S	0	0	0
			2781	1839	456	473	13			

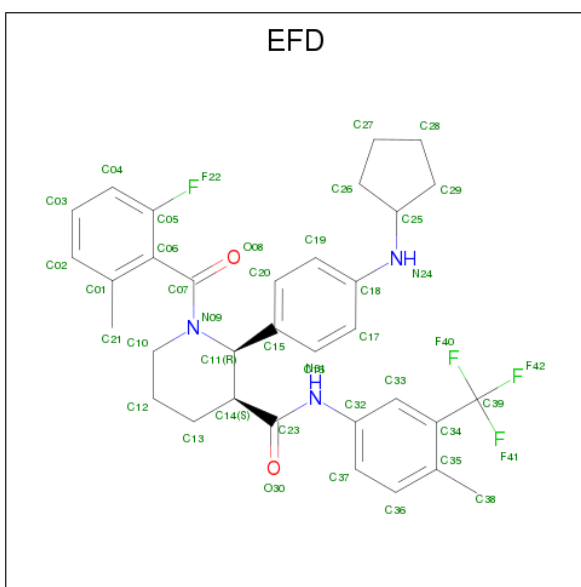
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ASP	-	expression tag	UNP P0ABE7
B	2	TYR	-	expression tag	UNP P0ABE7
B	3	LYS	-	expression tag	UNP P0ABE7
B	4	ASP	-	expression tag	UNP P0ABE7
B	5	ASP	-	expression tag	UNP P0ABE7
B	6	ASP	-	expression tag	UNP P0ABE7
B	7	ASP	-	expression tag	UNP P0ABE7
B	8	VAL	-	expression tag	UNP P0ABE7
B	9	ASP	-	expression tag	UNP P0ABE7
B	16	TRP	MET	engineered mutation	UNP P0ABE7
B	111	ILE	HIS	engineered mutation	UNP P0ABE7
B	115	LEU	ARG	engineered mutation	UNP P0ABE7
B	418	ASN	-	expression tag	UNP P21730
B	419	LEU	-	expression tag	UNP P21730
B	420	TYR	-	expression tag	UNP P21730
B	421	PHE	-	expression tag	UNP P21730
B	422	GLN	-	expression tag	UNP P21730

- Molecule 2 is a protein called PMX53.

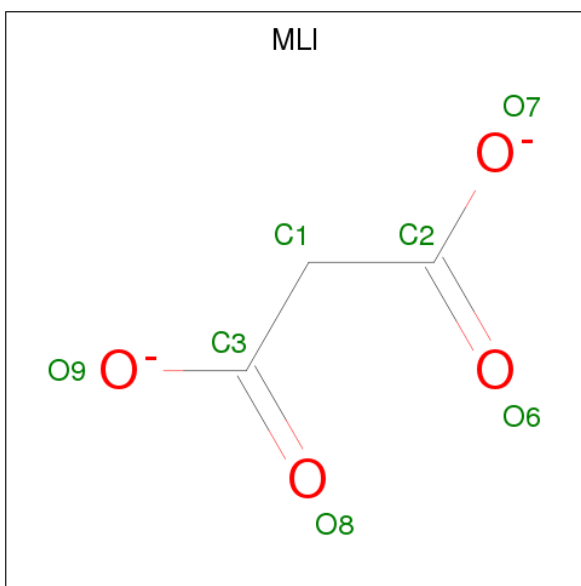
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	7	Total	C	N	O	0	0	0
			65	47	11	7			

- Molecule 3 is avacopan (three-letter code: EFD) (formula: C<sub>33</sub>H<sub>35</sub>F<sub>4</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			42	33	4	3	2		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).

