Full wwPDB X-ray Structure Validation Report (i)

Jul 18, 2016 – 04:04 PM EDT

PDB ID	:	5IU8
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with compound 12f at 2.0A resolution
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Deposited on	:	2016-03-17
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

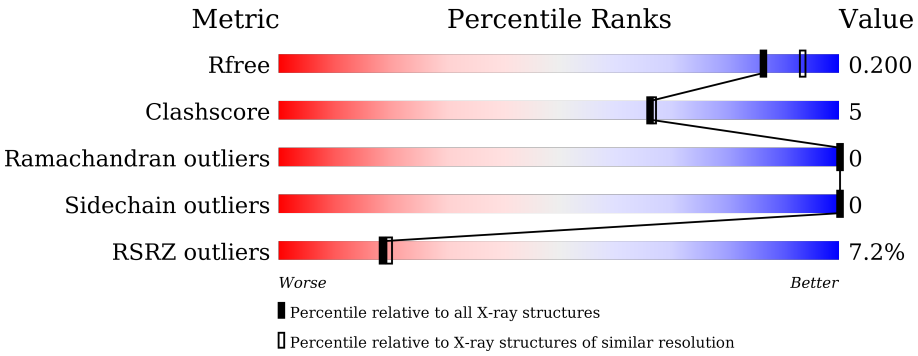
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 <=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	433	6% 82% 7% 11%

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	CLR	A	2404	-	-	-	X
5	CLR	A	2405	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	2406	-	-	-	X
6	OLA	A	2407	-	-	-	X
6	OLA	A	2408	-	-	-	X
6	OLA	A	2409	-	-	-	X
6	OLA	A	2410	-	-	-	X
6	OLA	A	2412	-	-	-	X
6	OLA	A	2413	-	-	-	X
6	OLA	A	2414	-	-	-	X
6	OLA	A	2415	-	-	-	X
6	OLA	A	2416	-	-	X	X
6	OLA	A	2417	-	-	-	X
6	OLA	A	2418	-	-	X	X
6	OLA	A	2423	-	-	-	X
6	OLA	A	2424	-	-	-	X
6	OLA	A	2425	-	-	-	X
7	OLB	A	2426	-	-	-	X
7	OLB	A	2427	-	-	-	X
8	OLC	A	2428	-	-	-	X
8	OLC	A	2430	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3831 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
			Total	C	N	O	S			
1	A	387	3131	2040	526	542	23	0	20	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	316	ALA	-	expression tag	UNP P29274
A	317	ALA	-	expression tag	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274

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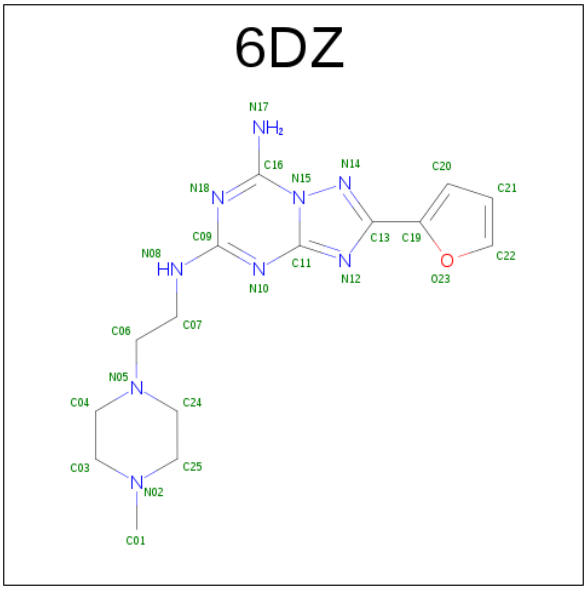
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
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).

