



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2018 – 12:59 PM EST

PDB ID : 5OM1  
Title : Structure of the A2A-StaR2-bRIL562-Compound 4e complex at 2.1Å obtained from in meso soaking experiments (1 hour soak).  
Authors : Rucktoo, P.; Cheng, R.K.Y.; Segala, E.; Geng, T.; Errey, J.C.; Brown, G.A.; Cooke, R.; Marshall, F.H.; Dore, A.S.  
Deposited on : 2017-07-28  
Resolution : 2.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
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-20030736

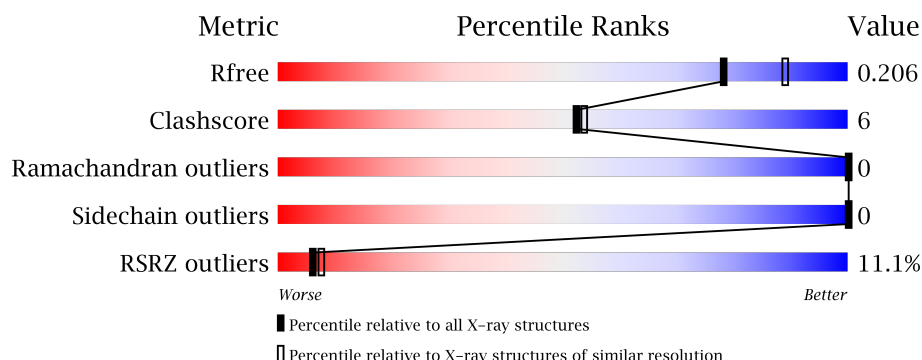
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	434	<div> <div>10%</div> <div>82%</div> <div>7%</div> <div>11%</div> </div>

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
4	OLA	A	1203	-	-	-	X
4	OLA	A	1208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLA	A	1209	-	-	-	X
4	OLA	A	1210	-	-	-	X
4	OLA	A	1214	-	-	-	X
4	OLA	A	1215	-	-	-	X
4	OLA	A	1217	-	-	-	X
4	OLA	A	1218	-	-	-	X
4	OLA	A	1220	-	-	-	X
5	CLR	A	1204	-	-	-	X
6	OLC	A	1221	-	-	-	X
6	OLC	A	1222	-	-	-	X
6	OLC	A	1223	-	-	-	X
6	OLC	A	1224	-	-	-	X
6	OLC	A	1225	-	-	-	X
6	OLC	A	1226	-	-	-	X
6	OLC	A	1227	-	-	-	X
6	OLC	A	1228	-	-	-	X
6	OLC	A	1229	-	-	-	X
6	OLC	A	1230	-	-	-	X
6	OLC	A	1231	-	-	-	X
6	OLC	A	1232	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3783 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,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	10	0
			3075	2004	519	530	22			

There are 34 discrepancies between the modelled and reference sequences:

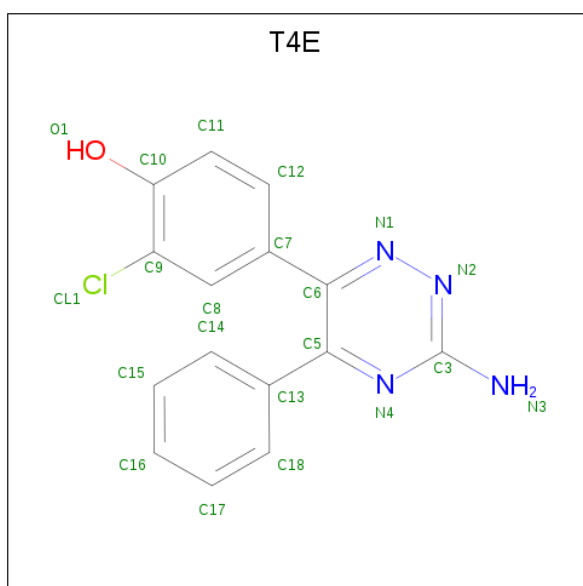
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
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	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-(3-amino-5-phenyl-1,2,4-triazin-6-yl)-2-chlorophenol (three-letter code: T4E) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>4</sub>O).