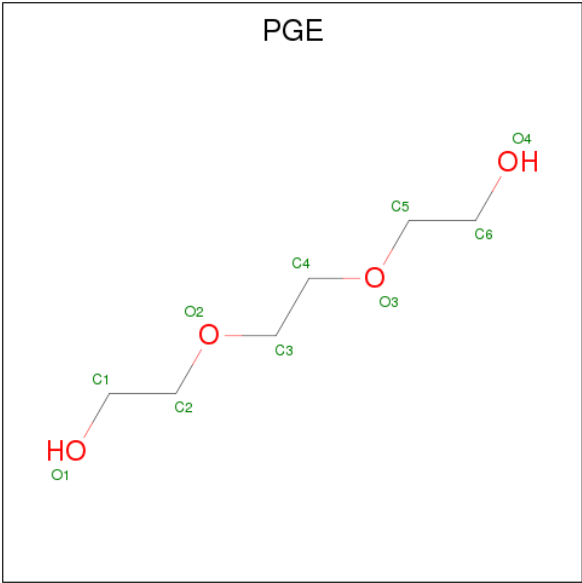


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

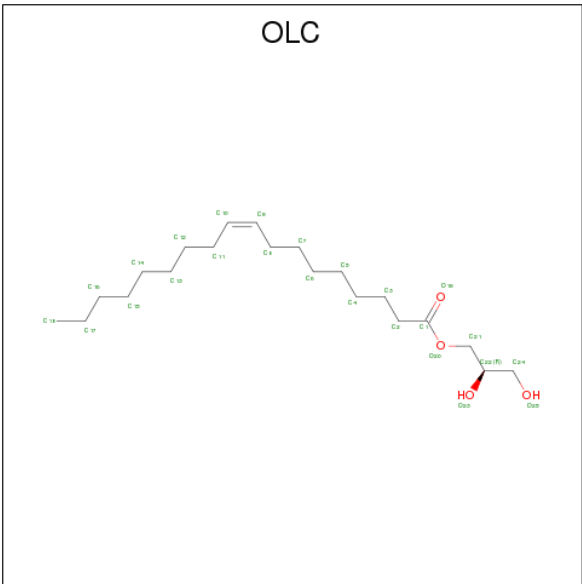
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



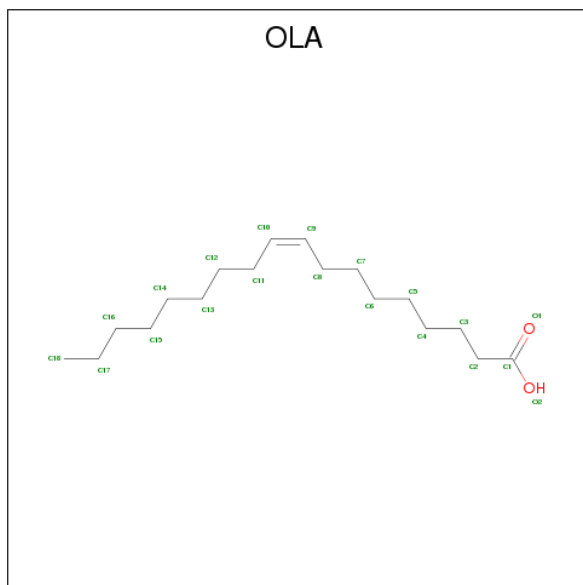
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 8 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		

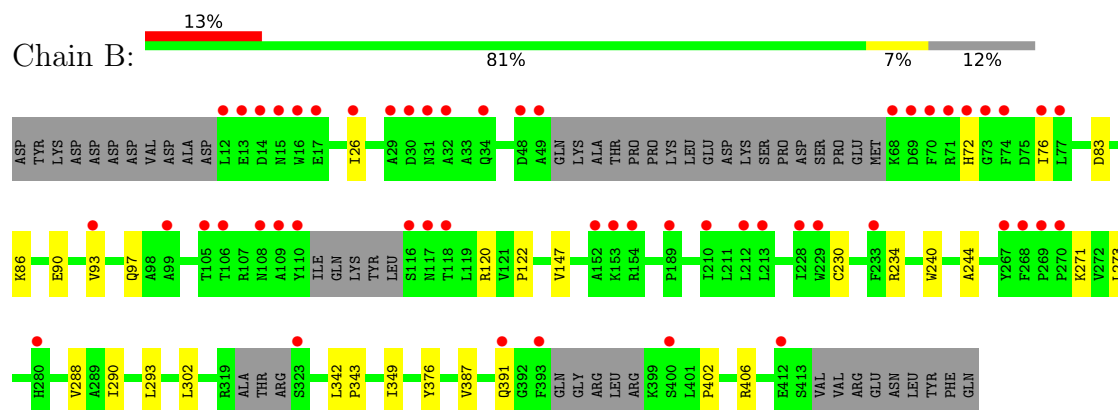
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	39	Total	O	0	0
			39	39		
9	L	6	Total	O	0	0
			6	6		

