



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2017 – 10:29 AM EDT

PDB ID : 5MZJ
Title : Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with theophylline at 2.0Å resolution
Authors : Cheng, R.K.Y.; Segala, E.; Robertson, N.; Deflorian, F.; Dore, A.S.; Errey, J.C.; Fiez-Vandal, C.; Marshall, F.H.; Cooke, R.M.
Deposited on : unknown
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
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-20029824

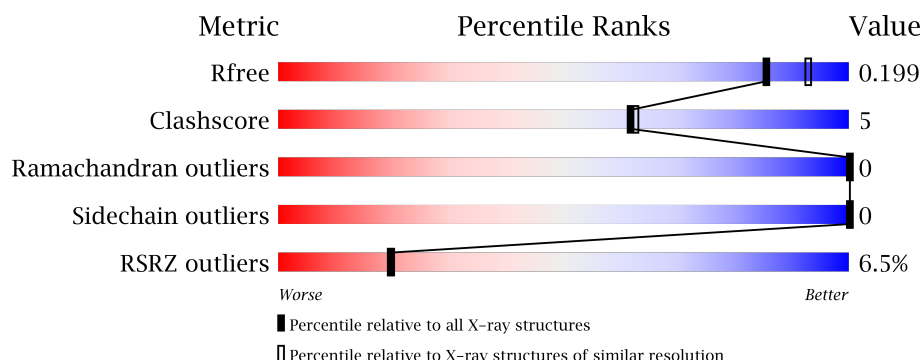
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	<div> <div>6%</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
5	OLA	A	2405	-	-	-	X
5	OLA	A	2406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OLA	A	2407	-	-	-	X
5	OLA	A	2409	-	-	-	X
5	OLA	A	2410	-	-	-	X
5	OLA	A	2411	-	-	-	X
5	OLA	A	2414	-	-	-	X
5	OLA	A	2416	-	-	-	X
5	OLA	A	2419	-	-	-	X
5	OLA	A	2420	-	-	-	X
5	OLA	A	2421	-	-	-	X
5	OLA	A	2423	-	-	-	X
5	OLA	A	2424	-	-	-	X
5	OLA	A	2425	-	-	-	X
5	OLA	A	2426	-	-	-	X
6	OLC	A	2429	-	-	-	X
6	OLC	A	2430	-	-	-	X
6	OLC	A	2431	-	-	-	X
6	OLC	A	2432	-	-	-	X
6	OLC	A	2433	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3813 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	386	Total	C	N	O	S	0	15	0
			3111	2029	526	533	23			

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	conflict	UNP P0ABE7
A	1106	LEU	ARG	conflict	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	GLY	engineered mutation	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274

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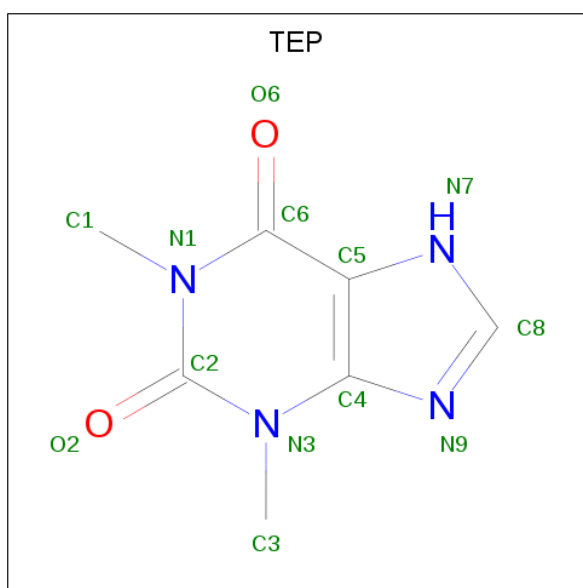
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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

