



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 PM GMT

PDB ID : 4NC3  
Title : Crystal structure of the 5-HT<sub>2B</sub> receptor solved using serial femtosecond crystallography in lipidic cubic phase.  
Authors : Liu, W.; Wacker, D.; Gati, C.; Han, G.W.; James, D.; Wang, D.; Nelson, G.; Weierstall, U.; Katritch, V.; Barty, A.; Zatsepin, N.A.; Li, D.; Messerschmidt, M.; Boutet, S.; Williams, G.J.; Koglin, J.E.; Seibert, M.M.; Wang, C.; Shah, S.T.A.; Basu, S.; Fromme, R.; Kupitz, C.; Rendek, K.N.; Grotjohann, I.; Fromme, P.; Kirian, R.A.; Beyerlein, K.R.; White, T.A.; Chapman, H.N.; Caffrey, M.; Spence, J.C.H.; Stevens, R.C.; Cherezov, V.; GPCR Network (GPCR)  
Deposited on : 2013-10-23  
Resolution : 2.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

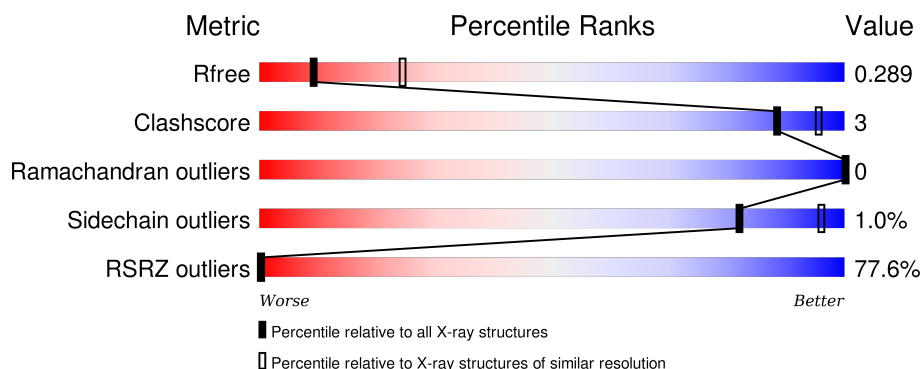
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	430	

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
2	PLM	A	1201	-	-	-	X
5	OLC	A	1204	-	-	-	X
5	OLC	A	1205	-	-	-	X
5	OLC	A	1208	-	-	-	X
6	PEG	A	1206	-	-	-	X
8	OLA	A	1210	-	-	-	X
8	OLA	A	1211	-	-	-	X
8	OLA	A	1212	-	-	-	X
9	DGA	A	1213	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3123 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.

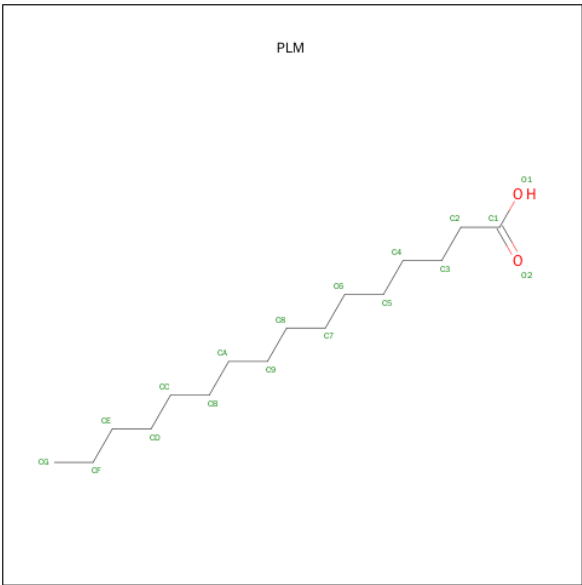
- Molecule 1 is a protein called Chimera protein of human 5-hydroxytryptamine receptor 2B and E. Coli soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	1	0
			2839	1867	451	505	16			

There are 23 discrepancies between the modelled and reference sequences:

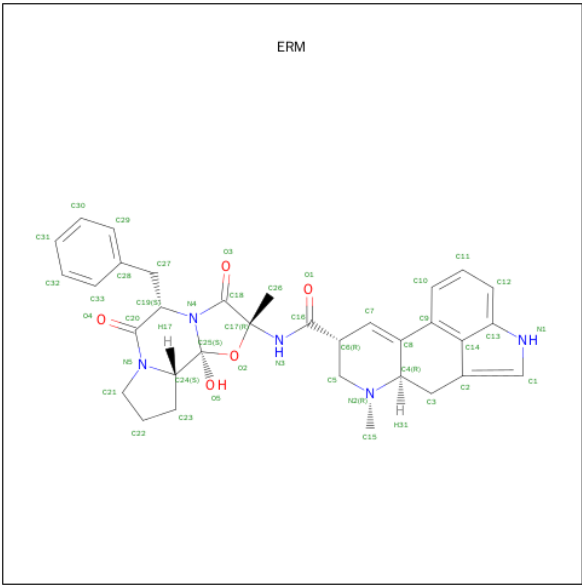
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASP	-	EXPRESSION TAG	UNP P41595
A	27	TYR	-	EXPRESSION TAG	UNP P41595
A	28	LYS	-	EXPRESSION TAG	UNP P41595
A	29	ASP	-	EXPRESSION TAG	UNP P41595
A	30	ASP	-	EXPRESSION TAG	UNP P41595
A	31	ASP	-	EXPRESSION TAG	UNP P41595
A	32	ASP	-	EXPRESSION TAG	UNP P41595
A	33	GLY	-	EXPRESSION TAG	UNP P41595
A	34	ALA	-	EXPRESSION TAG	UNP P41595
A	35	PRO	-	EXPRESSION TAG	UNP P41595
A	144	TRP	MET	engineered mutation	UNP P41595
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	406	GLY	-	EXPRESSION TAG	UNP P41595
A	407	ARG	-	EXPRESSION TAG	UNP P41595
A	408	PRO	-	EXPRESSION TAG	UNP P41595
A	409	LEU	-	EXPRESSION TAG	UNP P41595
A	410	GLU	-	EXPRESSION TAG	UNP P41595
A	411	VAL	-	EXPRESSION TAG	UNP P41595
A	412	LEU	-	EXPRESSION TAG	UNP P41595
A	413	PHE	-	EXPRESSION TAG	UNP P41595
A	414	GLN	-	EXPRESSION TAG	UNP P41595

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



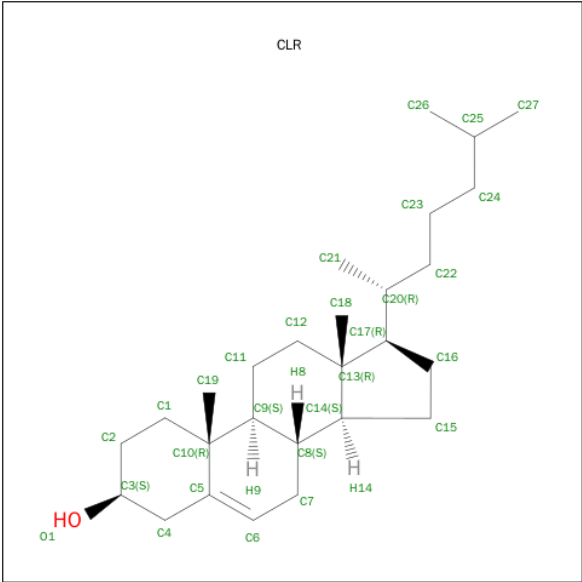
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is ERGOTAMINE (three-letter code: ERM) (formula:  $C_{33}H_{35}N_5O_5$ ).



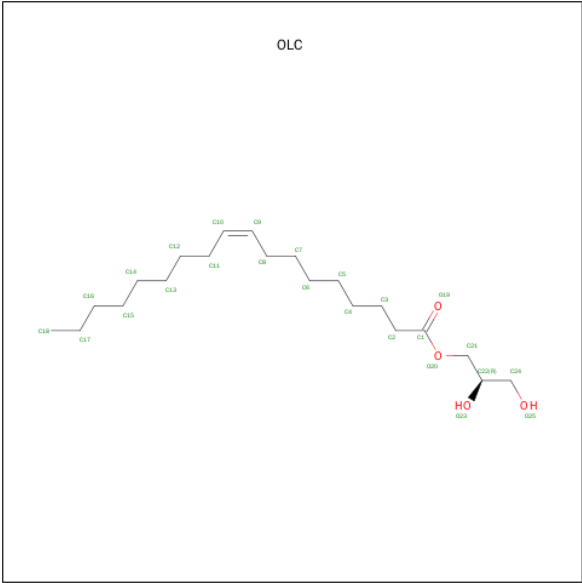
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	5	5		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



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

- Molecule 5 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>).