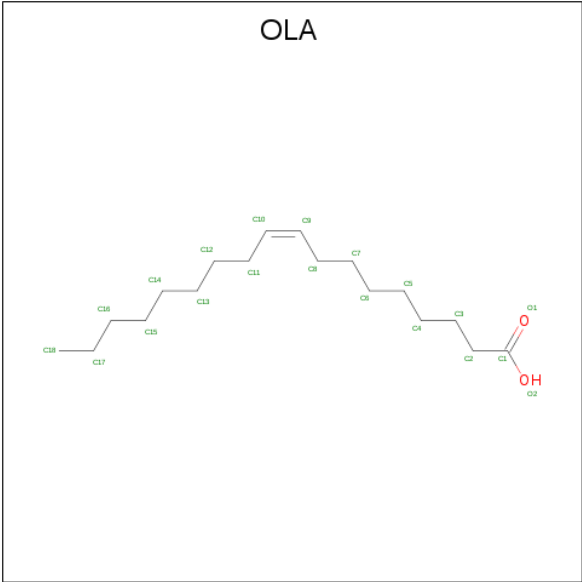


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	
			21	15	1	4	1	

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

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

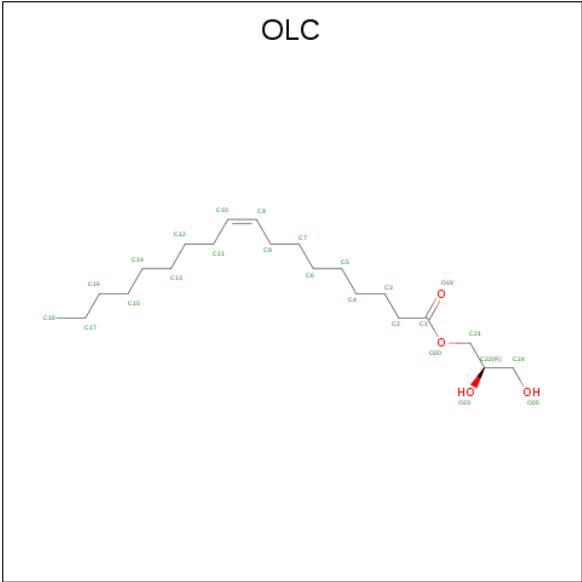
- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			9	7	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			15	13	2		
4	A	1	Total	C		0	0
			12	12			
4	A	1	Total	C		0	0
			8	8			
4	A	1	Total	C		0	0
			11	11			
4	A	1	Total	C		0	0
			12	12			
4	A	1	Total	C	O	0	0
			14	12	2		
4	A	1	Total	C	O	0	0
			19	17	2		
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			15	13	2		

- 
- The chemical structure of CLR is a complex polycyclic molecule. It features a bicyclic core with several fused rings. The stereochemistry is indicated by wedged and dashed bonds. Key features include a hydroxyl group (HO) attached to C3(S), a double bond between C5 and C6, and a long side chain starting from C13(R) and ending in a branched alkyl group. The atoms are numbered from C1 to C27, with C1-C10 and C12-C15 being part of the bicyclic system, and C16-C27 forming the side chain. The stereochemistry is as follows: C1(R), C2(R), C3(S), C4(R), C5(R), C6(R), C7(R), C8(S), C9(S), C10(R), C11(R), C12(R), C13(R), C14(S), C15(R), C16(R), C17(R), C18(R), C19(R), C20(R), C21(R), C22(R), C23(R), C24(R), C25(R), C26(R), C27(R).

- 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
			18	14	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			19	15	4		
6	A	1	Total	C	O	0	0
			16	12	4		
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
			22	18	4		
6	A	1	Total	C	O	0	0
			25	21	4		
6	A	1	Total	C	O	0	0
			25	21	4		
6	A	1	Total	C	O	0	0
			24	20	4		
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C		0	0
			14	14			