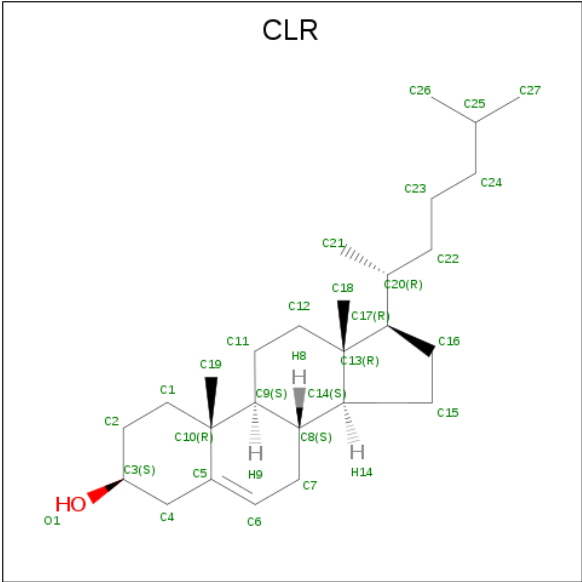
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is THEOPHYLLINE (three-letter code: TEP) (formula: C₇H₈N₄O₂).



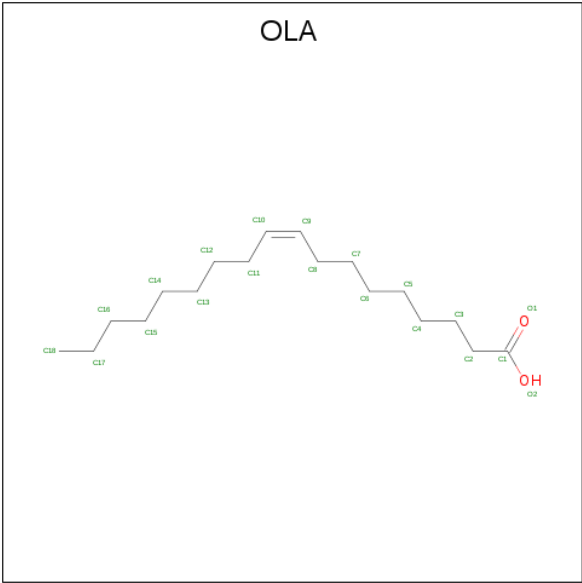
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 7 4 2	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



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 OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



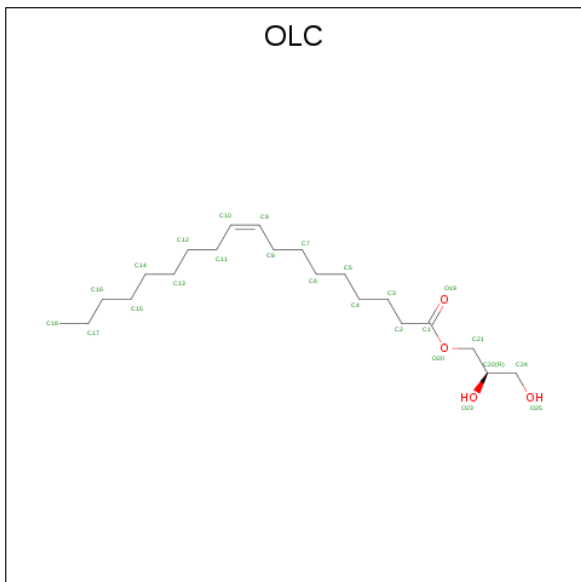
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 8 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 18 16 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 19 17 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C 11 11	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C 15 15	0	0
5	A	1	Total C O 13 11 2	0	0
5	A	1	Total C O 20 18 2	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
			23	19	4		
6	A	1	Total	C	O	0	0
			23	19	4		
6	A	1	Total	C	O	0	0
			23	19	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			16	12	4		

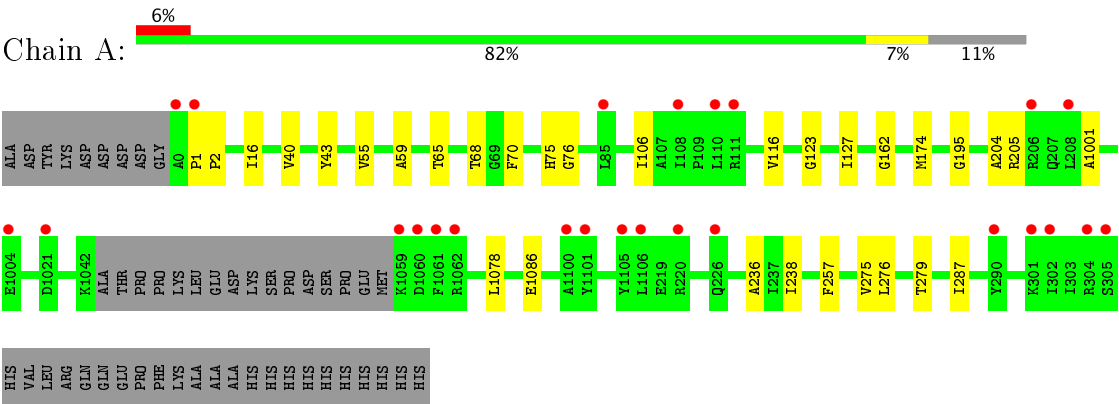
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		

