



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:45 PM UTC

PDB ID : 6WGT / pdb_00006wgt
Title : Crystal structure of HTR2A with hallucinogenic agonist
Authors : Kim, K.L.; Che, T.; Krumm, B.E.; Roth, B.L.
Deposited on : 2020-04-06
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

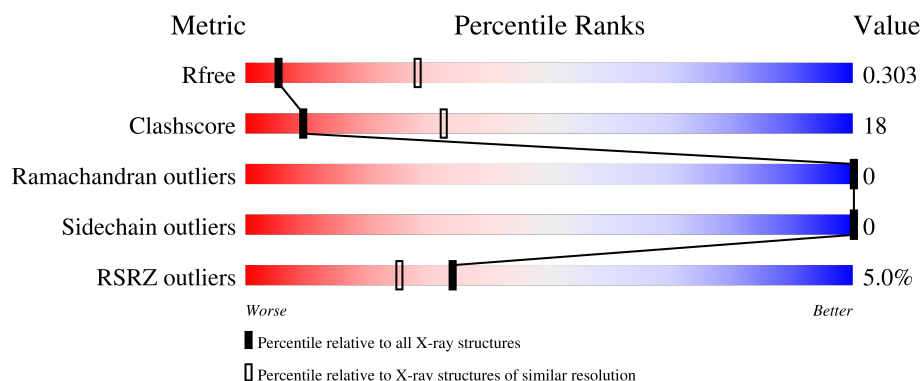
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	448	5% 58% 25% 16%
1	B	448	3% 60% 20% 20%
1	C	448	4% 57% 27% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8100 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 5-hydroxytryptamine receptor 2A,Soluble cytochrome b562 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2692	1762	429	480	21			
1	B	358	Total	C	N	O	S	0	0	0
			2495	1623	403	448	21			
1	C	376	Total	C	N	O	S	0	0	0
			2693	1754	431	488	20			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	initiating methionine	UNP P28223
A	41	LYS	-	expression tag	UNP P28223
A	42	THR	-	expression tag	UNP P28223
A	43	ILE	-	expression tag	UNP P28223
A	44	ILE	-	expression tag	UNP P28223
A	45	ALA	-	expression tag	UNP P28223
A	46	LEU	-	expression tag	UNP P28223
A	47	SER	-	expression tag	UNP P28223
A	48	TYR	-	expression tag	UNP P28223
A	49	ILE	-	expression tag	UNP P28223
A	50	PHE	-	expression tag	UNP P28223
A	51	CYS	-	expression tag	UNP P28223
A	52	LEU	-	expression tag	UNP P28223
A	53	VAL	-	expression tag	UNP P28223
A	54	PHE	-	expression tag	UNP P28223
A	55	ALA	-	expression tag	UNP P28223
A	56	ASP	-	expression tag	UNP P28223
A	57	TYR	-	expression tag	UNP P28223
A	58	LYS	-	expression tag	UNP P28223
A	59	ASP	-	expression tag	UNP P28223
A	60	ASP	-	expression tag	UNP P28223
A	61	ASP	-	expression tag	UNP P28223

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Chain	Residue	Modelled	Actual	Comment	Reference
A	62	ASP	-	expression tag	UNP P28223
A	63	GLY	-	expression tag	UNP P28223
A	64	ALA	-	expression tag	UNP P28223
A	65	PRO	-	expression tag	UNP P28223
A	247	ALA	LEU	conflict	UNP P28223
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	ARG	conflict	UNP P0ABE7
A	371	ALA	LEU	conflict	UNP P28223
A	406	GLY	-	expression tag	UNP P28223
A	407	ARG	-	expression tag	UNP P28223
A	408	PRO	-	expression tag	UNP P28223
A	409	LEU	-	expression tag	UNP P28223
A	410	GLU	-	expression tag	UNP P28223
A	411	VAL	-	expression tag	UNP P28223
A	412	LEU	-	expression tag	UNP P28223
A	413	PHE	-	expression tag	UNP P28223
A	414	GLN	-	expression tag	UNP P28223
A	415	GLY	-	expression tag	UNP P28223
A	416	PRO	-	expression tag	UNP P28223
A	417	HIS	-	expression tag	UNP P28223
A	418	HIS	-	expression tag	UNP P28223
A	419	HIS	-	expression tag	UNP P28223
A	420	HIS	-	expression tag	UNP P28223
A	421	HIS	-	expression tag	UNP P28223
A	422	HIS	-	expression tag	UNP P28223
A	423	HIS	-	expression tag	UNP P28223
A	424	HIS	-	expression tag	UNP P28223
A	425	HIS	-	expression tag	UNP P28223
A	426	HIS	-	expression tag	UNP P28223
B	40	MET	-	initiating methionine	UNP P28223
B	41	LYS	-	expression tag	UNP P28223
B	42	THR	-	expression tag	UNP P28223
B	43	ILE	-	expression tag	UNP P28223
B	44	ILE	-	expression tag	UNP P28223
B	45	ALA	-	expression tag	UNP P28223
B	46	LEU	-	expression tag	UNP P28223
B	47	SER	-	expression tag	UNP P28223
B	48	TYR	-	expression tag	UNP P28223
B	49	ILE	-	expression tag	UNP P28223
B	50	PHE	-	expression tag	UNP P28223
B	51	CYS	-	expression tag	UNP P28223