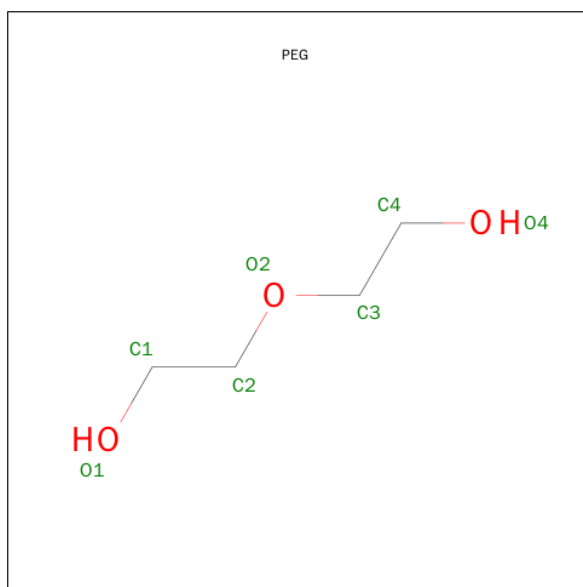
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	15	4		
5	A	1	Total	C	O	0	0
			16	12	4		

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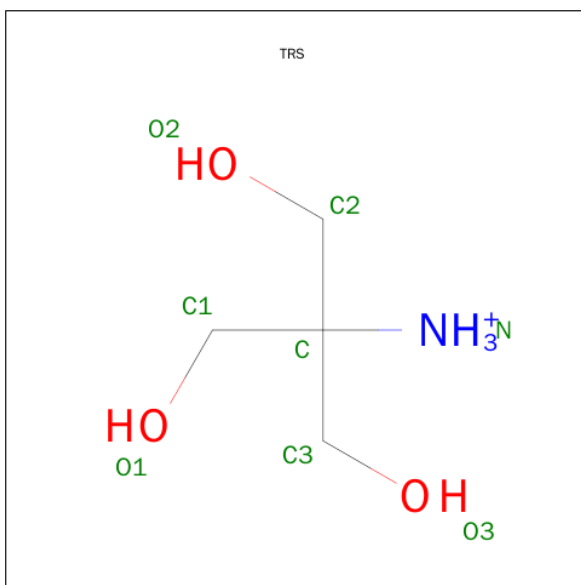
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			19	15	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



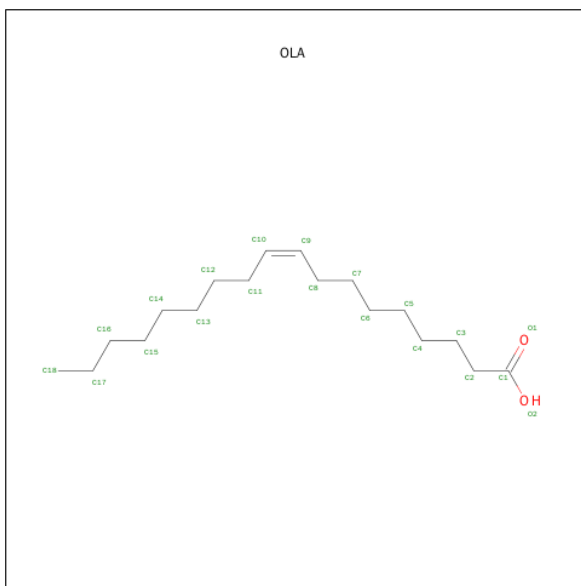
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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