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, α , β , γ	39.25Å 179.87Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.60 – 2.00 33.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.60-2.00) 99.9 (33.60-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.00Å)	Xtriage
Refinement program	PHENIX v1.10.1_2155	Depositor
R, R_{free}	0.182 , 0.204 0.176 , 0.199	Depositor DCC
R_{free} test set	1729 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3813	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.32	0/3174	0.42	0/4312

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	A	3111	0	3184	25	0
2	A	1	0	0	0	0
3	A	13	0	8	0	0
4	A	84	0	138	0	0
5	A	307	0	459	22	0
6	A	136	0	186	7	0
7	A	161	0	0	2	1
All	All	3813	0	3975	39	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 5.

All (39) 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:174[B]:MET:SD	7:A:2563:HOH:O	2.43	0.76
5:A:2405:OLA:H152	6:A:2430:OLC:H12A	1.74	0.69
5:A:2424:OLA:H183	5:A:2425:OLA:C11	2.24	0.68
1:A:162:GLY:O	7:A:2501:HOH:O	2.17	0.59
5:A:2409:OLA:H151	5:A:2416:OLA:H151	1.85	0.58
1:A:68:THR:HG22	6:A:2428:OLC:H21	1.89	0.55
1:A:174[A]:MET:HG3	1:A:257:PHE:HB2	1.90	0.54
5:A:2425:OLA:H71	6:A:2433:OLC:H4	1.90	0.52
1:A:76:GLY:H	5:A:2426:OLA:H21	1.76	0.51
1:A:279[A]:THR:HG23	5:A:2417:OLA:H131	1.93	0.51
1:A:127:ILE:HG12	5:A:2416:OLA:H82	1.92	0.50
5:A:2417:OLA:H82	5:A:2418:OLA:H61	1.94	0.49
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.12	0.49
5:A:2422:OLA:H61	5:A:2424:OLA:H162	1.95	0.49
1:A:238:ILE:HD11	1:A:287:ILE:HB	1.95	0.48
5:A:2409:OLA:H142	5:A:2416:OLA:H151	1.95	0.48
1:A:75:HIS:HB2	5:A:2426:OLA:C1	2.44	0.48
1:A:43:TYR:CE2	6:A:2431:OLC:H24A	2.49	0.47
1:A:16:ILE:HD11	1:A:275[A]:VAL:HG13	1.97	0.47
5:A:2421:OLA:H141	5:A:2421:OLA:H171	1.62	0.47
5:A:2423:OLA:C12	6:A:2427:OLC:H8	2.46	0.46
6:A:2429:OLC:H15	6:A:2430:OLC:H14	1.98	0.46
1:A:65:THR:HG23	5:A:2405:OLA:H41	1.98	0.45
1:A:65:THR:HG22	1:A:70:PHE:CE1	2.52	0.45
5:A:2420:OLA:H81	5:A:2420:OLA:H52	1.49	0.44
1:A:106:ILE:HD11	1:A:204:ALA:HB2	1.99	0.43
1:A:236:ALA:HB1	5:A:2419:OLA:H10	2.00	0.43
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.00	0.43
1:A:195:GLY:HA2	5:A:2406:OLA:H51	2.00	0.43
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	2.01	0.42
1:A:205[B]:ARG:O	1:A:1001:ALA:N	2.51	0.42
5:A:2410:OLA:H132	5:A:2410:OLA:H162	1.56	0.42
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.53	0.42
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.01	0.42
5:A:2405:OLA:H82	6:A:2430:OLC:H9	2.01	0.42
1:A:1:PRO:HA	1:A:2:PRO:HD3	1.92	0.41
1:A:123:GLY:HA3	5:A:2416:OLA:H22	2.01	0.41
1:A:276:LEU:HD21	5:A:2421:OLA:H112	2.03	0.41
5:A:2422:OLA:H41	5:A:2426:OLA:H142	2.02	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)
7:A:2636:HOH:O	7:A:2649:HOH:O[4_555]	2.18	0.02