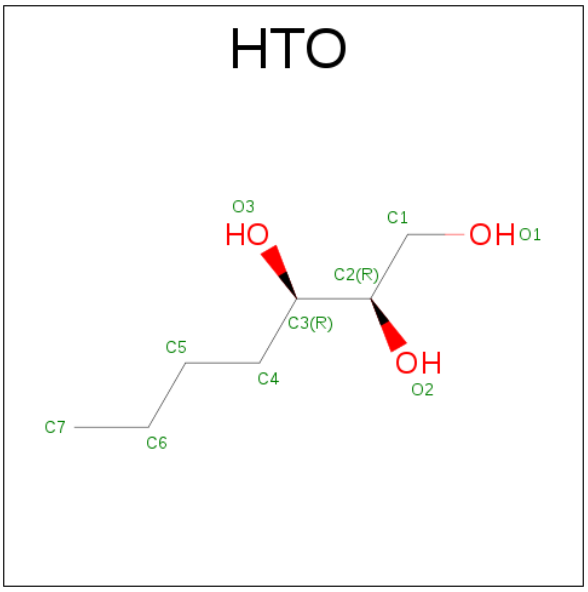
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 2-(furan-2-yl)-N 5 -[2-(4-methylpiperazin-1-yl)ethyl][1,2,4]triazolo[1,5-a][1,3,5] triazine-5,7-diamine (three-letter code: 6DZ) (formula: $C_{15}H_{21}N_9O$).



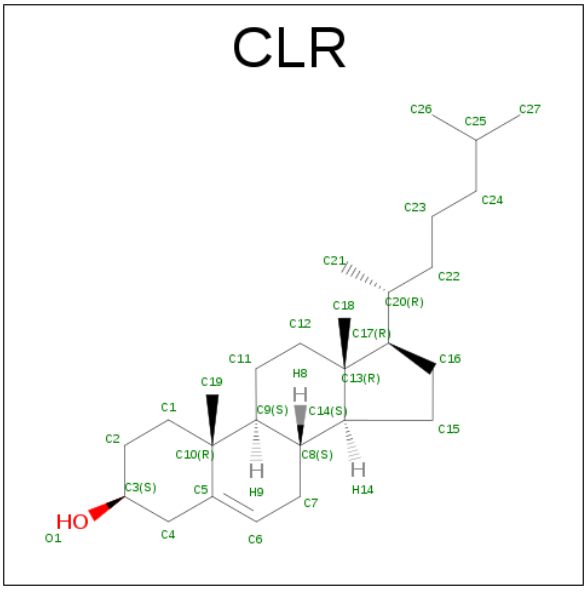
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 25 15 9 1	0	0

- Molecule 4 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 7 3	0	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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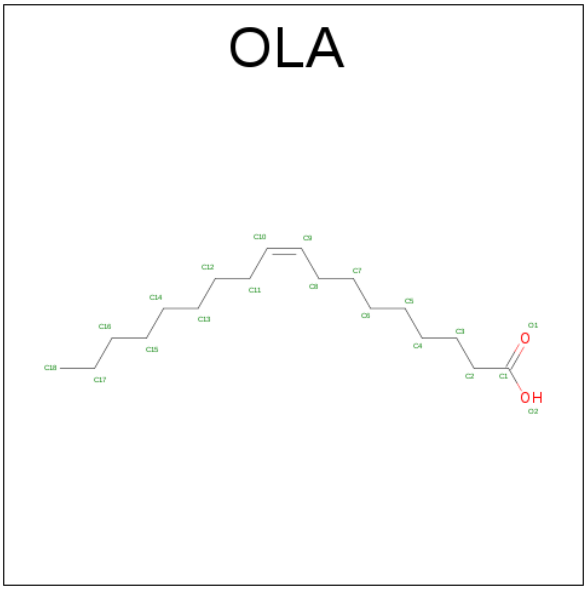
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 28 27 1	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