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Chain	Residue	Modelled	Actual	Comment	Reference
B	52	LEU	-	expression tag	UNP P28223
B	53	VAL	-	expression tag	UNP P28223
B	54	PHE	-	expression tag	UNP P28223
B	55	ALA	-	expression tag	UNP P28223
B	56	ASP	-	expression tag	UNP P28223
B	57	TYR	-	expression tag	UNP P28223
B	58	LYS	-	expression tag	UNP P28223
B	59	ASP	-	expression tag	UNP P28223
B	60	ASP	-	expression tag	UNP P28223
B	61	ASP	-	expression tag	UNP P28223
B	62	ASP	-	expression tag	UNP P28223
B	63	GLY	-	expression tag	UNP P28223
B	64	ALA	-	expression tag	UNP P28223
B	65	PRO	-	expression tag	UNP P28223
B	247	ALA	LEU	conflict	UNP P28223
B	1007	TRP	MET	conflict	UNP P0ABE7
B	1102	ILE	HIS	conflict	UNP P0ABE7
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B	406	GLY	-	expression tag	UNP P28223
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B	408	PRO	-	expression tag	UNP P28223
B	409	LEU	-	expression tag	UNP P28223
B	410	GLU	-	expression tag	UNP P28223
B	411	VAL	-	expression tag	UNP P28223
B	412	LEU	-	expression tag	UNP P28223
B	413	PHE	-	expression tag	UNP P28223
B	414	GLN	-	expression tag	UNP P28223
B	415	GLY	-	expression tag	UNP P28223
B	416	PRO	-	expression tag	UNP P28223
B	417	HIS	-	expression tag	UNP P28223
B	418	HIS	-	expression tag	UNP P28223
B	419	HIS	-	expression tag	UNP P28223
B	420	HIS	-	expression tag	UNP P28223
B	421	HIS	-	expression tag	UNP P28223
B	422	HIS	-	expression tag	UNP P28223
B	423	HIS	-	expression tag	UNP P28223
B	424	HIS	-	expression tag	UNP P28223
B	425	HIS	-	expression tag	UNP P28223
B	426	HIS	-	expression tag	UNP P28223
C	40	MET	-	initiating methionine	UNP P28223
C	41	LYS	-	expression tag	UNP P28223

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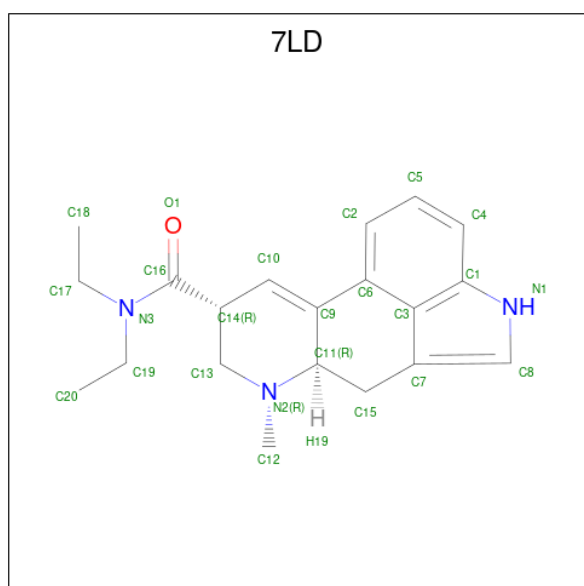
Chain	Residue	Modelled	Actual	Comment	Reference
C	42	THR	-	expression tag	UNP P28223
C	43	ILE	-	expression tag	UNP P28223
C	44	ILE	-	expression tag	UNP P28223
C	45	ALA	-	expression tag	UNP P28223
C	46	LEU	-	expression tag	UNP P28223
C	47	SER	-	expression tag	UNP P28223
C	48	TYR	-	expression tag	UNP P28223
C	49	ILE	-	expression tag	UNP P28223
C	50	PHE	-	expression tag	UNP P28223
C	51	CYS	-	expression tag	UNP P28223
C	52	LEU	-	expression tag	UNP P28223
C	53	VAL	-	expression tag	UNP P28223
C	54	PHE	-	expression tag	UNP P28223
C	55	ALA	-	expression tag	UNP P28223
C	56	ASP	-	expression tag	UNP P28223
C	57	TYR	-	expression tag	UNP P28223
C	58	LYS	-	expression tag	UNP P28223
C	59	ASP	-	expression tag	UNP P28223
C	60	ASP	-	expression tag	UNP P28223
C	61	ASP	-	expression tag	UNP P28223
C	62	ASP	-	expression tag	UNP P28223
C	63	GLY	-	expression tag	UNP P28223
C	64	ALA	-	expression tag	UNP P28223
C	65	PRO	-	expression tag	UNP P28223
C	247	ALA	LEU	conflict	UNP P28223
C	1007	TRP	MET	conflict	UNP P0ABE7
C	1102	ILE	HIS	conflict	UNP P0ABE7
C	1106	LEU	ARG	conflict	UNP P0ABE7
C	371	ALA	LEU	conflict	UNP P28223
C	406	GLY	-	expression tag	UNP P28223
C	407	ARG	-	expression tag	UNP P28223
C	408	PRO	-	expression tag	UNP P28223
C	409	LEU	-	expression tag	UNP P28223
C	410	GLU	-	expression tag	UNP P28223
C	411	VAL	-	expression tag	UNP P28223
C	412	LEU	-	expression tag	UNP P28223
C	413	PHE	-	expression tag	UNP P28223
C	414	GLN	-	expression tag	UNP P28223
C	415	GLY	-	expression tag	UNP P28223
C	416	PRO	-	expression tag	UNP P28223
C	417	HIS	-	expression tag	UNP P28223
C	418	HIS	-	expression tag	UNP P28223

