



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2016 – 04:44 PM EST

PDB ID : 5K2D  
Title : 1.9A angstrom A2a adenosine receptor structure with MR phasing using XFEL data  
Authors : Batyuk, A.; Galli, L.; Ishchenko, A.; Han, G.W.; Gati, C.; Popov, P.; Lee, M.-Y.; Stauch, B.; White, T.A.; Barty, A.; Aquila, A.; Hunter, M.S.; Liang, M.; Boutet, S.; Pu, M.; Liu, Z.-J.; Nelson, G.; James, D.; Li, C.; Zhao, Y.; Spence, J.C.H.; Liu, W.; Fromme, P.; Katritch, V.; Weierstall, U.; Stevens, R.C.; Cherezov, V.; GPCR Network (GPCR)  
Deposited on : 2016-05-18  
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028320

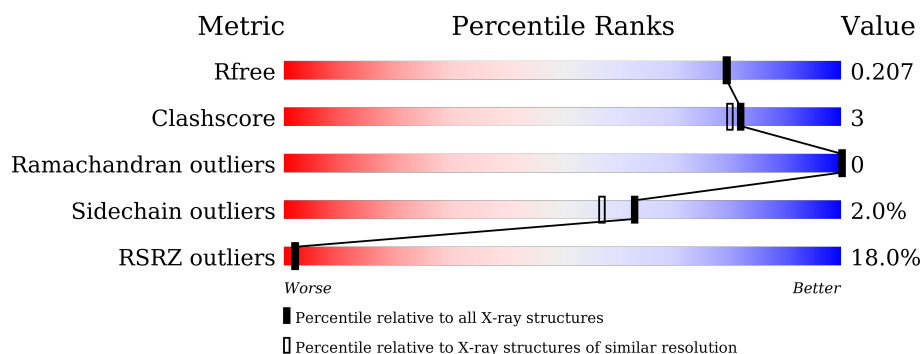
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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  $\geq 3$ , 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	A	447	

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	OLB	A	1206	-	-	-	X
5	OLB	A	1210	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OLC	A	1207	-	-	-	X
6	OLC	A	1212	-	-	-	X
6	OLC	A	1220	-	-	-	X
7	OLA	A	1213	-	-	-	X
7	OLA	A	1215	-	-	-	X
7	OLA	A	1216	-	-	-	X
7	OLA	A	1218	-	-	-	X
7	OLA	A	1223	-	-	-	X
7	OLA	A	1226	-	-	-	X
7	OLA	A	1227	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3636 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 Adenosine receptor A2a/Soluble cytochrome b562 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	12	0
			3121	2045	522	532	22			

There are 39 discrepancies between the modelled and reference sequences:

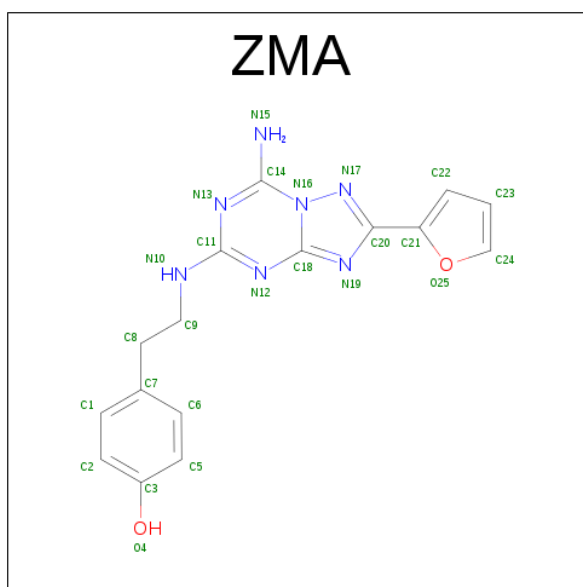
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).