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	392/434 (90%)	391 (100%)	1 (0%)	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	326/353 (92%)	326 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	230	HIS

5.3.3 RNA [i](#)

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 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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	TEP	A	2401	-	11,14,14	2.60	4 (36%)	13,21,21	3.04	6 (46%)
4	CLR	A	2402	-	31,31,31	0.68	0	48,48,48	1.04	2 (4%)
4	CLR	A	2403	-	31,31,31	0.65	0	48,48,48	0.84	1 (2%)
4	CLR	A	2404	-	31,31,31	0.76	0	48,48,48	0.98	2 (4%)
5	OLA	A	2405	-	16,19,19	0.39	0	15,19,19	0.27	0
5	OLA	A	2406	-	6,9,19	0.26	0	5,9,19	0.23	0
5	OLA	A	2407	-	5,8,19	0.26	0	4,8,19	0.15	0
5	OLA	A	2408	-	14,17,19	0.42	0	13,17,19	0.27	0
5	OLA	A	2409	-	16,19,19	0.45	0	15,19,19	0.23	0
5	OLA	A	2410	-	16,19,19	0.41	0	15,19,19	0.32	0
5	OLA	A	2411	-	8,11,19	0.46	0	7,11,19	0.35	0
5	OLA	A	2412	-	4,7,19	0.27	0	3,7,19	0.13	0
5	OLA	A	2413	-	11,14,19	0.36	0	10,14,19	0.31	0
5	OLA	A	2414	-	7,10,19	0.24	0	6,10,19	0.27	0
5	OLA	A	2415	-	15,18,19	0.43	0	14,18,19	0.25	0
5	OLA	A	2416	-	16,19,19	0.43	0	15,19,19	0.24	0
5	OLA	A	2417	-	11,11,19	0.46	0	10,10,19	0.29	0
5	OLA	A	2418	-	9,9,19	0.44	0	8,8,19	0.44	0
5	OLA	A	2419	-	10,10,19	0.57	0	9,9,19	0.31	0
5	OLA	A	2420	-	11,11,19	0.40	0	10,10,19	0.41	0
5	OLA	A	2421	-	8,8,19	0.46	0	7,7,19	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLA	A	2422	-	7,7,19	0.26	0	6,6,19	0.30	0
5	OLA	A	2423	-	11,14,19	0.41	0	10,14,19	0.38	0
5	OLA	A	2424	-	14,14,19	0.39	0	13,13,19	0.32	0
5	OLA	A	2425	-	9,12,19	0.38	0	8,12,19	0.48	0
5	OLA	A	2426	-	16,19,19	0.45	0	15,19,19	0.20	0
6	OLC	A	2427	-	15,15,24	0.67	0	16,16,25	0.94	1 (6%)
6	OLC	A	2428	-	16,16,24	0.79	0	17,17,25	0.80	0
6	OLC	A	2429	-	22,22,24	0.61	0	23,23,25	0.69	0
6	OLC	A	2430	-	22,22,24	0.68	0	23,23,25	0.78	1 (4%)
6	OLC	A	2431	-	22,22,24	0.64	0	23,23,25	0.75	0
6	OLC	A	2432	-	17,17,24	0.75	0	18,18,25	0.80	0
6	OLC	A	2433	-	15,15,24	0.80	0	16,16,25	0.70	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	TEP	A	2401	-	-	0/0/0/0	0/2/2/2
4	CLR	A	2402	-	-	0/10/68/68	0/4/4/4
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
4	CLR	A	2404	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2405	-	-	0/15/17/17	0/0/0/0
5	OLA	A	2406	-	-	0/5/7/17	0/0/0/0