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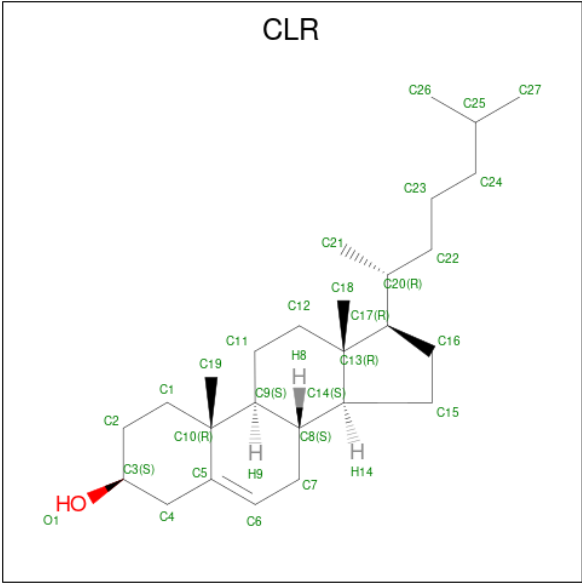
Chain	Residue	Modelled	Actual	Comment	Reference
C	419	HIS	-	expression tag	UNP P28223
C	420	HIS	-	expression tag	UNP P28223
C	421	HIS	-	expression tag	UNP P28223
C	422	HIS	-	expression tag	UNP P28223
C	423	HIS	-	expression tag	UNP P28223
C	424	HIS	-	expression tag	UNP P28223
C	425	HIS	-	expression tag	UNP P28223
C	426	HIS	-	expression tag	UNP P28223

- Molecule 2 is (8alpha)-N,N-diethyl-6-methyl-9,10-didehydroergoline-8-carboxamide (CCD ID: 7LD) (formula: C₂₀H₂₅N₃O) (labeled as "Ligand of Interest" by depositor).



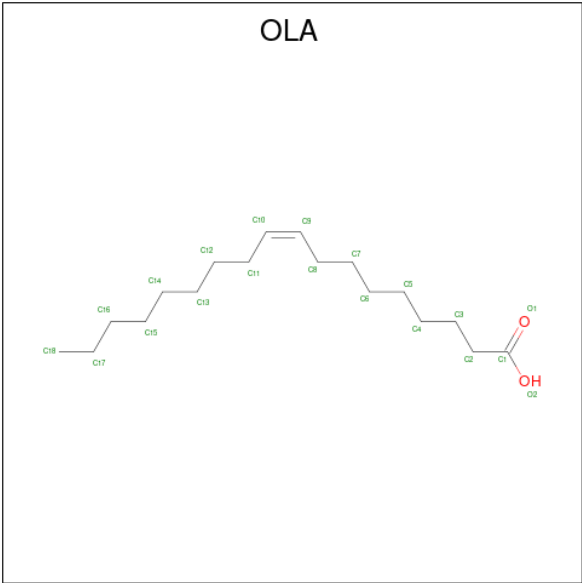
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	20	3	1		
2	B	1	Total	C	N	O	0	0
			24	20	3	1		
2	C	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



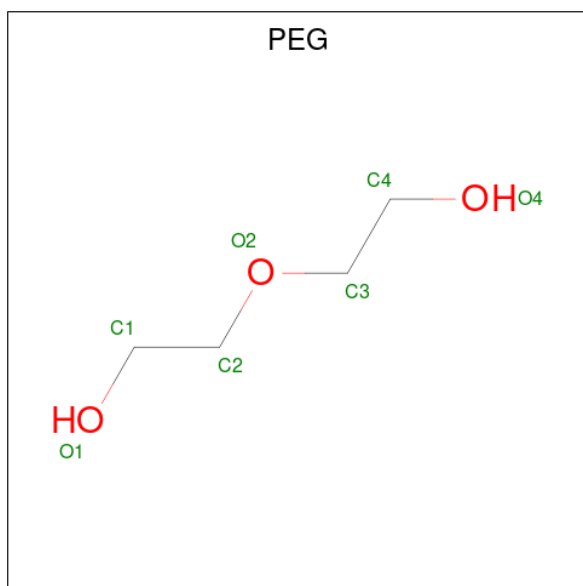
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C		0	0
			17	17			
4	A	1	Total	C	O	0	0
			20	18	2		