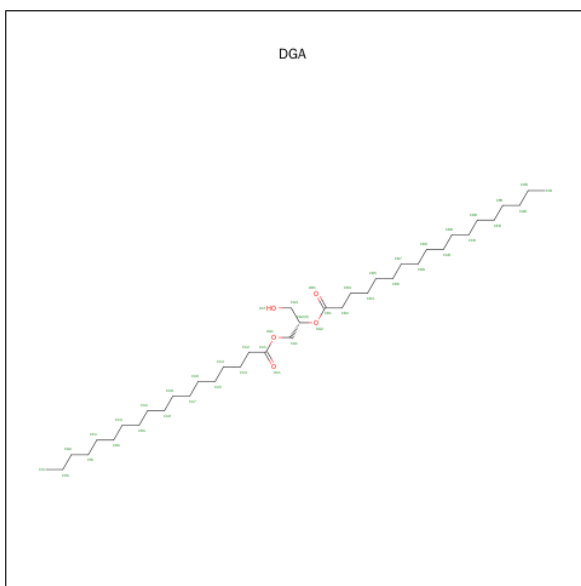
- Molecule 8 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C			0	0
			10	10				
8	A	1	Total	C	O		0	0
			20	18	2			
8	A	1	Total	C	O		0	0
			19	17	2			



- Molecule 9 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			26	21	5		
9	A	1	Total	C	O	0	0
			20	15	5		

- Molecule 10 is water.

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

### 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: Chimera protein of human 5-hydroxytryptamine receptor 2B and E. Coli soluble cytochrome b562



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.50Å 122.20Å 168.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.68 – 2.80 34.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.68-2.80) 93.5 (34.68-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.227 , 0.270 0.249 , 0.289	Depositor DCC
$R_{free}$ test set	815 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 87.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 20949 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, DGA, ERM, TRS, PEG, PLM, 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	0.22	0/2903	0.36	0/3965

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	2839	0	2823	13	0
2	A	17	0	31	0	0
3	A	43	0	35	0	0
4	A	28	0	46	1	0
5	A	79	0	111	3	0
6	A	7	0	9	0	0
7	A	8	0	12	0	0
8	A	49	0	76	0	0
9	A	46	0	56	0	0
10	A	7	0	0	0	0
All	All	3123	0	3199	16	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 3.

All (16) 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:128:CYS:SG	1:A:195:ILE:CD1	2.84	0.65
1:A:201:ASN:HB3	1:A:202:PRO:HD3	1.84	0.58
1:A:188:ILE:N	1:A:189:PRO:CD	2.70	0.55
1:A:376:ASN:HB3	1:A:377:PRO:HD3	1.92	0.52
4:A:1203:CLR:H183	4:A:1203:CLR:H212	1.91	0.51
5:A:1207:OLC:C14	5:A:1207:OLC:H18A	2.42	0.49
1:A:1007:TRP:C	1:A:1007:TRP:CD1	2.86	0.48
1:A:135:ASP:OD1	1:A:135:ASP:C	2.53	0.47
1:A:237:TYR:HA	5:A:1204:OLC:H22	1.97	0.46
1:A:201:ASN:HB3	1:A:202:PRO:CD	2.47	0.44
1:A:66:ILE:HB	1:A:67:PRO:HD3	2.00	0.44
5:A:1207:OLC:H14	5:A:1207:OLC:H18A	1.99	0.43
1:A:338:CYS:N	1:A:339:PRO:CD	2.82	0.42
1:A:228:THR:HB	1:A:229:PRO:CD	2.50	0.42
1:A:108:MET:HB2	1:A:109:PRO:HD3	2.02	0.42
1:A:190:VAL:HB	1:A:191:PRO:CD	2.50	0.41

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	365/430 (85%)	352 (96%)	13 (4%)	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	293/371 (79%)	290 (99%)	3 (1%)	82	96

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

Mol	Chain	Res	Type
1	A	115	ILE
1	A	1018	GLU
1	A	1094	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLM	A	1201	1	16,16,17	0.81	1 (6%)	15,15,17	0.57	0
3	ERM	A	1202	-	47,50,50	1.34	8 (17%)	49,79,79	1.64	9 (18%)
4	CLR	A	1203	-	31,31,31	0.61	0	48,48,48	1.53	11 (22%)
5	OLC	A	1204	-	18,18,24	1.19	2 (11%)	19,19,25	1.07	1 (5%)
5	OLC	A	1205	-	15,15,24	1.21	2 (13%)	16,16,25	1.08	1 (6%)
6	PEG	A	1206	-	6,6,6	0.58	0	5,5,5	0.25	0
5	OLC	A	1207	-	24,24,24	1.03	2 (8%)	25,25,25	1.14	2 (8%)
5	OLC	A	1208	-	18,18,24	1.18	2 (11%)	19,19,25	1.15	1 (5%)
7	TRS	A	1209	-	7,7,7	0.96	1 (14%)	9,9,9	0.68	0
8	OLA	A	1210	-	9,9,19	0.93	1 (11%)	8,8,19	0.69	0
8	OLA	A	1211	-	16,19,19	0.72	1 (6%)	16,19,19	0.61	0
8	OLA	A	1212	-	15,18,19	0.74	1 (6%)	15,18,19	0.63	0
9	DGA	A	1213	-	25,25,43	0.93	2 (8%)	27,27,45	1.26	2 (7%)
9	DGA	A	1214	-	19,19,43	1.05	2 (10%)	21,21,45	1.40	2 (9%)