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0

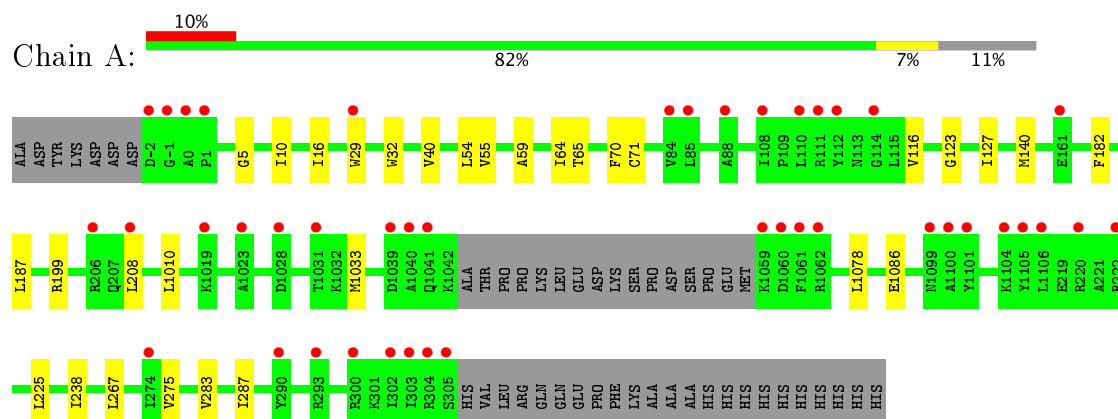
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	137	Total 137	O 137	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: Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.54Å 179.85Å 140.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.83 – 2.10 33.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.83-2.10) 99.9 (33.83-2.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.12rc2_2821: ???)	Depositor
R, $R_{free}$	0.188 , 0.210 0.184 , 0.206	Depositor DCC
$R_{free}$ test set	1474 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.6	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	3783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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, OLC, CL, NA, CLR, T4E

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	0.24	0/3141	0.37	0/4273

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	3075	0	3139	31	0
2	A	21	0	10	0	0
3	A	1	0	0	0	0
4	A	199	0	293	12	0
5	A	112	0	184	4	0
6	A	237	0	335	31	0
7	A	1	0	0	0	0
8	A	137	0	0	0	0
All	All	3783	0	3961	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 6.