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

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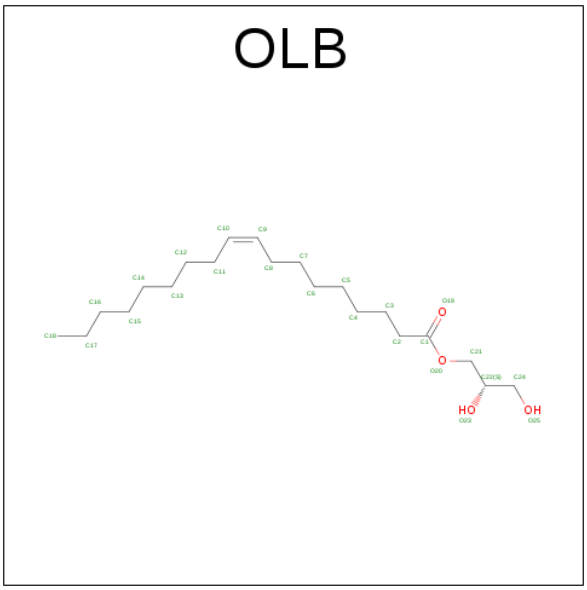
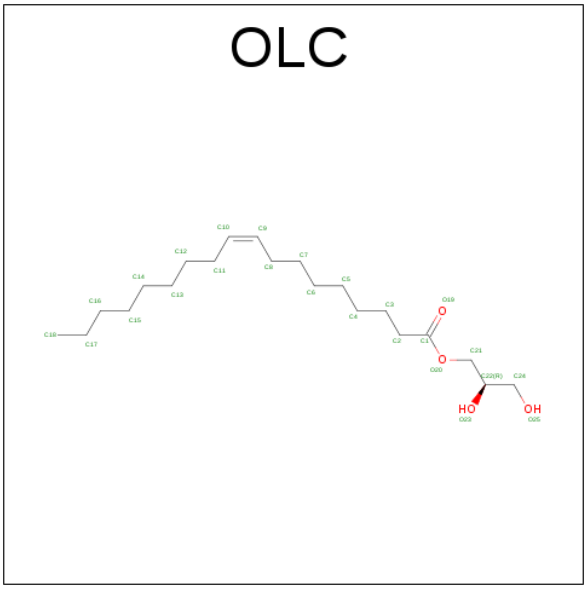
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 14 12 2	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C 8 8	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C 12 12	0	0
6	A	1	Total C 9 9	0	0
6	A	1	Total C 9 9	0	0
6	A	1	Total C 12 12	0	0
6	A	1	Total C O 20 18 2	0	0

- Molecule 7 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 12 4	0	0
7	A	1	Total C O 21 17 4	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 18 14 4	0	0
8	A	1	Total C O 20 16 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	A	1	Total C O 17 13 4	0	0

- Molecule 9 is water.

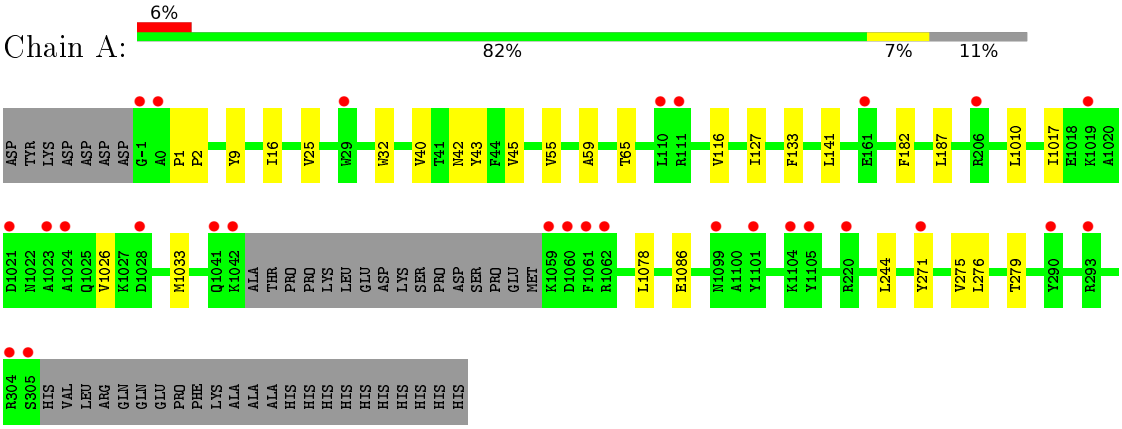
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	157	Total O 158 158	0	1

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,Adenosine receptor A2a

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.31Å 179.54Å 139.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 2.00 33.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.67-2.00) 99.6 (33.67-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.181 , 0.200 0.181 , 0.200	Depositor DCC
R_{free} test set	1703 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3831	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLB, OLC, HTO, NA, 6DZ, 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	0.24	0/3201	0.35	0/4353

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	3131	0	3212	21	0
2	A	1	0	0	0	0
3	A	25	0	0	0	0
4	A	10	0	16	0	0
5	A	112	0	184	4	0
6	A	277	0	425	22	0
7	A	37	0	50	1	0
8	A	80	0	112	2	0
9	A	158	0	0	0	0
All	All	3831	0	3999	38	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 5.