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	PLM	A	1201	1	-	0/14/14/15	0/0/0/0
3	ERM	A	1202	-	-	0/13/87/87	0/7/8/8
4	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
5	OLC	A	1204	-	-	0/18/18/24	0/0/0/0
5	OLC	A	1205	-	-	0/15/15/24	0/0/0/0
6	PEG	A	1206	-	-	0/4/4/4	0/0/0/0
5	OLC	A	1207	-	-	0/24/24/24	0/0/0/0
5	OLC	A	1208	-	-	0/18/18/24	0/0/0/0
7	TRS	A	1209	-	-	0/9/9/9	0/0/0/0
8	OLA	A	1210	-	-	0/7/7/17	0/0/0/0
8	OLA	A	1211	-	-	0/15/17/17	0/0/0/0
8	OLA	A	1212	-	-	0/14/16/17	0/0/0/0
9	DGA	A	1213	-	-	0/27/27/45	0/0/0/0
9	DGA	A	1214	-	-	0/21/21/45	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	ERM	C12-C13	-3.70	1.35	1.41
2	A	1201	PLM	O1-C1	-3.06	1.25	1.42
7	A	1209	TRS	C-N	-2.49	1.47	1.50
3	A	1202	ERM	C19-N4	-2.42	1.43	1.47
3	A	1202	ERM	C24-N5	-2.03	1.44	1.47
3	A	1202	ERM	C27-C19	-2.01	1.50	1.54
3	A	1202	ERM	C5-N2	2.13	1.50	1.47
3	A	1202	ERM	C6-C16	2.18	1.56	1.53
5	A	1205	OLC	C2-C1	2.38	1.57	1.50
5	A	1207	OLC	C2-C1	2.41	1.57	1.50
9	A	1213	DGA	OG2-CB1	2.44	1.41	1.34
9	A	1214	DGA	OG2-CB1	2.45	1.41	1.34
5	A	1208	OLC	C2-C1	2.52	1.58	1.50
5	A	1204	OLC	C2-C1	2.52	1.58	1.50
9	A	1213	DGA	OG1-CA1	2.52	1.40	1.33
9	A	1214	DGA	OG1-CA1	2.53	1.40	1.33
3	A	1202	ERM	C11-C12	2.67	1.42	1.36
8	A	1210	OLA	C10-C9	2.72	1.47	1.28
8	A	1212	OLA	C10-C9	2.73	1.47	1.31
8	A	1211	OLA	C10-C9	2.74	1.47	1.31
5	A	1208	OLC	O20-C1	3.40	1.43	1.33
5	A	1207	OLC	O20-C1	3.41	1.43	1.33
5	A	1204	OLC	O20-C1	3.42	1.43	1.33
5	A	1205	OLC	O20-C1	3.45	1.43	1.33
3	A	1202	ERM	C9-C8	3.67	1.51	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	ERM	C21-N5-C24	-3.83	105.87	111.62
3	A	1202	ERM	O5-C25-N4	-3.50	110.23	113.17
4	A	1203	CLR	C16-C17-C20	-3.05	106.62	112.05
3	A	1202	ERM	C23-C24-C25	-3.03	114.44	117.70
4	A	1203	CLR	C21-C20-C22	-2.98	105.38	110.35
3	A	1202	ERM	C10-C9-C14	-2.97	116.30	120.16
4	A	1203	CLR	C19-C10-C9	-2.94	107.91	111.67
4	A	1203	CLR	C3-C4-C5	-2.86	105.92	111.82
3	A	1202	ERM	O1-C16-C6	-2.66	118.85	121.66
4	A	1203	CLR	C18-C13-C14	-2.64	106.58	111.75
3	A	1202	ERM	O4-C20-N5	-2.34	119.37	123.03
4	A	1203	CLR	C15-C14-C8	-2.27	115.44	119.03
4	A	1203	CLR	C7-C8-C14	-2.19	107.44	110.86
5	A	1207	OLC	O20-C1-O19	-2.14	117.97	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1203	CLR	C11-C9-C10	-2.02	110.44	113.11