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)
6:A:1230:OLC:H13A	6:A:1231:OLC:C15	1.44	1.42
6:A:1230:OLC:C13	6:A:1231:OLC:C15	2.06	1.32
5:A:1205:CLR:C27	6:A:1229:OLC:H15	1.93	0.98
6:A:1230:OLC:H13	6:A:1231:OLC:C15	2.01	0.89
5:A:1205:CLR:H272	6:A:1229:OLC:H15	1.56	0.88
1:A:71:CYS:O	6:A:1229:OLC:H24A	1.79	0.82
1:A:140[A]:MET:HE2	6:A:1225:OLC:H2	1.63	0.78
6:A:1230:OLC:H13A	6:A:1231:OLC:C14	2.15	0.77
4:A:1219:OLA:H82	4:A:1220:OLA:H122	1.66	0.76
1:A:5:GLY:HA3	6:A:1222:OLC:H21A	1.70	0.72
1:A:54:LEU:HD21	6:A:1231:OLC:H10	1.72	0.70
4:A:1208:OLA:H172	6:A:1229:OLC:H17A	1.74	0.69
6:A:1230:OLC:H7	6:A:1232:OLC:H7	1.74	0.69
1:A:123:GLY:HA3	4:A:1210:OLA:H22	1.76	0.67
4:A:1208:OLA:H172	6:A:1229:OLC:C17	2.25	0.66
4:A:1210:OLA:H151	6:A:1228:OLC:H12	1.77	0.64
5:A:1204:CLR:H3	6:A:1225:OLC:O23	1.97	0.64
1:A:267:LEU:HD23	6:A:1222:OLC:H22	1.79	0.64
1:A:70:PHE:HD2	6:A:1229:OLC:H24A	1.65	0.62
1:A:283:VAL:HG12	4:A:1212:OLA:H122	1.81	0.62
1:A:70:PHE:HD2	6:A:1229:OLC:C24	2.15	0.60
1:A:127:ILE:HG12	4:A:1210:OLA:H82	1.83	0.59
6:A:1230:OLC:C14	6:A:1231:OLC:C15	2.82	0.57
6:A:1227:OLC:H2	6:A:1229:OLC:H2	1.86	0.56
1:A:140[B]:MET:CE	6:A:1225:OLC:H2	2.37	0.54
1:A:70:PHE:CD2	6:A:1229:OLC:H24A	2.43	0.54
5:A:1205:CLR:C27	6:A:1229:OLC:C15	2.78	0.52
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.93	0.50
1:A:65:THR:HG21	6:A:1229:OLC:H5	1.93	0.50
1:A:140[A]:MET:CE	6:A:1225:OLC:H4A	2.42	0.49
1:A:16:ILE:HD11	1:A:275[A]:VAL:HG13	1.95	0.48
1:A:140[B]:MET:HE3	6:A:1225:OLC:H2	1.94	0.48
1:A:29[A]:TRP:CD1	4:A:1217:OLA:H112	2.48	0.48
1:A:32:TRP:CZ2	4:A:1217:OLA:H62	2.48	0.48
1:A:182:PHE:CE1	1:A:187[B]:LEU:HG	2.49	0.47
1:A:32:TRP:CE3	4:A:1217:OLA:H71	2.51	0.46
1:A:1010:LEU:HD12	1:A:1033:MET:HE3	1.99	0.44
1:A:140[A]:MET:HE2	6:A:1225:OLC:H4A	1.99	0.44
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.00	0.44
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.00	0.44
1:A:5:GLY:HA3	6:A:1222:OLC:C21	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG12	1:A:64:ILE:HG23	2.00	0.43
1:A:267:LEU:CD2	6:A:1222:OLC:H22	2.48	0.43
1:A:208:LEU:HG	1:A:225:LEU:HD13	2.01	0.42
4:A:1210:OLA:C15	6:A:1228:OLC:H12	2.45	0.42
6:A:1227:OLC:C2	6:A:1229:OLC:H2	2.51	0.41
1:A:199:ARG:HG2	4:A:1216:OLA:H21	2.03	0.41
1:A:238:ILE:HD11	1:A:287:ILE:HB	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	393/434 (91%)	390 (99%)	3 (1%)	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	321/353 (91%)	321 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	T4E	A	1201	-	23,23,23	2.21	9 (39%)	31,32,32	2.87	9 (29%)
4	OLA	A	1203	-	16,19,19	0.41	0	15,19,19	0.27	0
5	CLR	A	1204	-	31,31,31	0.68	0	48,48,48	0.93	2 (4%)
5	CLR	A	1205	-	31,31,31	0.66	0	48,48,48	0.99	2 (4%)
5	CLR	A	1206	-	31,31,31	0.68	0	48,48,48	0.85	1 (2%)
5	CLR	A	1207	-	31,31,31	0.70	0	48,48,48	0.87	0