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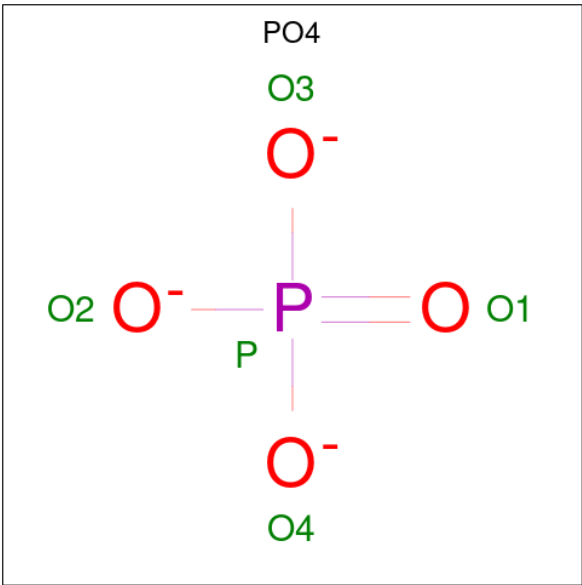
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C	0	0
			10	10		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



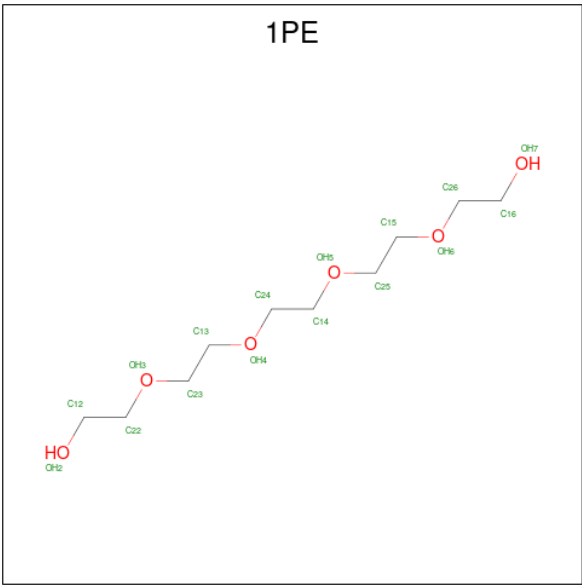
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).