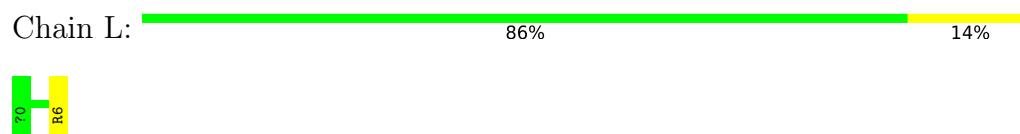
### 3 Residue-property plots [i](#)

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: Soluble cytochrome b562, C5a anaphylatoxin chemotactic receptor 1 chimera



- Molecule 2: PMX53



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.41Å 52.61Å 83.86Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	27.36 – 2.20 27.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.36-2.20) 99.6 (27.36-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.192 , 0.224 0.197 , 0.227	Depositor DCC
$R_{free}$ test set	1264 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OLA, ZAL, OLC, ACE, NA, MLI, ORN, PGE, YCM, EFD

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	B	0.26	0/2830	0.41	0/3875
2	L	0.29	0/45	0.35	0/57
All	All	0.26	0/2875	0.40	0/3932

There are no bond length outliers.

There are no bond angle outliers.

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	B	2781	0	2803	18	0
2	L	65	0	64	0	0
3	B	42	0	0	1	0
4	B	14	0	4	0	0
5	B	1	0	0	0	0
6	B	9	0	11	0	0
7	B	50	0	80	3	0
8	B	80	0	132	6	0
9	B	39	0	0	0	0
9	L	6	0	0	0	0
All	All	3087	0	3094	22	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 4.

All (22) 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:B:230:YCM:HD2	1:B:234:ARG:HD2	1.69	0.73
1:B:293:LEU:HD22	1:B:349:ILE:HG13	1.73	0.68
1:B:120:ARG:HB3	1:B:122:PRO:HD2	1.79	0.63
1:B:244:ALA:HA	8:B:510:OLA:H122	1.85	0.59
1:B:240:TRP:CD1	8:B:510:OLA:H21	2.38	0.58
1:B:288:VAL:HG22	7:B:506:OLC:H24	1.85	0.58
1:B:147:VAL:HG13	1:B:406:ARG:HG2	1.87	0.56
1:B:302:LEU:HB2	8:B:508:OLA:H141	1.90	0.54
1:B:387:VAL:O	1:B:391:GLN:HG2	2.08	0.53
1:B:290:ILE:HD13	8:B:508:OLA:H21	1.93	0.51
1:B:86:LYS:NZ	1:B:90:GLU:OE2	2.45	0.49
1:B:72:HIS:O	1:B:76:ILE:HG13	2.16	0.46
7:B:507:OLC:H8A	7:B:507:OLC:H11	1.72	0.46
8:B:511:OLA:H61	8:B:511:OLA:H9	1.46	0.45
1:B:402:PRO:O	1:B:406:ARG:HG3	2.18	0.44
7:B:507:OLC:H7A	7:B:507:OLC:H4	1.65	0.44
1:B:342:LEU:HB3	1:B:343:PRO:HD3	2.00	0.43
3:B:501:EFD:C23	3:B:501:EFD:C20	2.96	0.43
1:B:26:ILE:O	1:B:97:GLN:NE2	2.52	0.43
1:B:93:VAL:O	1:B:97:GLN:HG3	2.19	0.43
1:B:240:TRP:CE3	8:B:510:OLA:H9	2.54	0.42
1:B:271:LYS:HE3	1:B:273:LEU:HD21	2.01	0.42