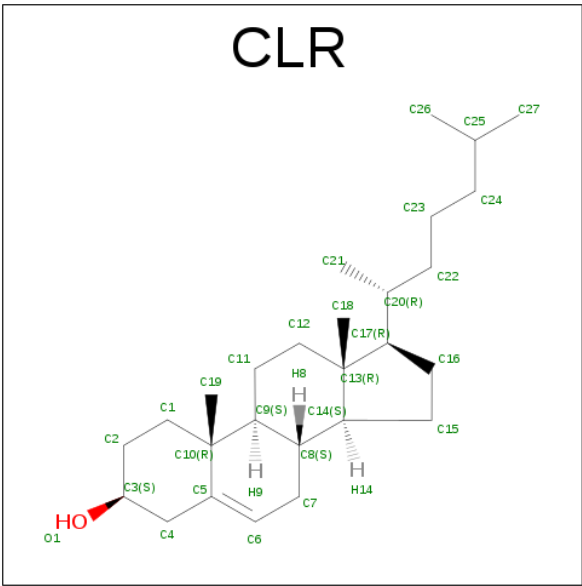


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

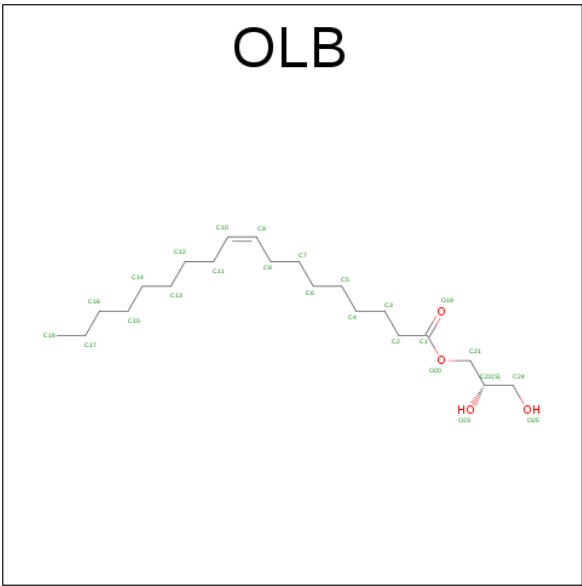
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



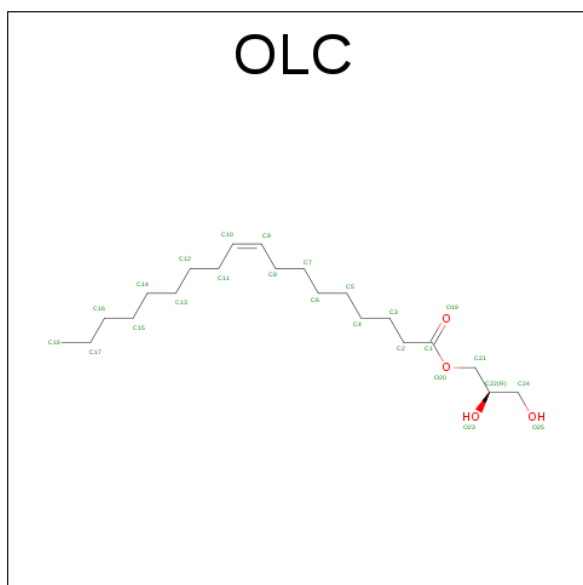
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



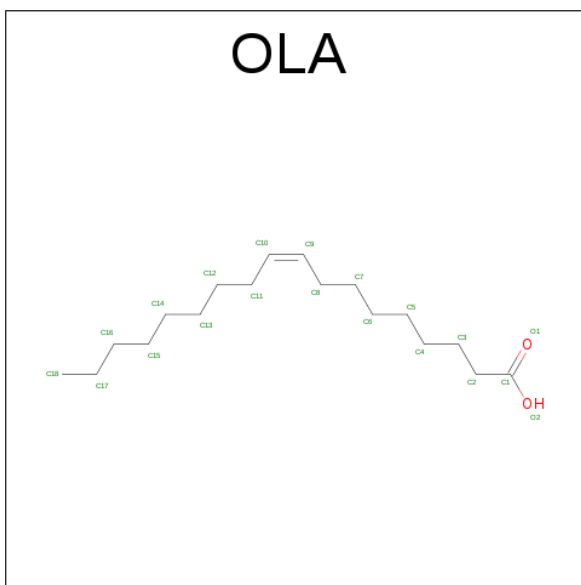
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			18	14	4		
5	A	1	Total	C	O	0	0
			17	13	4		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			16	12	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			14	10	4		
6	A	1	Total	C	O	0	0
			17	13	4		
6	A	1	Total	C	O	0	0
			11	7	4		