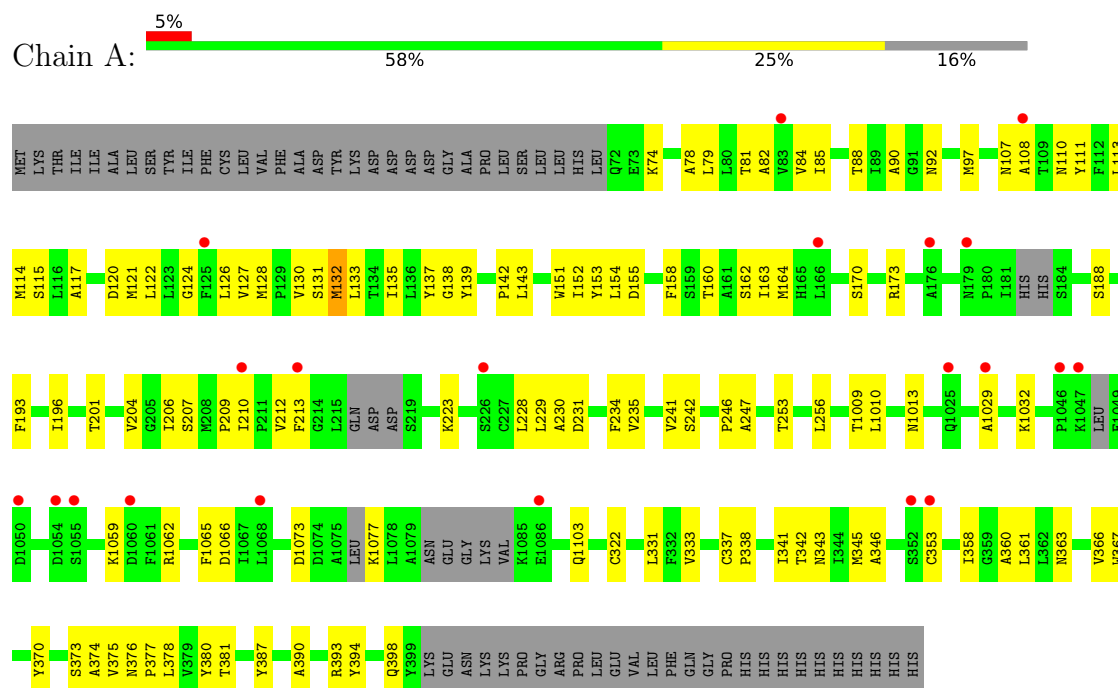


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	10	6		

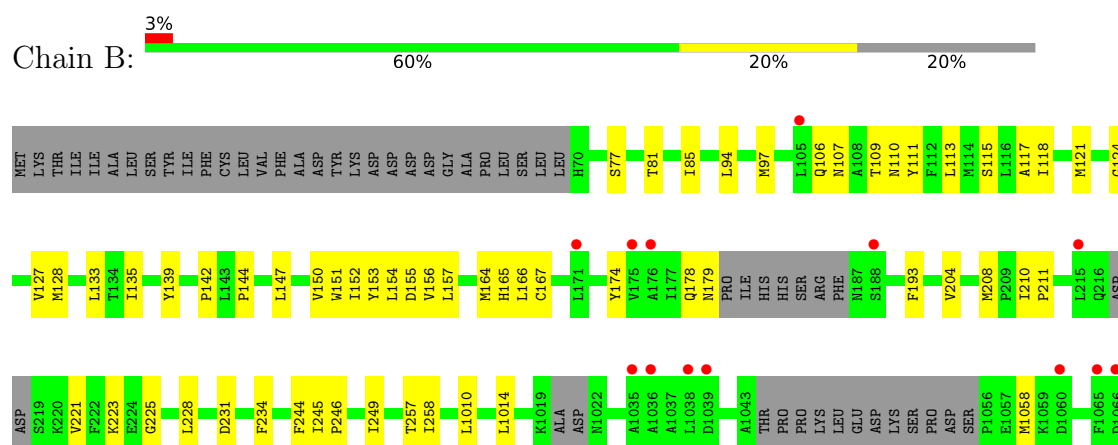
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 5-hydroxytryptamine receptor 2A,Soluble cytochrome b562 fusion



- Molecule 1: 5-hydroxytryptamine receptor 2A,Soluble cytochrome b562 fusion



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.64Å 175.26Å 280.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 3.40 34.54 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.2 (34.54-3.40) 94.2 (34.54-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.265 , 0.305 0.266 , 0.303	Depositor DCC
R_{free} test set	1350 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8100	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, PO4, PEG, CLR, OLA, 7LD

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	0.60	0/2745	0.88	3/3758 (0.1%)
1	B	0.53	0/2542	0.73	0/3484
1	C	0.57	0/2744	0.80	0/3756
All	All	0.57	0/8031	0.81	3/10998 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	SER	CA-C-N	7.10	135.09	121.54
1	A	188	SER	C-N-CA	7.10	135.09	121.54
1	A	132	MET	CB-CG-SD	-5.26	96.91	112.70

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	2692	0	2493	111	0
1	B	2495	0	2226	67	1
1	C	2693	0	2490	93	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	0	0	0
3	A	56	0	92	18	0
4	A	37	0	61	7	0
4	B	10	0	14	0	0
5	A	7	0	10	1	0
5	C	7	0	10	0	0
6	B	10	0	0	1	0
6	C	5	0	0	0	0
7	C	16	0	22	3	0
All	All	8100	0	7418	277	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 18.