5	OLA	A	2407	-	-	0/4/6/17	0/0/0/0
5	OLA	A	2408	-	-	0/13/15/17	0/0/0/0
5	OLA	A	2409	-	-	0/15/17/17	0/0/0/0
5	OLA	A	2410	-	-	0/15/17/17	0/0/0/0
5	OLA	A	2411	-	-	0/7/9/17	0/0/0/0
5	OLA	A	2412	-	-	0/3/5/17	0/0/0/0
5	OLA	A	2413	-	-	0/10/12/17	0/0/0/0
5	OLA	A	2414	-	-	0/6/8/17	0/0/0/0
5	OLA	A	2415	-	-	0/14/16/17	0/0/0/0
5	OLA	A	2416	-	-	0/15/17/17	0/0/0/0
5	OLA	A	2417	-	-	0/9/9/17	0/0/0/0
5	OLA	A	2418	-	-	0/7/7/17	0/0/0/0
5	OLA	A	2419	-	-	0/8/8/17	0/0/0/0
5	OLA	A	2420	-	-	0/9/9/17	0/0/0/0
5	OLA	A	2421	-	-	0/6/6/17	0/0/0/0
5	OLA	A	2422	-	-	0/5/5/17	0/0/0/0
5	OLA	A	2423	-	-	0/10/12/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2424	-	-	0/12/12/17	0/0/0/0
5	OLA	A	2425	-	-	0/8/10/17	0/0/0/0
5	OLA	A	2426	-	-	0/15/17/17	0/0/0/0
6	OLC	A	2427	-	-	0/15/15/24	0/0/0/0
6	OLC	A	2428	-	-	0/16/16/24	0/0/0/0
6	OLC	A	2429	-	-	0/22/22/24	0/0/0/0
6	OLC	A	2430	-	-	0/22/22/24	0/0/0/0
6	OLC	A	2431	-	-	0/22/22/24	0/0/0/0
6	OLC	A	2432	-	-	0/17/17/24	0/0/0/0
6	OLC	A	2433	-	-	0/15/15/24	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	TEP	C4-N3	-6.00	1.40	1.45
3	A	2401	TEP	C5-C6	-3.26	1.42	1.51
3	A	2401	TEP	C6-N1	3.28	1.43	1.38
3	A	2401	TEP	C2-N3	3.41	1.41	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	TEP	C6-N1-C2	-3.27	121.52	124.23
3	A	2401	TEP	O2-C2-N3	-2.57	119.16	122.95
4	A	2402	CLR	C18-C13-C17	-2.30	107.37	111.73
4	A	2404	CLR	C18-C13-C17	-2.04	107.87	111.73
6	A	2427	OLC	O20-C1-O19	-2.03	118.52	123.55
6	A	2430	OLC	O20-C1-O19	-2.01	118.56	123.55
4	A	2402	CLR	C12-C13-C17	2.07	119.67	116.58
4	A	2403	CLR	C1-C2-C3	2.11	113.11	110.42
3	A	2401	TEP	N9-C8-N7	2.43	112.70	104.74
4	A	2404	CLR	C12-C13-C17	2.43	120.21	116.58
3	A	2401	TEP	N3-C2-N1	3.16	120.94	117.14
3	A	2401	TEP	C5-C4-N9	5.23	110.01	103.23
3	A	2401	TEP	C5-C4-N3	7.37	119.68	110.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2405	OLA	3	0
5	A	2406	OLA	1	0
5	A	2409	OLA	2	0
5	A	2410	OLA	1	0
5	A	2416	OLA	4	0
5	A	2417	OLA	2	0
5	A	2418	OLA	1	0
5	A	2419	OLA	1	0
5	A	2420	OLA	1	0
5	A	2421	OLA	2	0
5	A	2422	OLA	2	0
5	A	2423	OLA	1	0
5	A	2424	OLA	2	0
5	A	2425	OLA	2	0
5	A	2426	OLA	3	0
6	A	2427	OLC	1	0
6	A	2428	OLC	1	0
6	A	2429	OLC	1	0
6	A	2430	OLC	3	0
6	A	2431	OLC	1	0
6	A	2433	OLC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	208[B]:LEU	C	1001:ALA	N	3.03
1	A	208[A]:LEU	C	1001:ALA	N	3.02
1	A	1106:LEU	C	219:GLU	N	2.85