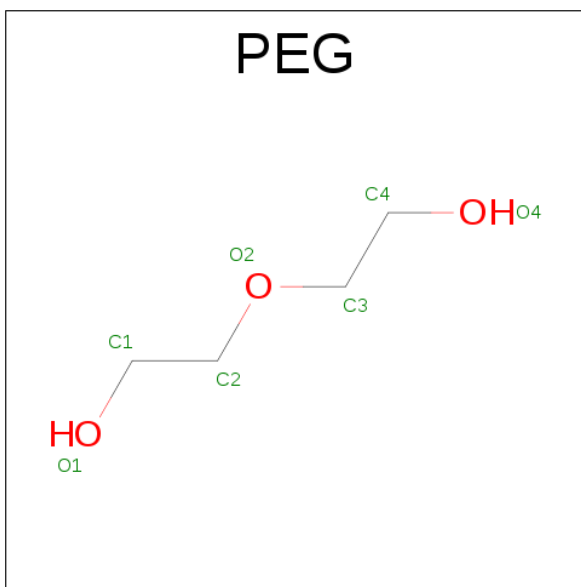
- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	9	2		
7	A	1	Total	C	O	0	0
			12	10	2		
7	A	1	Total	C	O	0	0
			16	14	2		
7	A	1	Total	C	O	0	0
			9	7	2		
7	A	1	Total	C	O	0	0
			11	9	2		
7	A	1	Total	C	O	0	0
			9	7	2		
7	A	1	Total	C	O	0	0
			12	10	2		
7	A	1	Total	C	O	0	0
			13	11	2		
7	A	1	Total	C	O	0	0
			19	17	2		
7	A	1	Total	C	O	0	0
			17	15	2		
7	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





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

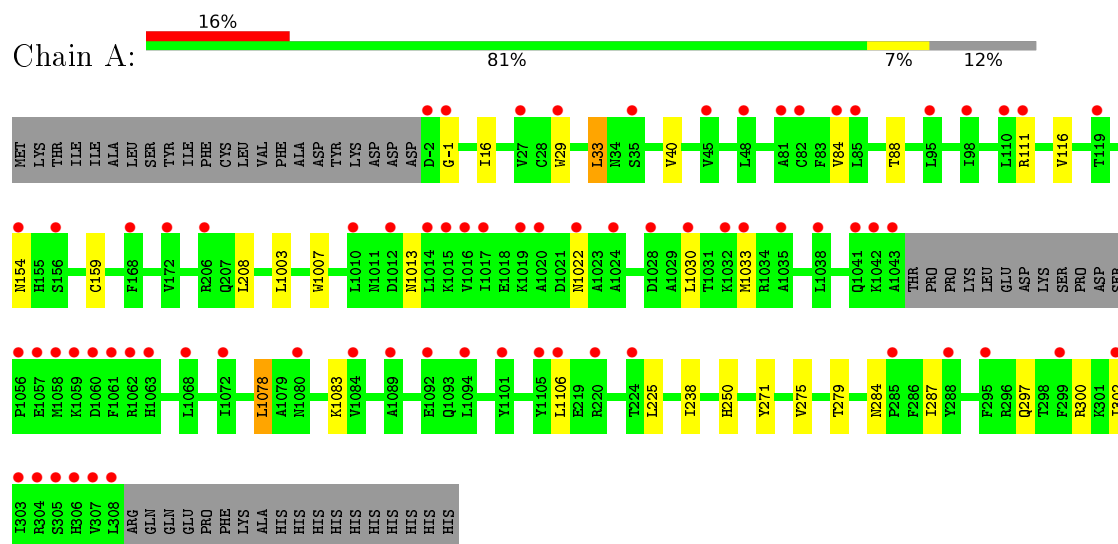
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	93	Total	O	0	0
			93	93		