4	A	1203	CLR	C2-C1-C10	2.12	117.24	112.75
3	A	1202	ERM	C21-N5-C20	2.19	126.61	123.02
4	A	1203	CLR	C1-C10-C5	2.40	113.40	108.80
9	A	1213	DGA	OG1-CA1-CA2	2.52	119.58	111.90
5	A	1204	OLC	O20-C1-C2	2.61	119.84	111.90
5	A	1207	OLC	O20-C1-C2	2.62	119.88	111.90
9	A	1214	DGA	OG1-CA1-CA2	2.71	120.14	111.90
5	A	1208	OLC	O20-C1-C2	2.76	120.31	111.90
5	A	1205	OLC	O20-C1-C2	2.85	120.60	111.90
3	A	1202	ERM	C24-C25-N4	3.02	110.96	107.95
4	A	1203	CLR	C1-C2-C3	3.06	115.40	110.43
9	A	1213	DGA	OG2-CB1-CB2	3.69	119.54	111.53
9	A	1214	DGA	OG2-CB1-CB2	3.72	119.61	111.53
3	A	1202	ERM	C23-C24-N5	4.69	107.90	102.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	CLR	1	0
5	A	1204	OLC	1	0
5	A	1207	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<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	370/430 (86%)	3.07	287 (77%) 0 0	57, 89, 153, 196	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	11.5
1	A	161	ILE	9.5
1	A	1070	GLY	9.2
1	A	1028	ASP	8.9
1	A	201	ASN	8.7
1	A	204	ASN	8.6
1	A	1093	GLN	8.4
1	A	200	ASP	8.3
1	A	203	ASN	8.1
1	A	119	ALA	7.1
1	A	202	PRO	6.5
1	A	165	GLN	6.4
1	A	1024	ALA	6.2
1	A	128	CYS	6.1
1	A	1069	VAL	6.1
1	A	160	PRO	6.1
1	A	50	GLN	6.1
1	A	199	VAL	6.0
1	A	315	THR	6.0
1	A	1080	ASN	5.8
1	A	1073	ASP	5.8
1	A	164	ASN	5.6
1	A	48	GLU	5.6
1	A	1065	PHE	5.6
1	A	389	ASP	5.5
1	A	316	ILE	5.5
1	A	1068	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	49	GLU	5.2
1	A	1021	ASP	5.1
1	A	1076	LEU	5.0
1	A	1103	GLN	5.0
1	A	1026	VAL	5.0
1	A	317	SER	4.8
1	A	1100	ALA	4.8
1	A	205	ILE	4.7
1	A	242	HIS	4.7
1	A	392	GLY	4.7
1	A	1096	THR	4.7
1	A	177	THR	4.7
1	A	357	THR	4.6
1	A	140	THR	4.6
1	A	397	CYS	4.6
1	A	229	PRO	4.6
1	A	1066	ASP	4.5
1	A	143	ILE	4.5
1	A	1097	THR	4.5
1	A	1012	ASP	4.5
1	A	337	TRP	4.5
1	A	103	VAL	4.4
1	A	345	ILE	4.4
1	A	1030	LEU	4.4
1	A	197	THR	4.4
1	A	176	ILE	4.4
1	A	1063	HIS	4.4
1	A	162	GLN	4.4
1	A	1017	ILE	4.3
1	A	92	PHE	4.3
1	A	146	LEU	4.3
1	A	167	ASN	4.3
1	A	141	ALA	4.3
1	A	1033	MET	4.2
1	A	384	ASN	4.2
1	A	338	CYS	4.2
1	A	175	LYS	4.1
1	A	96	LEU	4.1
1	A	1015	LYS	4.1
1	A	139	SER	4.1
1	A	331	PHE	4.1
1	A	342	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1079	ALA	4.0
1	A	1084	VAL	4.0
1	A	335	LEU	4.0
1	A	147	CYS	4.0
1	A	190	VAL	4.0
1	A	373	SER	4.0
1	A	206	THR	4.0