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	B	360/422 (85%)	350 (97%)	10 (3%)	0	100	100
2	L	3/7 (43%)	3 (100%)	0	0	100	100
All	All	363/429 (85%)	353 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	281/361 (78%)	279 (99%)	2 (1%)	85	93
2	L	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	285/365 (78%)	282 (99%)	3 (1%)	76	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	ASP
1	B	376	TYR
2	L	6	ARG

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 ⓘ

3 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	YCM	B	230	1	9,9,10	1.28	2 (22%)	4,10,12	0.81	0
2	ORN	L	2	2	7,7,8	0.97	1 (14%)	4,7,9	0.93	0
2	ZAL	L	4	2	10,11,12	0.80	0	11,13,15	1.46	2 (18%)

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	YCM	B	230	1	-	0/6/8/10	0/0/0/0
2	ORN	L	2	2	-	0/4/6/8	0/0/0/0
2	ZAL	L	4	2	-	0/4/14/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	YCM	CD-SG	-2.18	1.77	1.81
1	B	230	YCM	CA-C	2.04	1.52	1.50
2	L	2	ORN	CA-C	2.25	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	4	ZAL	CB-C1-C6	-2.11	107.04	111.73
2	L	4	ZAL	C6-C1-C2	2.26	114.76	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	230	YCM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
3	EFD	B	501	-	46,46,46	3.48	8 (17%)	63,67,67	1.40	6 (9%)
4	MLI	B	502	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	503	-	0,6,6	0.00	-	0,7,7	0.00	-
6	PGE	B	505	-	8,8,9	0.35	0	7,7,8	0.32	0
7	OLC	B	506	-	24,24,24	0.83	1 (4%)	25,25,25	1.37	3 (12%)
7	OLC	B	507	-	24,24,24	0.90	1 (4%)	25,25,25	1.27	3 (12%)
8	OLA	B	508	-	16,19,19	0.78	1 (6%)	15,19,19	1.16	0
8	OLA	B	509	-	16,19,19	0.83	1 (6%)	15,19,19	0.84	0
8	OLA	B	510	-	16,19,19	0.87	1 (6%)	15,19,19	0.75	0
8	OLA	B	511	-	16,19,19	0.81	1 (6%)	15,19,19	1.18	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
3	EFD	B	501	-	-	0/30/51/51	0/5/5/5
4	MLI	B	502	-	-	0/0/4/4	0/0/0/0
4	MLI	B	503	-	-	0/0/4/4	0/0/0/0
6	PGE	B	505	-	-	0/6/6/7	0/0/0/0
7	OLC	B	506	-	-	0/24/24/24	0/0/0/0
7	OLC	B	507	-	-	0/24/24/24	0/0/0/0
8	OLA	B	508	-	-	0/15/17/17	0/0/0/0
8	OLA	B	509	-	-	0/15/17/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLA	B	510	-	-	0/15/17/17	0/0/0/0
8	OLA	B	511	-	-	0/15/17/17	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	EFD	C14-C11	-14.23	1.40	1.54
3	B	501	EFD	C11-N09	-11.14	1.37	1.47
3	B	501	EFD	C13-C14	-8.36	1.37	1.53
3	B	501	EFD	C10-N09	-7.96	1.37	1.47
3	B	501	EFD	C12-C13	-5.82	1.38	1.53
3	B	501	EFD	C12-C10	-3.08	1.40	1.51
8	B	509	OLA	C10-C9	2.95	1.48	1.31
8	B	511	OLA	C10-C9	2.95	1.48	1.31
8	B	508	OLA	C10-C9	2.99	1.48	1.31
8	B	510	OLA	C10-C9	3.15	1.49	1.31
7	B	506	OLC	O20-C1	3.58	1.43	1.33
3	B	501	EFD	C23-N31	3.69	1.42	1.35