### 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 errors 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: Adenosine receptor A2a/Soluble cytochrome b562 chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.36Å 180.74Å 142.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.44 – 1.90 23.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.44-1.90) 100.0 (23.44-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.174 , 0.207 0.173 , 0.207	Depositor DCC
$R_{free}$ test set	1986 reflections (4.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 94.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLB, OLC, NA, ZMA, PEG, CLR

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	0.49	0/3189	0.54	0/4343

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 [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	3121	0	3151	19	1
2	A	25	0	15	1	0
3	A	1	0	0	0	0
4	A	84	0	138	1	0
5	A	35	0	45	1	0
6	A	121	0	149	2	0
7	A	149	0	201	2	0
8	A	7	0	10	0	0
9	A	93	0	0	0	0
All	All	3636	0	3709	23	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 3.

All (23) 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:154[B]:ASN:HD22	1:A:159:CYS:HB2	1.56	0.70
1:A:275[A]:VAL:O	1:A:279:THR:HG23	1.97	0.65
1:A:154[B]:ASN:ND2	1:A:159:CYS:HB2	2.11	0.64
1:A:275[B]:VAL:O	1:A:279:THR:HG23	1.98	0.64
1:A:84:VAL:O	1:A:88[B]:THR:HG23	2.00	0.61
1:A:16:ILE:CD1	1:A:275[B]:VAL:HG23	2.37	0.55
1:A:208:LEU:HG	1:A:225[B]:LEU:HD23	1.89	0.55
1:A:250:HIS:CE1	2:A:1201:ZMA:H24	2.42	0.54
1:A:271:TYR:O	1:A:275[B]:VAL:HG12	2.10	0.51
1:A:297:GLN:OE1	1:A:300[B]:ARG:NH1	2.44	0.51
5:A:1210:OLB:O23	7:A:1227:OLA:H31	2.13	0.49
1:A:16:ILE:HD11	1:A:275[B]:VAL:HG23	1.94	0.48
4:A:1205:CLR:H72	6:A:1222:OLC:H22	1.96	0.47
1:A:1013:ASN:HB3	1:A:1033:MET:HE2	1.97	0.46
1:A:29[A]:TRP:CD1	1:A:33:LEU:HD13	2.52	0.45
1:A:1007:TRP:CE3	1:A:1106[B]:LEU:HD12	2.51	0.44
6:A:1212:OLC:H2	6:A:1212:OLC:H5A	1.79	0.44
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.01	0.42
1:A:1078:LEU:HD12	1:A:1083:LYS:HE2	2.01	0.41
1:A:238:ILE:HD13	1:A:287[B]:ILE:HD13	2.02	0.41
1:A:284:ASN:HA	1:A:287[B]:ILE:HD12	2.03	0.41
1:A:29[B]:TRP:HD1	1:A:302:ILE:HD13	1.86	0.40
7:A:1226:OLA:H111	7:A:1226:OLA:H81	1.64	0.40

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)
1:A:-1:GLY:O	1:A:300[A]:ARG:NH1[4_575]	2.12	0.08

## 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	403/447 (90%)	399 (99%)	4 (1%)	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	A	318/374 (85%)	312 (98%)	6 (2%)	65	59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	111	ARG
1	A	1003	LEU
1	A	1022	ASN
1	A	1030	LEU
1	A	1078	LEU