1	A	115	ILE	3.9
1	A	396	THR	3.9
1	A	376	ASN	3.9
1	A	178	VAL	3.9
1	A	1077	LYS	3.9
1	A	166	TYR	3.9
1	A	78	ALA	3.9
1	A	1094	LEU	3.9
1	A	340	PHE	3.9
1	A	1001	ALA	3.8
1	A	228	THR	3.8
1	A	395	ILE	3.8
1	A	346	THR	3.8
1	A	356	THR	3.8
1	A	97	ALA	3.8
1	A	1031	THR	3.8
1	A	1075	ALA	3.8
1	A	339	PRO	3.8
1	A	70	GLY	3.8
1	A	1062	ARG	3.8
1	A	241	ILE	3.8
1	A	1007	TRP	3.7
1	A	1101	TYR	3.7
1	A	1078	LEU	3.7
1	A	1014	LEU	3.7
1	A	361	LEU	3.7
1	A	354	ASN	3.7
1	A	1061	PHE	3.7
1	A	64	VAL	3.6
1	A	230	LEU	3.6
1	A	149	ILE	3.6
1	A	172	ALA	3.6
1	A	60	LEU	3.6
1	A	390	ALA	3.6
1	A	186	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	188	ILE	3.6
1	A	61	ILE	3.5
1	A	101	LEU	3.5
1	A	314	GLN	3.5
1	A	1008	GLU	3.5
1	A	65	ILE	3.5
1	A	181	LEU	3.5
1	A	352	SER	3.5
1	A	69	ILE	3.5
1	A	351	ASP	3.5
1	A	174	ILE	3.4
1	A	126	VAL	3.4
1	A	329	VAL	3.4
1	A	367	TRP	3.4
1	A	370	TYR	3.4
1	A	76	ILE	3.4
1	A	145	HIS	3.4
1	A	77	LEU	3.4
1	A	1022	ASN	3.4
1	A	344	ASN	3.4
1	A	1060	ASP	3.4
1	A	378	LEU	3.4
1	A	330	PHE	3.4
1	A	182	ILE	3.3
1	A	137	LEU	3.3
1	A	341	PHE	3.3
1	A	1011	ASN	3.3
1	A	372	SER	3.3
1	A	187	ALA	3.3
1	A	236	THR	3.3
1	A	142	SER	3.3
1	A	366	VAL	3.3
1	A	144	TRP	3.3
1	A	1067	ILE	3.3
1	A	332	LEU	3.2
1	A	179	VAL	3.2
1	A	120	MET	3.2
1	A	152	ASP	3.2
1	A	219	LEU	3.2
1	A	1010	LEU	3.2
1	A	93	LEU	3.2
1	A	124	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	PHE	3.2
1	A	110	ILE	3.2
1	A	1099	ASN	3.2
1	A	102	LEU	3.2
1	A	385	LYS	3.2
1	A	75	VAL	3.1
1	A	114	THR	3.1
1	A	183	SER	3.1
1	A	1005	ASP	3.1
1	A	217	PHE	3.1
1	A	318	ASN	3.1
1	A	400	ARG	3.1
1	A	233	MET	3.1
1	A	90	ASN	3.0
1	A	150	SER	3.0
1	A	113	LEU	3.0
1	A	189	PRO	3.0
1	A	82	GLU	3.0
1	A	320	GLN	3.0
1	A	210	THR	3.0
1	A	227	PHE	3.0
1	A	1106	LEU	3.0
1	A	371	VAL	3.0
1	A	377	PRO	2.9
1	A	1095	LYS	2.9
1	A	336	MET	2.9
1	A	1006	ASN	2.9
1	A	399	TYR	2.8
1	A	343	THR	2.8
1	A	1032	LYS	2.8
1	A	222	SER	2.8
1	A	1086	GLU	2.8
1	A	54	LEU	2.8
1	A	51	GLY	2.8
1	A	1002	ASP	2.8
1	A	180	TRP	2.8
1	A	328	ILE	2.7
1	A	112	LEU	2.7
1	A	173	PHE	2.7
1	A	107	VAL	2.7
1	A	360	MET	2.7
1	A	121	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	362	LEU	2.7
1	A	334	LEU	2.7
1	A	73	THR	2.7
1	A	55	HIS	2.7
1	A	347	LEU	2.6
1	A	129	PRO	2.6
1	A	1003	LEU	2.6
1	A	148	ALA	2.6
1	A	1090	ALA	2.6
1	A	322	ALA	2.6
1	A	94	MET	2.6
1	A	398	ASN	2.6