All (277) 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:337:CYS:O	1:A:341:ILE:HG13	1.71	0.88
1:A:345:MET:HG2	3:A:1202:CLR:H121	1.59	0.83
1:B:1075:ALA:HB3	1:B:1090:ALA:HB2	1.60	0.82
1:A:137:TYR:CD2	1:A:142:PRO:HB3	2.14	0.82
1:A:124:GLY:HA2	1:A:128:MET:SD	2.19	0.82
1:A:229:LEU:HD12	1:A:235:VAL:HG23	1.62	0.81
1:A:201:THR:HA	1:A:204:VAL:HG12	1.59	0.81
1:B:115:SER:OG	1:B:165:HIS:NE2	2.14	0.79
1:B:94:LEU:HB3	1:B:391:PHE:CD1	2.19	0.78
1:A:92:ASN:HD21	1:A:117:ALA:HA	1.49	0.78
1:C:240:PHE:O	1:C:240:PHE:HD1	1.67	0.77
1:A:137:TYR:CE2	1:A:142:PRO:HB3	2.21	0.76
1:C:232:ASP:HB3	1:C:347:VAL:HG13	1.68	0.74
1:A:152:ILE:HD11	1:A:229:LEU:HB2	1.70	0.73
1:C:1064:GLY:HA2	1:C:1067:ILE:HD13	1.70	0.73
1:B:244:PHE:HZ	1:B:341:ILE:HG22	1.52	0.73
1:B:118:ILE:HA	1:B:121:MET:HE2	1.73	0.70
1:B:110:ASN:ND2	6:B:1204:PO4:O2	2.23	0.70
1:A:82:ALA:HB2	1:A:132:MET:HE1	1.73	0.70
1:A:378:LEU:HD12	4:A:1203:OLA:H111	1.74	0.69
1:C:367:TRP:HA	1:C:370:TYR:HB2	1.73	0.69
1:A:81:THR:HB	1:A:132:MET:CE	2.22	0.69
1:A:120:ASP:OD1	1:A:373:SER:HB3	1.93	0.68
1:A:170:SER:HB3	1:A:253:THR:OG1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLY:HA2	1:B:128:MET:SD	2.35	0.67
1:A:228:LEU:HD21	5:A:1205:PEG:H41	1.76	0.67
1:A:342:THR:HG22	3:A:1202:CLR:H222	1.76	0.67
1:A:88:THR:HG22	1:A:374:ALA:HB2	1.78	0.66
1:C:128:MET:HE2	1:C:370:TYR:HB3	1.76	0.65
1:B:147:LEU:H	1:B:147:LEU:HD12	1.61	0.65
1:C:229:LEU:HD21	1:C:234:PHE:HD2	1.61	0.64
3:A:1206:CLR:H232	3:A:1206:CLR:H161	1.79	0.64
1:A:173:ARG:NH2	1:A:322:CYS:SG	2.71	0.64
1:A:81:THR:HB	1:A:132:MET:HE2	1.79	0.64
1:B:81:THR:O	1:B:85:ILE:HG13	1.97	0.64
1:B:94:LEU:HB3	1:B:391:PHE:HD1	1.62	0.64
1:C:149:ALA:HB2	1:C:221:VAL:HG11	1.80	0.62
1:A:206:ILE:O	1:A:209:PRO:HD2	1.98	0.62
1:B:166:LEU:HD22	1:B:329:PHE:CD1	2.35	0.62
1:B:367:TRP:HA	1:B:370:TYR:HB2	1.80	0.62
1:C:92:ASN:O	1:C:96:ILE:HG13	2.00	0.62
1:C:232:ASP:HB3	1:C:347:VAL:CG1	2.28	0.61
1:B:144:PRO:HD2	1:B:147:LEU:HD13	1.83	0.61
1:A:1013:ASN:HB2	1:A:1032:LYS:HE3	1.83	0.60
1:B:166:LEU:HD22	1:B:329:PHE:HD1	1.66	0.60
1:A:115:SER:HB2	1:A:196:ILE:HD13	1.83	0.60
1:A:85:ILE:HD11	1:A:128:MET:O	2.01	0.60
1:C:223:LYS:HE2	7:C:1204:1PE:H142	1.84	0.59
1:C:362:LEU:O	1:C:366:VAL:HG23	2.03	0.59
1:B:107:ASN:OD1	1:B:107:ASN:N	2.34	0.59
1:C:1092:GLU:HG2	1:C:1096:THR:HB	1.85	0.59
1:A:193:PHE:HE2	3:A:1206:CLR:H6	1.67	0.58
1:A:210:ILE:HD11	1:A:234:PHE:CE2	2.37	0.58
1:A:84:VAL:O	1:A:88:THR:HG23	2.04	0.58
1:A:122:LEU:HB3	1:A:158:PHE:CE2	2.39	0.58
1:C:81:THR:O	1:C:85:ILE:HG13	2.03	0.58
1:C:113:LEU:HD23	1:C:380:TYR:OH	2.03	0.58
1:A:97:MET:HE1	4:A:1204:OLA:H10	1.83	0.58
1:B:244:PHE:CZ	1:B:341:ILE:HG22	2.37	0.57
1:C:1034:ARG:HA	1:C:1068:LEU:HD23	1.86	0.57
1:A:338:PRO:O	1:A:342:THR:HG23	2.04	0.57
1:B:117:ALA:O	1:B:121:MET:N	2.37	0.56
1:C:240:PHE:O	1:C:240:PHE:CD1	2.55	0.56
1:A:82:ALA:CA	1:A:132:MET:HE1	2.36	0.56
1:B:330:PHE:CZ	1:B:334:VAL:HG21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:ASN:ND2	1:A:1029:ALA:O	2.38	0.56
1:B:127:VAL:HG11	1:B:155:ASP:HB2	1.87	0.56
1:C:382:LEU:HB3	1:C:383:PHE:CD1	2.41	0.56
1:B:77:SER:O	1:B:81:THR:HG23	2.05	0.56
1:B:223:LYS:HB3	1:B:228:LEU:HD21	1.88	0.55