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	ZMA	A	1201	-	21,28,28	0.75	0	23,39,39	2.55	7 (30%)
4	CLR	A	1203	-	31,31,31	0.60	0	48,48,48	0.90	2 (4%)
4	CLR	A	1204	-	31,31,31	0.60	0	48,48,48	0.91	1 (2%)
4	CLR	A	1205	-	31,31,31	0.67	0	48,48,48	0.85	1 (2%)
5	OLB	A	1206	-	17,17,24	1.11	1 (5%)	18,18,25	0.93	1 (5%)
6	OLC	A	1207	-	16,16,24	1.10	1 (6%)	17,17,25	1.15	1 (5%)
6	OLC	A	1208	-	16,16,24	1.12	1 (6%)	17,17,25	1.07	1 (5%)
6	OLC	A	1209	-	15,15,24	1.17	1 (6%)	16,16,25	1.10	1 (6%)
5	OLB	A	1210	-	16,16,24	1.20	1 (6%)	17,17,25	1.08	2 (11%)
6	OLC	A	1211	-	10,10,24	1.44	1 (10%)	11,11,25	1.21	1 (9%)
6	OLC	A	1212	-	17,17,24	1.07	1 (5%)	18,18,25	0.96	1 (5%)
7	OLA	A	1213	-	7,10,19	0.24	0	7,10,19	0.55	0
7	OLA	A	1214	-	8,11,19	0.36	0	8,11,19	0.64	0
7	OLA	A	1215	-	12,15,19	0.22	0	12,15,19	0.59	0
7	OLA	A	1216	-	5,8,19	0.21	0	5,8,19	0.67	0
7	OLA	A	1217	-	7,10,19	0.22	0	7,10,19	0.62	0
7	OLA	A	1218	-	5,8,19	0.26	0	5,8,19	0.53	0
7	OLA	A	1219	-	8,11,19	0.33	0	8,11,19	0.79	0
6	OLC	A	1220	-	13,13,24	1.19	1 (7%)	14,14,25	1.19	1 (7%)
6	OLC	A	1221	-	16,16,24	1.12	1 (6%)	17,17,25	1.14	1 (5%)
6	OLC	A	1222	-	10,10,24	1.44	1 (10%)	11,11,25	1.21	1 (9%)
7	OLA	A	1223	-	9,12,19	0.31	0	9,12,19	0.76	0
7	OLA	A	1224	-	15,18,19	0.23	0	15,18,19	0.60	0
8	PEG	A	1225	-	6,6,6	0.43	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	OLA	A	1226	-	13,16,19	0.22	0	13,16,19	0.58	0
7	OLA	A	1227	-	16,19,19	0.22	0	16,19,19	0.60	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	ZMA	A	1201	-	-	0/6/10/10	0/3/4/4
4	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
4	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
4	CLR	A	1205	-	-	0/10/68/68	0/4/4/4
5	OLB	A	1206	-	-	0/17/17/24	0/0/0/0
6	OLC	A	1207	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1208	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1209	-	-	0/15/15/24	0/0/0/0
5	OLB	A	1210	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1211	-	-	0/10/10/24	0/0/0/0
6	OLC	A	1212	-	-	0/17/17/24	0/0/0/0
7	OLA	A	1213	-	-	0/6/8/17	0/0/0/0
7	OLA	A	1214	-	-	0/7/9/17	0/0/0/0
7	OLA	A	1215	-	-	0/11/13/17	0/0/0/0
7	OLA	A	1216	-	-	0/4/6/17	0/0/0/0
7	OLA	A	1217	-	-	0/6/8/17	0/0/0/0
7	OLA	A	1218	-	-	0/4/6/17	0/0/0/0
7	OLA	A	1219	-	-	0/7/9/17	0/0/0/0
6	OLC	A	1220	-	-	0/13/13/24	0/0/0/0
6	OLC	A	1221	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1222	-	-	0/10/10/24	0/0/0/0
7	OLA	A	1223	-	-	0/8/10/17	0/0/0/0
7	OLA	A	1224	-	-	0/14/16/17	0/0/0/0
8	PEG	A	1225	-	-	0/4/4/4	0/0/0/0
7	OLA	A	1226	-	-	0/12/14/17	0/0/0/0
7	OLA	A	1227	-	-	0/15/17/17	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1207	OLC	O20-C1	4.07	1.45	1.33
6	A	1220	OLC	O20-C1	4.12	1.45	1.33
6	A	1212	OLC	O20-C1	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1221	OLC	O20-C1	4.23	1.45	1.33
6	A	1208	OLC	O20-C1	4.25	1.46	1.33