All (38) 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:2418:OLA:H181	6:A:2419:OLA:H181	1.59	0.84
5:A:2406:CLR:H192	6:A:2418:OLA:H31	1.73	0.69
6:A:2416:OLA:C6	6:A:2418:OLA:H71	2.25	0.66
6:A:2416:OLA:H62	6:A:2418:OLA:H71	1.77	0.65
6:A:2418:OLA:H181	6:A:2419:OLA:C18	2.25	0.64
6:A:2416:OLA:H41	6:A:2418:OLA:H42	1.83	0.60
5:A:2403:CLR:H72	5:A:2406:CLR:H12	1.87	0.55
5:A:2406:CLR:H271	6:A:2418:OLA:H183	1.89	0.55
6:A:2416:OLA:H31	6:A:2418:OLA:H21	1.88	0.55
1:A:16:ILE:HD11	1:A:275[A]:VAL:HG13	1.88	0.54
1:A:32:TRP:CE3	6:A:2414:OLA:H71	2.43	0.54
1:A:127:ILE:HD13	6:A:2410:OLA:H72	1.90	0.53
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.89	0.53
1:A:244[B]:LEU:HG	6:A:2423:OLA:H161	1.91	0.53
6:A:2410:OLA:H142	6:A:2416:OLA:C18	2.42	0.49
1:A:141[A]:LEU:HD22	6:A:2416:OLA:H81	1.95	0.49
6:A:2410:OLA:H111	6:A:2413:OLA:C12	2.43	0.49
6:A:2419:OLA:H142	8:A:2430:OLC:H7	1.95	0.48
1:A:182:PHE:CE1	1:A:187[B]:LEU:HG	2.49	0.48
6:A:2416:OLA:H61	6:A:2418:OLA:H71	1.96	0.47
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.97	0.47
6:A:2410:OLA:H142	6:A:2416:OLA:H181	1.97	0.46
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.98	0.46
1:A:65:THR:HG21	7:A:2427:OLB:H4A	1.97	0.45
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.51	0.45
1:A:1010:LEU:HD12	1:A:1033:MET:HE3	1.99	0.44
6:A:2416:OLA:C3	6:A:2418:OLA:H21	2.48	0.44
1:A:133:PHE:CD2	6:A:2418:OLA:H182	2.53	0.44
1:A:9:TYR:CE1	1:A:271:TYR:HD2	2.36	0.44
1:A:25:VAL:HG22	6:A:2414:OLA:H132	2.00	0.43
6:A:2409:OLA:H72	6:A:2409:OLA:H41	1.50	0.43
1:A:1:PRO:HA	1:A:2:PRO:HD3	1.93	0.42
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.20	0.42
5:A:2403:CLR:H25	8:A:2430:OLC:H18B	2.03	0.41
1:A:32:TRP:CD2	6:A:2414:OLA:H71	2.56	0.40
1:A:276:LEU:O	1:A:279[B]:THR:OG1	2.35	0.40
1:A:1017:ILE:HG23	1:A:1026:VAL:HG13	2.03	0.40
1:A:42:ASN:HA	1:A:45:VAL:HB	2.03	0.40