4	OLA	A	1208	-	16,19,19	0.41	0	15,19,19	0.26	0
4	OLA	A	1209	-	5,8,19	0.25	0	4,8,19	0.17	0
4	OLA	A	1210	-	16,19,19	0.42	0	15,19,19	0.26	0
4	OLA	A	1211	-	11,14,19	0.36	0	10,14,19	0.31	0
4	OLA	A	1212	-	11,11,19	0.49	0	10,10,19	0.37	0
4	OLA	A	1213	-	7,7,19	0.44	0	6,6,19	0.33	0
4	OLA	A	1214	-	10,10,19	0.54	0	9,9,19	0.34	0
4	OLA	A	1215	-	11,11,19	0.40	0	10,10,19	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OLA	A	1216	-	10,13,19	0.42	0	9,13,19	0.43	0
4	OLA	A	1217	-	15,18,19	0.42	0	14,18,19	0.24	0
4	OLA	A	1218	-	8,11,19	0.46	0	7,11,19	0.41	0
4	OLA	A	1219	-	8,11,19	0.47	0	7,11,19	0.40	0
4	OLA	A	1220	-	11,14,19	0.36	0	10,14,19	0.32	0
6	OLC	A	1221	-	17,17,24	1.09	1 (5%)	18,18,25	1.29	2 (11%)
6	OLC	A	1222	-	17,17,24	1.04	1 (5%)	18,18,25	1.25	2 (11%)
6	OLC	A	1223	-	18,18,24	1.03	2 (11%)	19,19,25	1.39	2 (10%)
6	OLC	A	1224	-	15,15,24	1.04	1 (6%)	16,16,25	1.21	3 (18%)
6	OLC	A	1225	-	16,16,24	1.03	1 (6%)	17,17,25	1.75	3 (17%)
6	OLC	A	1226	-	16,16,24	1.13	1 (6%)	17,17,25	1.53	2 (11%)
6	OLC	A	1227	-	21,21,24	0.90	2 (9%)	22,22,25	1.27	3 (13%)
6	OLC	A	1228	-	24,24,24	0.81	1 (4%)	25,25,25	1.24	3 (12%)
6	OLC	A	1229	-	24,24,24	0.89	2 (8%)	25,25,25	1.26	2 (8%)
6	OLC	A	1230	-	23,23,24	0.98	1 (4%)	24,24,25	1.17	2 (8%)
6	OLC	A	1231	-	21,21,24	0.86	2 (9%)	22,22,25	0.99	2 (9%)
6	OLC	A	1232	-	13,13,24	0.18	0	12,12,25	0.37	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	T4E	A	1201	-	-	0/8/8/8	0/3/3/3
4	OLA	A	1203	-	-	0/15/17/17	0/0/0/0
5	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1205	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1206	-	-	0/10/68/68	0/4/4/4
5	CLR	A	1207	-	-	0/10/68/68	0/4/4/4
4	OLA	A	1208	-	-	0/15/17/17	0/0/0/0
4	OLA	A	1209	-	-	0/4/6/17	0/0/0/0
4	OLA	A	1210	-	-	0/15/17/17	0/0/0/0
4	OLA	A	1211	-	-	0/10/12/17	0/0/0/0
4	OLA	A	1212	-	-	0/9/9/17	0/0/0/0
4	OLA	A	1213	-	-	0/5/5/17	0/0/0/0
4	OLA	A	1214	-	-	0/8/8/17	0/0/0/0
4	OLA	A	1215	-	-	0/9/9/17	0/0/0/0
4	OLA	A	1216	-	-	0/9/11/17	0/0/0/0
4	OLA	A	1217	-	-	0/14/16/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1218	-	-	0/7/9/17	0/0/0/0
4	OLA	A	1219	-	-	0/7/9/17	0/0/0/0
4	OLA	A	1220	-	-	0/10/12/17	0/0/0/0
6	OLC	A	1221	-	-	0/17/17/24	0/0/0/0
6	OLC	A	1222	-	-	0/17/17/24	0/0/0/0
6	OLC	A	1223	-	-	0/18/18/24	0/0/0/0
6	OLC	A	1224	-	-	0/15/15/24	0/0/0/0
6	OLC	A	1225	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1226	-	-	0/16/16/24	0/0/0/0
6	OLC	A	1227	-	-	0/21/21/24	0/0/0/0
6	OLC	A	1228	-	-	0/24/24/24	0/0/0/0
6	OLC	A	1229	-	-	0/24/24/24	0/0/0/0
6	OLC	A	1230	-	-	0/23/23/24	0/0/0/0
6	OLC	A	1231	-	-	0/21/21/24	0/0/0/0
6	OLC	A	1232	-	-	0/11/11/24	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	T4E	N1-N2	-2.77	1.27	1.34
6	A	1223	OLC	O20-C21	-2.23	1.40	1.45
6	A	1229	OLC	O20-C21	-2.09	1.40	1.45
6	A	1231	OLC	O20-C21	-2.07	1.40	1.45