5	A	1206	OLB	O20-C1	4.27	1.46	1.33
6	A	1209	OLC	O20-C1	4.37	1.46	1.33
6	A	1211	OLC	O20-C1	4.38	1.46	1.33
6	A	1222	OLC	O20-C1	4.40	1.46	1.33
5	A	1210	OLB	O20-C1	4.56	1.46	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ZMA	C9-C8-C7	-4.38	103.08	112.83
2	A	1201	ZMA	N12-C11-N13	-3.34	121.19	126.18
2	A	1201	ZMA	N13-C14-N16	-3.22	117.97	124.53
4	A	1203	CLR	C3-C4-C5	-2.36	107.43	111.89
2	A	1201	ZMA	C9-N10-C11	-2.29	119.71	123.62
4	A	1205	CLR	C19-C10-C9	-2.10	109.07	111.70
4	A	1203	CLR	C11-C12-C13	-2.02	109.18	112.81
6	A	1212	OLC	O20-C1-C2	2.24	118.75	111.85
5	A	1210	OLB	O20-C1-C2	2.33	119.01	111.85
2	A	1201	ZMA	C8-C9-N10	2.41	114.83	111.25
5	A	1206	OLB	O20-C1-C2	2.44	119.36	111.85
4	A	1204	CLR	C7-C8-C9	2.52	113.08	109.73
5	A	1210	OLB	C21-O20-C1	2.68	124.98	117.00
6	A	1208	OLC	O20-C1-C2	2.69	120.11	111.85
6	A	1222	OLC	O20-C1-C2	2.96	120.96	111.85
6	A	1211	OLC	O20-C1-C2	2.98	121.03	111.85
6	A	1209	OLC	O20-C1-C2	2.98	121.03	111.85
6	A	1207	OLC	O20-C1-C2	3.18	121.65	111.85
6	A	1221	OLC	O20-C1-C2	3.24	121.81	111.85
6	A	1220	OLC	O20-C1-C2	3.25	121.86	111.85
2	A	1201	ZMA	N17-C20-N19	4.31	117.36	114.63
2	A	1201	ZMA	N15-C14-N16	7.81	123.29	117.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ZMA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	CLR	1	0
5	A	1210	OLB	1	0
6	A	1212	OLC	1	0
6	A	1222	OLC	1	0
7	A	1226	OLA	1	0
7	A	1227	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	A	395/447 (88%)	0.85	71 (17%) 2 2	28, 45, 108, 156	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1056	PRO	8.0
1	A	1024	ALA	6.0
1	A	307	VAL	5.7
1	A	306	HIS	5.6
1	A	304	ARG	5.5
1	A	1062	ARG	5.2
1	A	1019	LYS	5.2
1	A	1057	GLU	5.0
1	A	1061	PHE	4.8
1	A	-1	GLY	4.8
1	A	305	SER	4.7
1	A	1010	LEU	4.7
1	A	1058	MET	4.6
1	A	1080	ASN	4.5
1	A	1060	ASP	4.5
1	A	1020	ALA	4.3
1	A	1068	LEU	4.2
1	A	308	LEU	4.1
1	A	1059	LYS	4.0
1	A	1092	GLU	4.0
1	A	299	PHE	3.8
1	A	111	ARG	3.8
1	A	-2	ASP	3.7
1	A	1063	HIS	3.6
1	A	81	ALA	3.6
1	A	156	SER	3.4
1	A	1028	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1089	ALA	3.4
1	A	1041	GLN	3.4
1	A	1038	LEU	3.3
1	A	1105	TYR	3.3
1	A	1072	ILE	3.2
1	A	1094	LEU	3.1
1	A	1101	TYR	3.1
1	A	1043	ALA	3.0
1	A	27	VAL	2.9
1	A	119	THR	2.9
1	A	98	ILE	2.9
1	A	1030	LEU	2.8
1	A	1033	MET	2.8
1	A	154[A]	ASN	2.8
1	A	1016	VAL	2.7
1	A	1106[A]	LEU	2.7
1	A	84	VAL	2.6
1	A	295	PHE	2.6
1	A	224	THR	2.6
1	A	85	LEU	2.5
1	A	1014	LEU	2.5
1	A	1017	ILE	2.4
1	A	1042	LYS	2.4
1	A	48	LEU	2.4
1	A	1035	ALA	2.4
1	A	35	SER	2.3
1	A	1012	ASP	2.3
1	A	82	CYS	2.3
1	A	45	VAL	2.2
1	A	110	LEU	2.2
1	A	220	ARG	2.2
1	A	288	TYR	2.2
1	A	168	PHE	2.2
1	A	1032	LYS	2.2
1	A	29[A]	TRP	2.2
1	A	303	ILE	2.1
1	A	1022	ASN	2.1
1	A	302	ILE	2.1
1	A	206	ARG	2.1
1	A	1084	VAL	2.0
1	A	95	LEU	2.0
1	A	1015	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	172	VAL	2.0
1	A	285	PRO	2.0