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	A	403/433 (93%)	401 (100%)	2 (0%)	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	331/353 (94%)	331 (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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	6DZ	A	2401	-	21,28,28	3.52	9 (42%)	23,39,39	2.81	9 (39%)
4	HTO	A	2402	-	9,9,9	0.49	0	8,10,10	3.73	3 (37%)
5	CLR	A	2403	-	31,31,31	0.63	0	48,48,48	1.00	2 (4%)
5	CLR	A	2404	-	31,31,31	0.65	0	48,48,48	0.90	1 (2%)
5	CLR	A	2405	-	31,31,31	0.66	0	48,48,48	0.85	0
5	CLR	A	2406	-	31,31,31	0.66	0	48,48,48	1.00	2 (4%)
6	OLA	A	2407	-	11,14,19	0.35	0	10,14,19	0.29	0
6	OLA	A	2408	-	5,8,19	0.26	0	5,8,19	0.16	0
6	OLA	A	2409	-	14,17,19	0.40	0	14,17,19	0.25	0
6	OLA	A	2410	-	16,19,19	0.42	0	16,19,19	0.24	0
6	OLA	A	2411	-	11,14,19	0.35	0	10,14,19	0.29	0
6	OLA	A	2412	-	8,11,19	0.46	0	8,11,19	0.38	0
6	OLA	A	2413	-	10,13,19	0.42	0	10,13,19	0.37	0
6	OLA	A	2414	-	15,18,19	0.41	0	15,18,19	0.24	0
6	OLA	A	2415	-	7,10,19	0.24	0	7,10,19	0.32	0
6	OLA	A	2416	-	16,19,19	0.41	0	16,19,19	0.30	0
6	OLA	A	2417	-	10,13,19	0.42	0	10,13,19	0.42	0
6	OLA	A	2418	-	16,19,19	0.41	0	16,19,19	0.34	0
6	OLA	A	2419	-	7,7,19	0.46	0	6,6,19	0.21	0
6	OLA	A	2420	-	16,19,19	0.42	0	16,19,19	0.24	0
6	OLA	A	2421	-	11,11,19	0.48	0	10,10,19	0.36	0
6	OLA	A	2422	-	8,8,19	0.46	0	7,7,19	0.18	0
6	OLA	A	2423	-	8,8,19	0.45	0	7,7,19	0.19	0
6	OLA	A	2424	-	11,11,19	0.48	0	10,10,19	0.34	0
6	OLA	A	2425	-	16,19,19	0.42	0	16,19,19	0.25	0
7	OLB	A	2426	-	15,15,24	0.99	2 (13%)	16,16,25	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	OLB	A	2427	-	20,20,24	0.87	2 (10%)	21,21,25	0.86	1 (4%)
8	OLC	A	2428	-	17,17,24	0.95	2 (11%)	18,18,25	0.94	1 (5%)
8	OLC	A	2429	-	19,19,24	0.89	2 (10%)	19,20,25	0.72	1 (5%)
8	OLC	A	2430	-	24,24,24	0.81	2 (8%)	25,25,25	0.86	1 (4%)
8	OLC	A	2431	-	16,16,24	0.99	2 (12%)	17,17,25	0.91	1 (5%)