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, 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	386/434 (88%)	0.15	25 (6%) 20 20	15, 33, 73, 121	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	6.4
1	A	1059	LYS	5.7
1	A	110	LEU	3.9
1	A	1062	ARG	3.9
1	A	1105	TYR	3.6
1	A	208[A]	LEU	3.5
1	A	290	TYR	3.4
1	A	304	ARG	3.4
1	A	0	ALA	3.3
1	A	1060	ASP	3.3
1	A	111	ARG	3.1
1	A	220	ARG	3.1
1	A	1021	ASP	3.0
1	A	305	SER	3.0
1	A	302	ILE	2.8
1	A	1106	LEU	2.7
1	A	206	ARG	2.5
1	A	1101	TYR	2.4
1	A	1100	ALA	2.4
1	A	1	PRO	2.4
1	A	108	ILE	2.2
1	A	226	GLN	2.1
1	A	301	LYS	2.0
1	A	1004	GLU	2.0
1	A	85	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	OLA	A	2410	20/20	0.76	0.25	14.33	53,63,74,74	0
5	OLA	A	2426	20/20	0.58	0.26	12.60	58,66,74,76	0
5	OLA	A	2425	13/20	0.74	0.27	10.57	44,60,76,77	0
5	OLA	A	2424	15/20	0.90	0.15	8.55	49,54,56,56	0
5	OLA	A	2419	11/20	0.89	0.20	7.44	38,46,58,58	0
5	OLA	A	2421	9/20	0.76	0.22	6.52	53,63,66,66	0
5	OLA	A	2409	20/20	0.64	0.24	5.21	46,59,75,75	0
6	OLC	A	2433	16/25	0.89	0.17	5.17	35,42,61,61	0
6	OLC	A	2429	23/25	0.85	0.17	5.17	40,54,82,83	0
5	OLA	A	2423	15/20	0.70	0.19	5.01	54,58,70,71	0
5	OLA	A	2407	9/20	0.87	0.20	4.91	42,46,64,66	0
5	OLA	A	2416	20/20	0.68	0.32	4.81	45,67,72,72	0
6	OLC	A	2431	23/25	0.70	0.28	4.45	46,52,72,78	0
5	OLA	A	2420	12/20	0.79	0.20	4.08	61,62,64,64	0
5	OLA	A	2406	10/20	0.52	0.22	3.74	60,76,84,85	0
5	OLA	A	2411	12/20	0.76	0.32	3.60	45,60,80,83	0
5	OLA	A	2414	11/20	0.83	0.17	3.31	49,52,70,74	0
6	OLC	A	2432	18/25	0.74	0.27	2.63	48,59,78,83	0
6	OLC	A	2430	23/25	0.88	0.16	2.50	39,52,63,70	0
5	OLA	A	2405	20/20	0.88	0.14	2.13	34,54,65,66	0
6	OLC	A	2428	17/25	0.81	0.15	1.94	51,65,83,84	0
5	OLA	A	2415	19/20	0.72	0.23	1.91	54,61,69,70	0
5	OLA	A	2417	12/20	0.81	0.20	1.45	42,54,69,69	0
5	OLA	A	2418	10/20	0.82	0.19	0.96	58,60,64,65	0
3	TEP	A	2401	13/13	0.98	0.19	0.95	18,20,23,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	OLA	A	2408	18/20	0.86	0.15	0.83	47,61,72,76	0
4	CLR	A	2403	28/28	0.94	0.10	0.51	25,30,48,49	0
4	CLR	A	2402	28/28	0.95	0.09	0.01	21,26,51,56	0
4	CLR	A	2404	28/28	0.96	0.08	-0.81	18,25,49,53	0
2	NA	A	2400	1/1	0.97	0.11	-1.16	35,35,35,35	0
5	OLA	A	2422	8/20	0.85	0.14	-	53,65,68,69	0
6	OLC	A	2427	16/25	0.85	0.18	-	38,47,55,60	0
5	OLA	A	2412	8/20	0.81	0.14	-	59,62,64,64	0
5	OLA	A	2413	15/20	0.75	0.23	-	60,68,78,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.