7	B	507	OLC	O20-C1	4.05	1.45	1.33
3	B	501	EFD	C07-N09	4.49	1.43	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	EFD	C18-N24-C25	-5.82	111.86	124.20
7	B	506	OLC	O20-C1-O19	-3.59	114.83	123.58
3	B	501	EFD	C38-C35-C34	-2.99	121.31	124.19
7	B	507	OLC	O20-C1-O19	-2.36	117.82	123.58
7	B	507	OLC	C14-C15-C16	-2.07	103.20	114.41
7	B	506	OLC	C3-C2-C1	-2.01	106.34	113.60
3	B	501	EFD	C15-C11-N09	2.04	114.02	111.99
3	B	501	EFD	C27-C26-C25	2.08	108.73	104.60
3	B	501	EFD	C06-C07-N09	2.60	121.77	118.23
3	B	501	EFD	C14-C23-N31	2.77	118.04	114.77
7	B	507	OLC	O20-C1-C2	2.85	120.15	111.92
7	B	506	OLC	O20-C1-C2	3.98	123.44	111.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	EFD	1	0
7	B	506	OLC	1	0
7	B	507	OLC	2	0
8	B	508	OLA	2	0
8	B	510	OLA	3	0
8	B	511	OLA	1	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	370/422 (87%)	0.64	53 (14%) 2 2	23, 44, 94, 113	0
2	L	4/7 (57%)	0.34	0 100 100	33, 39, 39, 40	0
All	All	374/429 (87%)	0.63	53 (14%) 2 2	23, 43, 94, 113	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	PHE	8.2
1	B	29	ALA	5.8
1	B	280	HIS	5.6
1	B	14	ASP	5.5
1	B	31	ASN	5.5
1	B	109	ALA	5.4
1	B	105	THR	5.3
1	B	12	LEU	5.0
1	B	30	ASP	4.9
1	B	72	HIS	4.8
1	B	48	ASP	4.3
1	B	68	LYS	4.3
1	B	15	ASN	4.1
1	B	323	SER	4.0
1	B	228	ILE	3.9
1	B	106	THR	3.8
1	B	76	ILE	3.8
1	B	269	PRO	3.6
1	B	93	VAL	3.5
1	B	267	TYR	3.5
1	B	116	SER	3.5
1	B	34	GLN	3.4
1	B	118	THR	3.3
1	B	77	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	270	PRO	3.2
1	B	73	GLY	3.1
1	B	49	ALA	3.1
1	B	210	ILE	3.0
1	B	268	PHE	3.0
1	B	117	ASN	2.9
1	B	13	GLU	2.8
1	B	17	GLU	2.8
1	B	233	PHE	2.7
1	B	412	GLU	2.7
1	B	229	TRP	2.7
1	B	153	LYS	2.6
1	B	74	PHE	2.6
1	B	32	ALA	2.5
1	B	69	ASP	2.5
1	B	391	GLN	2.5
1	B	108	ASN	2.5
1	B	189	PRO	2.4
1	B	212	LEU	2.4
1	B	393	PHE	2.3
1	B	400	SER	2.3
1	B	154	ARG	2.2
1	B	110	TYR	2.1
1	B	26	ILE	2.1
1	B	213	LEU	2.1
1	B	99	ALA	2.1
1	B	152	ALA	2.1
1	B	71	ARG	2.0
1	B	16	TRP	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	YCM	B	230	10/11	0.88	0.15	53,60,69,76	0
2	ORN	L	2	8/9	0.93	0.15	36,37,42,42	0
2	ZAL	L	4	11/12	0.97	0.23	30,37,44,45	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	OLA	B	509	20/20	0.61	0.22	60,65,79,81	0
8	OLA	B	510	20/20	0.69	0.23	47,61,83,83	0
7	OLC	B	507	25/25	0.74	0.28	59,64,78,78	0
8	OLA	B	511	20/20	0.80	0.26	63,67,78,80	0
4	MLI	B	502	7/7	0.81	0.22	77,79,82,86	0
8	OLA	B	508	20/20	0.83	0.23	39,53,81,81	0
7	OLC	B	506	25/25	0.83	0.18	52,58,75,78	0
6	PGE	B	505	9/10	0.84	0.38	73,75,78,79	0
5	NA	B	504	1/1	0.91	0.10	43,43,43,43	0
4	MLI	B	503	7/7	0.91	0.18	37,51,70,71	0
3	EFD	B	501	42/42	0.93	0.12	33,37,41,45	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.