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	6DZ	A	2401	-	-	0/6/20/20	0/3/4/4
4	HTO	A	2402	-	-	0/10/10/10	0/0/0/0
5	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	CLR	A	2404	-	-	0/10/68/68	0/4/4/4
5	CLR	A	2405	-	-	0/10/68/68	0/4/4/4
5	CLR	A	2406	-	-	0/10/68/68	0/4/4/4
6	OLA	A	2407	-	-	0/10/12/17	0/0/0/0
6	OLA	A	2408	-	-	0/4/6/17	0/0/0/0
6	OLA	A	2409	-	-	0/13/15/17	0/0/0/0
6	OLA	A	2410	-	-	0/15/17/17	0/0/0/0
6	OLA	A	2411	-	-	0/10/12/17	0/0/0/0
6	OLA	A	2412	-	-	0/7/9/17	0/0/0/0
6	OLA	A	2413	-	-	0/9/11/17	0/0/0/0
6	OLA	A	2414	-	-	0/14/16/17	0/0/0/0
6	OLA	A	2415	-	-	0/6/8/17	0/0/0/0
6	OLA	A	2416	-	-	0/15/17/17	0/0/0/0
6	OLA	A	2417	-	-	0/9/11/17	0/0/0/0
6	OLA	A	2418	-	-	0/15/17/17	0/0/0/0
6	OLA	A	2419	-	-	0/5/5/17	0/0/0/0
6	OLA	A	2420	-	-	0/15/17/17	0/0/0/0
6	OLA	A	2421	-	-	0/9/9/17	0/0/0/0
6	OLA	A	2422	-	-	0/6/6/17	0/0/0/0
6	OLA	A	2423	-	-	0/6/6/17	0/0/0/0
6	OLA	A	2424	-	-	0/9/9/17	0/0/0/0
6	OLA	A	2425	-	-	0/15/17/17	0/0/0/0
7	OLB	A	2426	-	-	0/15/15/24	0/0/0/0
7	OLB	A	2427	-	-	0/20/20/24	0/0/0/0
8	OLC	A	2428	-	-	0/17/17/24	0/0/0/0
8	OLC	A	2429	-	-	0/19/19/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	2430	-	-	0/24/24/24	0/0/0/0
8	OLC	A	2431	-	-	0/16/16/24	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	6DZ	C06-N05	-8.14	1.28	1.47
3	A	2401	6DZ	C01-N02	-7.63	1.28	1.46
3	A	2401	6DZ	C25-N02	-4.76	1.36	1.46
3	A	2401	6DZ	C03-N02	-4.75	1.36	1.46
3	A	2401	6DZ	C04-N05	-4.26	1.35	1.47
3	A	2401	6DZ	C24-N05	-4.17	1.35	1.47
8	A	2431	OLC	O20-C21	-2.23	1.40	1.45
7	A	2426	OLB	O20-C21	-2.23	1.40	1.45
8	A	2428	OLC	O20-C21	-2.19	1.40	1.45
8	A	2429	OLC	O20-C21	-2.17	1.40	1.45
8	A	2430	OLC	O20-C21	-2.15	1.40	1.45
7	A	2427	OLB	O20-C21	-2.13	1.40	1.45
7	A	2426	OLB	O20-C1	2.35	1.40	1.33
8	A	2428	OLC	O20-C1	2.36	1.40	1.33
7	A	2427	OLB	O20-C1	2.37	1.40	1.33
8	A	2429	OLC	O20-C1	2.38	1.40	1.33
8	A	2431	OLC	O20-C1	2.39	1.40	1.33
8	A	2430	OLC	O20-C1	2.41	1.40	1.33
3	A	2401	6DZ	C11-N12	2.46	1.39	1.35
3	A	2401	6DZ	C16-N17	4.58	1.42	1.34
3	A	2401	6DZ	C09-N08	4.85	1.42	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2401	6DZ	N14-C13-N12	-9.96	108.31	114.63
4	A	2402	HTO	C5-C4-C3	-8.80	98.76	114.16
3	A	2401	6DZ	N10-C09-N18	-3.89	120.37	126.18
3	A	2401	6DZ	C07-N08-C09	-2.99	118.52	123.62
4	A	2402	HTO	O1-C1-C2	-2.78	104.90	111.07
3	A	2401	6DZ	N18-C16-N15	-2.37	119.70	124.53
5	A	2403	CLR	C18-C13-C17	-2.11	107.76	111.76
5	A	2406	CLR	C18-C13-C17	-2.04	107.88	111.76
5	A	2404	CLR	C12-C13-C17	2.08	119.63	116.58
3	A	2401	6DZ	N17-C16-N18	2.14	120.25	117.06
8	A	2429	OLC	O20-C1-C2	2.19	118.58	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2401	6DZ	C19-C13-N12	2.24	126.62	123.76
5	A	2406	CLR	C12-C13-C17	2.26	119.89	116.58
5	A	2403	CLR	C12-C13-C17	2.26	119.89	116.58
7	A	2426	OLB	O20-C1-C2	2.42	119.31	111.85
8	A	2431	OLC	O20-C1-C2	2.59	119.81	111.85
8	A	2428	OLC	O20-C1-C2	2.68	120.11	111.85
3	A	2401	6DZ	C09-N10-C11	2.75	119.48	115.54