6	A	1227	OLC	O20-C21	-2.06	1.40	1.45
2	A	1201	T4E	C5-N4	2.25	1.38	1.34
2	A	1201	T4E	C7-C6	2.29	1.51	1.49
2	A	1201	T4E	C3-N4	2.36	1.39	1.35
2	A	1201	T4E	C3-N3	2.69	1.39	1.34
2	A	1201	T4E	C11-C12	2.97	1.44	1.38
6	A	1231	OLC	O20-C1	3.05	1.42	1.33
6	A	1227	OLC	O20-C1	3.17	1.42	1.33
6	A	1223	OLC	O20-C1	3.33	1.43	1.33
2	A	1201	T4E	C13-C5	3.34	1.52	1.49
6	A	1229	OLC	O20-C1	3.40	1.43	1.33
6	A	1224	OLC	O20-C1	3.44	1.43	1.33
2	A	1201	T4E	C6-N1	3.51	1.39	1.33
6	A	1228	OLC	O20-C1	3.63	1.44	1.33
6	A	1226	OLC	O20-C1	3.64	1.44	1.33
6	A	1225	OLC	O20-C1	3.75	1.44	1.33
6	A	1222	OLC	O20-C1	3.94	1.44	1.33
6	A	1230	OLC	O20-C1	4.18	1.45	1.33
6	A	1221	OLC	O20-C1	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	T4E	C3-N2	5.20	1.41	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	T4E	N4-C3-N2	-8.22	119.55	125.58
2	A	1201	T4E	C5-C6-N1	-8.12	115.28	119.83
6	A	1225	OLC	O20-C1-O19	-3.62	114.56	123.55
6	A	1229	OLC	O20-C1-O19	-3.12	115.80	123.55
6	A	1227	OLC	O20-C1-O19	-3.03	116.03	123.55
6	A	1226	OLC	O20-C1-O19	-2.89	116.37	123.55
6	A	1223	OLC	O20-C1-O19	-2.78	116.65	123.55
6	A	1231	OLC	O20-C1-O19	-2.72	116.79	123.55
2	A	1201	T4E	C11-C10-C9	-2.54	116.04	118.57
2	A	1201	T4E	C12-C7-C8	-2.41	115.05	118.16
6	A	1230	OLC	C4-C3-C2	-2.40	104.46	113.24
5	A	1205	CLR	C18-C13-C17	-2.34	107.30	111.73
6	A	1222	OLC	O20-C1-O19	-2.33	117.77	123.55
6	A	1221	OLC	O20-C1-O19	-2.25	117.97	123.55
6	A	1228	OLC	O20-C1-O19	-2.16	118.19	123.55
6	A	1227	OLC	C13-C12-C11	-2.07	105.78	113.74
6	A	1224	OLC	O20-C1-O19	-2.06	118.44	123.55
5	A	1204	CLR	C18-C13-C17	-2.02	107.90	111.73
5	A	1206	CLR	C12-C13-C17	2.05	119.64	116.58
5	A	1204	CLR	C12-C13-C17	2.09	119.70	116.58
6	A	1225	OLC	O20-C21-C22	2.10	116.03	105.72
5	A	1205	CLR	C12-C13-C17	2.27	119.97	116.58
6	A	1224	OLC	C21-O20-C1	2.36	124.24	117.13
6	A	1228	OLC	O20-C1-C2	2.67	119.66	111.90
6	A	1224	OLC	O20-C1-C2	2.69	119.73	111.90
6	A	1231	OLC	O20-C1-C2	3.03	120.70	111.90
2	A	1201	T4E	N3-C3-N2	3.39	120.62	117.29
6	A	1221	OLC	O20-C1-C2	3.44	121.90	111.90
6	A	1222	OLC	O20-C1-C2	3.51	122.11	111.90
6	A	1227	OLC	O20-C1-C2	3.53	122.16	111.90
6	A	1223	OLC	O20-C1-C2	3.65	122.51	111.90
6	A	1230	OLC	O20-C1-C2	3.69	122.64	111.90
2	A	1201	T4E	C7-C6-N1	3.89	119.62	114.43
2	A	1201	T4E	C6-N1-N2	4.08	124.91	120.37
6	A	1229	OLC	O20-C1-C2	4.30	124.42	111.90
6	A	1228	OLC	C21-O20-C1	4.36	130.26	117.13
6	A	1226	OLC	O20-C1-C2	4.53	125.08	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	T4E	C3-N2-N1	4.55	120.80	117.39
6	A	1225	OLC	O20-C1-C2	4.94	126.28	111.90
2	A	1201	T4E	C8-C9-C10	5.45	124.13	121.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1204	CLR	1	0
5	A	1205	CLR	3	0
4	A	1208	OLA	2	0
4	A	1210	OLA	4	0
4	A	1212	OLA	1	0
4	A	1216	OLA	1	0
4	A	1217	OLA	3	0
4	A	1219	OLA	1	0
4	A	1220	OLA	1	0