## 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	OLA	A	1223	13/20	0.63	0.40	8.86	84,91,111,112	0
7	OLA	A	1227	20/20	0.57	0.34	6.79	80,86,105,107	0
6	OLC	A	1207	17/25	0.78	0.18	5.50	62,76,89,90	0
5	OLB	A	1210	17/25	0.67	0.24	5.32	71,81,88,91	0
7	OLA	A	1226	17/20	0.53	0.25	4.87	79,89,98,98	0
7	OLA	A	1216	9/20	0.86	0.27	4.83	65,71,76,78	0
7	OLA	A	1218	9/20	0.82	0.13	4.46	84,88,97,97	0
5	OLB	A	1206	18/25	0.77	0.27	4.02	59,70,101,102	0
7	OLA	A	1215	16/20	0.64	0.24	3.97	61,84,97,99	0
7	OLA	A	1213	11/20	0.70	0.30	3.91	50,64,91,93	0
6	OLC	A	1212	18/25	0.81	0.17	3.77	69,75,89,91	0
6	OLC	A	1220	14/25	0.91	0.17	2.60	76,85,92,94	0
7	OLA	A	1224	19/20	0.68	0.20	1.93	75,87,94,95	0
6	OLC	A	1208	17/25	0.69	0.18	1.76	69,77,92,92	0
6	OLC	A	1209	16/25	0.84	0.19	1.60	75,82,89,89	0
4	CLR	A	1205	28/28	0.88	0.14	0.59	49,55,78,81	0
2	ZMA	A	1201	25/25	0.94	0.17	0.56	28,30,51,58	0
4	CLR	A	1204	28/28	0.89	0.13	0.52	47,56,66,67	0
4	CLR	A	1203	28/28	0.94	0.09	-0.34	44,50,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	1202	1/1	0.99	0.05	-1.84	35,35,35,35	0
7	OLA	A	1214	12/20	0.29	0.31	-	75,83,102,104	0
6	OLC	A	1221	17/25	0.86	0.16	-	73,79,87,89	0
6	OLC	A	1211	11/25	0.78	0.20	-	110,111,113,114	0
8	PEG	A	1225	7/7	0.64	0.18	-	95,96,98,98	0
7	OLA	A	1217	11/20	0.61	0.19	-	97,100,104,106	0
6	OLC	A	1222	11/25	0.63	0.18	-	100,103,107,107	0
7	OLA	A	1219	12/20	0.68	0.15	-	80,85,104,104	0

## 6.5 Other polymers

There are no such residues in this entry.