7	A	2427	OLB	O20-C1-C2	2.80	120.47	111.85
8	A	2430	OLC	O20-C1-C2	2.92	120.84	111.85
3	A	2401	6DZ	C25-N02-C03	3.13	113.75	109.50
3	A	2401	6DZ	N17-C16-N15	3.13	120.04	117.87
4	A	2402	HTO	O3-C3-C2	4.45	118.68	109.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2403	CLR	2	0
5	A	2406	CLR	3	0
6	A	2409	OLA	1	0
6	A	2410	OLA	4	0
6	A	2413	OLA	1	0
6	A	2414	OLA	3	0
6	A	2416	OLA	9	0
6	A	2418	OLA	11	0
6	A	2419	OLA	3	0
6	A	2423	OLA	1	0
7	A	2427	OLB	1	0
8	A	2430	OLC	2	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^{th} 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	387/433 (89%)	0.28	28 (7%)	18	20	11, 24, 70, 108	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	7.7
1	A	1059	LYS	6.2
1	A	1021	ASP	4.7
1	A	-1	GLY	4.4
1	A	305	SER	4.4
1	A	1105	TYR	4.4
1	A	1062	ARG	4.1
1	A	1023	ALA	3.8
1	A	304	ARG	3.8
1	A	220	ARG	3.3
1	A	1060	ASP	3.3
1	A	29	TRP	3.2
1	A	110	LEU	3.1
1	A	0	ALA	3.1
1	A	206	ARG	3.0
1	A	1019	LYS	2.8
1	A	290	TYR	2.8
1	A	111	ARG	2.8
1	A	1101	TYR	2.8
1	A	293	ARG	2.7
1	A	1028	ASP	2.7
1	A	271	TYR	2.6
1	A	161	GLU	2.6
1	A	1099	ASN	2.2
1	A	1024	ALA	2.2
1	A	1104	LYS	2.1
1	A	1041	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1042	LYS	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^{th} 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	CLR	A	2406	28/28	0.46	0.48	34.86	104,112,117,118	0
8	OLC	A	2428	18/25	0.81	0.24	11.65	42,52,60,63	0
6	OLA	A	2407	15/20	0.73	0.27	11.05	60,66,79,80	0
6	OLA	A	2417	14/20	0.78	0.23	9.81	58,59,65,66	0
6	OLA	A	2424	12/20	0.85	0.20	7.89	39,42,45,48	0
6	OLA	A	2425	20/20	0.81	0.19	7.51	39,51,62,63	0
6	OLA	A	2415	11/20	0.76	0.21	7.44	52,65,82,84	0
6	OLA	A	2416	20/20	0.78	0.19	6.99	39,50,60,64	0
7	OLB	A	2426	16/25	0.73	0.22	6.40	54,69,75,75	0
6	OLA	A	2418	20/20	0.76	0.21	6.17	45,50,74,76	0
8	OLC	A	2430	25/25	0.70	0.28	5.85	42,52,69,69	0
6	OLA	A	2410	20/20	0.66	0.23	5.26	40,53,62,64	0
7	OLB	A	2427	21/25	0.84	0.22	4.73	37,46,55,64	0
6	OLA	A	2413	14/20	0.64	0.23	4.66	47,60,63,64	0
6	OLA	A	2423	9/20	0.77	0.15	3.42	52,56,57,57	0
6	OLA	A	2408	9/20	0.89	0.18	3.34	35,39,53,57	0
6	OLA	A	2409	18/20	0.75	0.23	2.84	47,52,60,60	0
5	CLR	A	2404	28/28	0.92	0.14	2.65	25,29,38,40	0
6	OLA	A	2412	12/20	0.69	0.27	2.61	36,53,63,63	0
6	OLA	A	2414	19/20	0.74	0.23	2.09	54,57,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CLR	A	2405	28/28	0.93	0.12	2.05	15,23,44,46	0
6	OLA	A	2421	12/20	0.75	0.20	1.72	37,43,53,56	0
8	OLC	A	2431	17/25	0.83	0.22	1.66	45,53,70,71	0
6	OLA	A	2422	9/20	0.75	0.21	1.66	56,56,59,59	0
5	CLR	A	2403	28/28	0.93	0.13	1.49	18,24,45,49	0
4	HTO	A	2402	10/10	0.92	0.14	1.23	28,32,34,35	0
2	NA	A	2400	1/1	0.96	0.17	1.13	32,32,32,32	0
8	OLC	A	2429	20/25	0.81	0.18	1.10	35,40,68,70	0
3	6DZ	A	2401	25/25	0.96	0.14	-0.10	13,16,39,41	0
6	OLA	A	2411	15/20	0.69	0.22	-	68,69,77,78	0
6	OLA	A	2420	20/20	0.66	0.24	-	61,64,70,71	0
6	OLA	A	2419	8/20	0.79	0.17	-	41,42,44,47	0

6.5 Other polymers

There are no such residues in this entry.