6	A	1222	OLC	4	0
6	A	1225	OLC	6	0
6	A	1227	OLC	2	0
6	A	1228	OLC	2	0
6	A	1229	OLC	12	0
6	A	1230	OLC	6	0
6	A	1231	OLC	6	0
6	A	1232	OLC	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	388/434 (89%)	0.58	43 (11%) 6 7	17, 34, 76, 108	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	7.7
1	A	-1	GLY	7.2
1	A	-2	ASP	6.8
1	A	1059	LYS	4.6
1	A	1105	TYR	4.6
1	A	1062	ARG	4.4
1	A	220	ARG	4.4
1	A	290	TYR	4.3
1	A	305	SER	4.2
1	A	111	ARG	4.1
1	A	304	ARG	3.8
1	A	110	LEU	3.8
1	A	0	ALA	3.7
1	A	302	ILE	3.4
1	A	1019	LYS	3.4
1	A	1028	ASP	3.2
1	A	1060	ASP	3.1
1	A	29[A]	TRP	3.0
1	A	1	PRO	2.9
1	A	206	ARG	2.9
1	A	300[A]	ARG	2.7
1	A	1101	TYR	2.7
1	A	108	ILE	2.7
1	A	1106	LEU	2.6
1	A	1100	ALA	2.6
1	A	1099	ASN	2.5
1	A	1040	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	293	ARG	2.3
1	A	208	LEU	2.3
1	A	84	VAL	2.3
1	A	1104	LYS	2.3
1	A	303	ILE	2.3
1	A	114	GLY	2.3
1	A	88	ALA	2.2
1	A	222	ARG	2.2
1	A	1031	THR	2.2
1	A	274	ILE	2.1
1	A	85	LEU	2.1
1	A	1041	GLN	2.1
1	A	112	TYR	2.1
1	A	1023	ALA	2.0
1	A	161	GLU	2.0
1	A	1039	ASP	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
5	CLR	A	1204	28/28	0.76	0.34	49.58	85,87,88,89	0
6	OLC	A	1232	14/25	0.81	0.17	29.55	45,52,53,54	0
6	OLC	A	1225	17/25	0.65	0.28	18.32	56,66,78,78	0
4	OLA	A	1214	11/20	0.75	0.26	9.63	46,49,54,55	0
4	OLA	A	1220	15/20	0.77	0.20	9.04	56,59,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	1215	12/20	0.74	0.23	8.43	56,57,60,61	0
6	OLC	A	1226	17/25	0.77	0.23	7.64	66,69,75,75	0
6	OLC	A	1223	19/25	0.77	0.28	7.40	37,48,55,56	0
6	OLC	A	1231	22/25	0.73	0.29	6.66	51,61,67,68	0
4	OLA	A	1209	9/20	0.81	0.25	5.89	42,44,57,57	0
4	OLA	A	1203	20/20	0.87	0.22	5.40	61,61,62,62	20
6	OLC	A	1228	25/25	0.57	0.26	4.71	47,66,79,79	0
4	OLA	A	1210	20/20	0.63	0.29	4.69	57,67,70,71	0
6	OLC	A	1227	22/25	0.84	0.20	3.90	49,55,69,69	0
6	OLC	A	1230	24/25	0.70	0.27	3.55	51,59,65,66	0
6	OLC	A	1229	25/25	0.84	0.20	3.54	40,50,65,66	0
4	OLA	A	1218	12/20	0.62	0.36	3.40	48,59,70,71	0
4	OLA	A	1208	20/20	0.84	0.18	3.20	44,52,56,56	0
6	OLC	A	1224	16/25	0.80	0.17	3.09	42,52,63,65	0
6	OLC	A	1221	18/25	0.79	0.17	2.75	64,75,83,84	0
6	OLC	A	1222	18/25	0.73	0.25	2.16	57,70,87,87	0
4	OLA	A	1217	19/20	0.67	0.26	2.12	58,62,68,68	0
4	OLA	A	1212	12/20	0.75	0.25	1.77	44,51,61,62	0
4	OLA	A	1216	14/20	0.61	0.22	0.87	67,76,85,85	0
2	T4E	A	1201	21/21	0.97	0.20	0.82	16,19,21,23	0
3	NA	A	1202	1/1	0.96	0.18	0.58	41,41,41,41	0
5	CLR	A	1205	28/28	0.92	0.12	0.53	25,28,50,52	0
5	CLR	A	1206	28/28	0.93	0.11	-0.39	30,31,36,39	0
5	CLR	A	1207	28/28	0.95	0.10	-0.97	21,25,49,51	0
4	OLA	A	1219	12/20	0.65	0.19	-	61,62,63,63	0
4	OLA	A	1211	15/20	0.69	0.23	-	64,66,75,75	0
4	OLA	A	1213	8/20	0.68	0.18	-	60,62,63,63	0
7	CL	A	1233	1/1	0.83	0.08	-	73,73,73,73	0

## 6.5 Other polymers

There are no such residues in this entry.