1	A	62	LEU	2.5
1	A	123	LEU	2.5
1	A	74	LEU	2.5
1	A	1092	GLU	2.5
1	A	353	CYS	2.5
1	A	368	ILE	2.5
1	A	234	ILE	2.5
1	A	68	THR	2.5
1	A	380	TYR	2.5
1	A	184	ILE	2.5
1	A	109	PRO	2.5
1	A	136	VAL	2.5
1	A	1013	ASN	2.5
1	A	375	VAL	2.5
1	A	91	TYR	2.5
1	A	391	PHE	2.5
1	A	1105	TYR	2.5
1	A	1089	ALA	2.5
1	A	323	SER	2.5
1	A	130	ALA	2.5
1	A	168	SER	2.4
1	A	1027	LYS	2.4
1	A	122	PRO	2.4
1	A	66	ILE	2.4
1	A	1085	LYS	2.4
1	A	111	ALA	2.4
1	A	171	THR	2.4
1	A	108	MET	2.4
1	A	116	MET	2.4
1	A	1104	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1035	ALA	2.4
1	A	1023	ALA	2.4
1	A	100	ASP	2.4
1	A	170	ALA	2.4
1	A	243	ALA	2.4
1	A	387	PHE	2.4
1	A	125	LEU	2.4
1	A	1064	GLY	2.4
1	A	79	VAL	2.4
1	A	1081	GLU	2.3
1	A	1071	GLN	2.3
1	A	355	GLN	2.3
1	A	364	ILE	2.3
1	A	348	VAL	2.3
1	A	1098	ARG	2.3
1	A	99	ALA	2.3
1	A	157	ILE	2.3
1	A	87	TYR	2.3
1	A	133	PHE	2.3
1	A	132	LEU	2.3
1	A	1088	GLN	2.3
1	A	1016	VAL	2.3
1	A	216	ASP	2.3
1	A	333	PHE	2.2
1	A	53	LYS	2.2
1	A	1025	GLN	2.2
1	A	1087	ALA	2.2
1	A	212	GLU	2.2
1	A	225	ALA	2.2
1	A	325	VAL	2.2
1	A	244	LEU	2.1
1	A	95	SER	2.1
1	A	134	LEU	2.1
1	A	237	TYR	2.1
1	A	1102	ILE	2.1
1	A	59	LEU	2.1
1	A	381	THR	2.1
1	A	81	LEU	2.1
1	A	369	GLY	2.1
1	A	135	ASP	2.1
1	A	393	ARG	2.1
1	A	1059	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	2.0
1	A	169	ARG	2.0
1	A	1082	GLY	2.0
1	A	1018	GLU	2.0
1	A	151	VAL	2.0
1	A	245	GLN	2.0
1	A	1091	ALA	2.0
1	A	191	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
5	OLC	A	1208	19/25	0.16	0.81	5.49	80,111,128,130	0
8	OLA	A	1212	19/20	0.72	0.92	4.99	101,119,128,128	0
8	OLA	A	1211	20/20	0.31	0.66	2.81	77,106,112,113	0
5	OLC	A	1204	19/25	0.68	0.56	2.76	58,88,106,108	0
8	OLA	A	1210	10/20	0.39	0.59	2.54	84,90,101,101	0
2	PLM	A	1201	17/18	0.56	0.54	1.30	100,105,112,113	0
6	PEG	A	1206	7/7	0.37	0.49	1.28	94,100,104,107	0
9	DGA	A	1213	26/44	0.19	0.44	0.93	108,130,145,147	0
5	OLC	A	1205	16/25	0.39	0.47	0.50	70,101,124,125	0
5	OLC	A	1207	25/25	0.46	0.39	-0.16	99,114,150,154	0
9	DGA	A	1214	20/44	0.44	0.39	-0.17	104,127,141,146	0
3	ERM	A	1202	43/43	0.70	0.33	-0.75	56,66,79,85	0
4	CLR	A	1203	28/28	0.68	0.33	-1.84	72,93,103,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TRS	A	1209	8/8	0.07	0.58	-	133,136,137,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.