1:B:164:MET:HE2	1:B:246:PRO:HG2	1.88	0.55
1:A:107:ASN:O	1:A:111:TYR:N	2.39	0.55
1:C:153:TYR:HE1	1:C:207:SER:HB2	1.72	0.55
1:C:97:MET:HE1	1:C:394:TYR:HB3	1.89	0.55
1:A:1010:LEU:HD21	1:A:1065:PHE:CZ	2.43	0.54
1:A:206:ILE:HD13	1:A:241:VAL:CG1	2.37	0.54
1:A:82:ALA:CB	1:A:132:MET:HE1	2.38	0.54
1:A:193:PHE:CD2	3:A:1206:CLR:H41	2.43	0.54
1:A:377:PRO:O	1:A:381:THR:HG23	2.08	0.54
1:A:81:THR:HB	1:A:132:MET:HE3	1.89	0.54
1:C:243:PHE:HE2	1:C:337:CYS:HG	1.54	0.54
1:C:330:PHE:CZ	1:C:334:VAL:HG21	2.43	0.54
1:C:390:ALA:HB1	1:C:394:TYR:CE2	2.42	0.54
1:C:259:LYS:HA	1:C:262:GLN:HG3	1.90	0.54
1:C:257:THR:HA	1:C:260:SER:HB3	1.90	0.53
1:A:193:PHE:CE2	3:A:1206:CLR:H41	2.44	0.53
1:A:201:THR:HA	1:A:204:VAL:CG1	2.34	0.53
1:C:112:PHE:CZ	1:C:195:LYS:HB3	2.44	0.53
1:C:153:TYR:CE1	1:C:207:SER:HB2	2.44	0.53
1:C:210:ILE:H	1:C:210:ILE:HD12	1.74	0.53
1:C:133:LEU:HB3	1:C:142:PRO:HG3	1.90	0.53
1:A:193:PHE:CE2	3:A:1206:CLR:H6	2.43	0.53
1:B:258:ILE:HD11	1:B:322:CYS:SG	2.49	0.53
1:C:127:VAL:O	1:C:130:VAL:HG12	2.09	0.52
1:A:160:THR:O	1:A:164:MET:HG2	2.09	0.52
1:C:330:PHE:CD1	1:C:330:PHE:C	2.88	0.52
1:C:1072:ILE:O	1:C:1076:LEU:HG	2.09	0.52
1:C:227:CYS:O	1:C:228:LEU:HD23	2.10	0.52
1:A:97:MET:CE	4:A:1204:OLA:H10	2.40	0.52
1:C:229:LEU:HD21	1:C:234:PHE:CD2	2.43	0.52
1:A:209:PRO:HA	1:A:212:VAL:HB	1.91	0.51
1:A:133:LEU:HD21	1:A:143:LEU:HD21	1.92	0.51
1:B:382:LEU:HB3	1:B:383:PHE:CD1	2.45	0.51
1:A:82:ALA:N	1:A:132:MET:CE	2.73	0.51
1:C:193:PHE:HA	1:C:196:ILE:HD12	1.93	0.51
1:C:237:ILE:O	1:C:240:PHE:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:O	1:B:362:LEU:HD13	2.11	0.51
1:B:361:LEU:HB3	1:B:365:PHE:CE2	2.46	0.51
1:C:152:ILE:HG21	1:C:229:LEU:HD13	1.93	0.50
1:A:380:TYR:HB3	1:A:387:TYR:CD2	2.46	0.50
1:A:79:LEU:HG	1:A:82:ALA:HB3	1.93	0.50
1:C:1104:LYS:O	1:C:312:MET:HG2	2.12	0.50
1:A:135:ILE:HA	1:A:139:TYR:CE1	2.47	0.50
1:A:1062:ARG:O	1:A:1066:ASP:HB2	2.12	0.50
1:C:200:TRP:O	1:C:204:VAL:HG23	2.12	0.50
1:B:328:VAL:HG22	1:B:376:ASN:OD1	2.12	0.49
1:C:339:PHE:CD1	1:C:362:LEU:HD22	2.47	0.49
1:B:135:ILE:HG12	1:B:139:TYR:CZ	2.47	0.49
1:C:1105:TYR:CD1	1:C:1105:TYR:C	2.90	0.49
1:C:347:VAL:HG22	7:C:1204:1PE:H122	1.93	0.49
3:A:1206:CLR:H212	3:A:1206:CLR:H183	1.94	0.49
1:A:92:ASN:HD21	1:A:117:ALA:CA	2.19	0.49
1:A:130:VAL:HB	1:A:151:TRP:NE1	2.28	0.49
1:A:223:LYS:HB2	1:A:228:LEU:HD22	1.94	0.49
1:C:124:GLY:HA2	1:C:128:MET:SD	2.53	0.49
1:A:366:VAL:O	1:A:370:TYR:N	2.38	0.48
1:B:1014:LEU:HD23	1:B:1014:LEU:O	2.13	0.48
1:A:160:THR:HG23	1:A:164:MET:HE2	1.94	0.48
1:A:393:ARG:O	1:A:398:GLN:N	2.47	0.48
1:B:228:LEU:N	1:B:228:LEU:HD23	2.28	0.48
1:B:1074:ASP:OD1	1:B:1075:ALA:N	2.46	0.48
1:A:196:ILE:HG21	3:A:1206:CLR:H3	1.95	0.48
1:A:1062:ARG:HA	1:A:1062:ARG:HD3	1.55	0.48
1:C:264:GLU:O	1:C:1003:LEU:HG	2.14	0.48
1:A:333:VAL:O	1:A:337:CYS:HB2	2.14	0.48
1:C:336:TRP:NE1	1:C:369:GLY:O	2.46	0.48
1:A:153:TYR:CE1	1:A:207:SER:HB3	2.49	0.47
1:B:135:ILE:HG12	1:B:139:TYR:CE1	2.49	0.47
1:C:243:PHE:HE2	1:C:337:CYS:SG	2.37	0.47
1:C:1006:ASN:N	1:C:1006:ASN:HD22	2.10	0.47
1:C:1018:GLU:OE1	1:C:1018:GLU:HA	2.15	0.47
1:B:147:LEU:HD12	1:B:147:LEU:N	2.28	0.47
1:A:81:THR:HG23	1:A:367:TRP:CH2	2.49	0.47
1:A:115:SER:CB	1:A:196:ILE:HD13	2.43	0.47
1:B:106:GLN:HG3	1:B:111:TYR:CE2	2.49	0.47
1:A:223:LYS:HG3	1:A:230:ALA:CB	2.45	0.47
1:B:150:VAL:O	1:B:154:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LEU:HD12	1:C:127:VAL:HB	1.95	0.47
1:C:89:ILE:HD11	1:C:124:GLY:C	2.39	0.47
1:B:245:ILE:HD13	1:B:245:ILE:HA	1.69	0.47
1:C:116:LEU:C	1:C:116:LEU:HD23	2.40	0.46
1:C:349:CYS:HB3	1:C:353:CYS:HB2	1.44	0.46
1:A:126:LEU:HD23	1:A:154:LEU:HD13	1.97	0.46
1:A:152:ILE:HD11	1:A:229:LEU:CB	2.43	0.46
1:A:375:VAL:HG22	4:A:1203:OLA:H112	1.96	0.46
1:B:1093:GLN:O	1:B:1096:THR:OG1	2.31	0.46
1:A:90:ALA:HB2	4:A:1204:OLA:H182	1.97	0.46
1:C:1056:PRO:HA	1:C:1059:LYS:HB2	1.97	0.46
1:A:133:LEU:CD2	1:A:143:LEU:HD21	2.46	0.46
1:A:361:LEU:HD11	3:A:1202:CLR:H72	1.98	0.46
1:B:193:PHE:CD1	1:B:193:PHE:C	2.93	0.46
1:B:1092:GLU:O	1:B:1096:THR:HG23	2.16	0.46
1:C:174:TYR:HB2	1:C:257:THR:OG1	2.16	0.46
1:A:139:TYR:CE2	1:A:363:ASN:OD1	2.69	0.46
1:C:331:LEU:HD13	1:C:375:VAL:HG11	1.96	0.46
1:B:1058:MET:HE3	1:B:1058:MET:HB3	1.82	0.46
1:C:223:LYS:HE2	7:C:1204:1PE:C14	2.46	0.46
1:A:1059:LYS:HE2	1:A:1059:LYS:HB3	1.68	0.46
1:A:376:ASN:HB2	1:A:377:PRO:HD3	1.98	0.46
1:C:170:SER:OG	1:C:253:THR:HB	2.16	0.46
4:A:1204:OLA:H142	4:A:1204:OLA:H111	1.30	0.46
1:C:1064:GLY:CA	1:C:1067:ILE:HD13	2.42	0.46
1:A:223:LYS:HG3	1:A:230:ALA:HB2	1.98	0.45
1:A:79:LEU:O	1:A:82:ALA:N	2.49	0.45
1:A:231:ASP:OD1	1:A:234:PHE:N	2.33	0.45
1:A:331:LEU:HD23	1:A:375:VAL:HG11	1.99	0.45
1:C:109:THR:O	1:C:113:LEU:HD12	2.16	0.45
1:C:141:TRP:CE2	1:C:143:LEU:HB2	2.51	0.45
1:B:152:ILE:O	1:B:156:VAL:HG13	2.16	0.45
1:C:91:GLY:C	1:C:377:PRO:HG2	2.41	0.45
1:A:361:LEU:HD13	3:A:1202:CLR:H152	1.98	0.45
1:A:390:ALA:HB1	1:A:394:TYR:CE2	2.51	0.45
1:C:1099:ASN:O	1:C:1103:GLN:HG2	2.15	0.45
1:A:1013:ASN:HD21	1:A:1029:ALA:C	2.24	0.45
1:B:94:LEU:HB3	1:B:391:PHE:CE1	2.51	0.45
1:A:81:THR:HG22	1:A:132:MET:HE3	1.99	0.45
1:C:209:PRO:HG2	1:C:210:ILE:HD12	1.99	0.45
1:A:127:VAL:HG21	1:A:155:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:GLY:HA2	1:C:1067:ILE:CD1	2.43	0.45
1:A:131:SER:HB3	1:A:367:TRP:HZ2	1.82	0.45
1:A:1010:LEU:HD21	1:A:1065:PHE:HZ	1.82	0.45
1:C:250:MET:HE2	1:C:333:VAL:CG1	2.47	0.45
1:B:231:ASP:OD1	1:B:234:PHE:N	2.42	0.45
1:C:109:THR:O	1:C:112:PHE:HB2	2.17	0.44
1:C:390:ALA:HB1	1:C:394:TYR:HE2	1.81	0.44
1:B:155:ASP:OD1	1:B:155:ASP:C	2.60	0.44
1:B:1104:LYS:O	1:B:312:MET:HB2	2.18	0.44
1:B:156:VAL:HG21	1:B:210:ILE:CD1	2.47	0.44
1:C:1098:ARG:NH2	1:C:1098:ARG:HG3	2.31	0.44
1:A:82:ALA:N	1:A:132:MET:HE1	2.32	0.44
3:A:1206:CLR:C16	3:A:1206:CLR:H273	2.47	0.44
1:A:81:THR:HG23	1:A:367:TRP:CZ2	2.53	0.44
1:C:335:MET:SD	1:C:372:SER:HB3	2.57	0.44
1:A:247:ALA:HB1	1:A:333:VAL:HG22	2.00	0.44
1:B:208:MET:O	1:B:211:PRO:HD2	2.18	0.44
1:A:256:LEU:N	1:A:256:LEU:HD23	2.33	0.43
3:A:1206:CLR:H161	3:A:1206:CLR:H273	1.99	0.43
1:B:1010:LEU:HD23	1:B:1010:LEU:HA	1.71	0.43
1:A:1062:ARG:HH12	1:A:1103:GLN:HG3	1.83	0.43
1:A:353:CYS:SG	3:A:1202:CLR:H193	2.58	0.43
1:B:127:VAL:CG1	1:B:155:ASP:HB2	2.48	0.43
1:B:174:TYR:HE1	1:B:257:THR:HG1	1.66	0.43
1:B:384:ASN:HB3	1:B:387:TYR:HB2	2.01	0.43
1:C:1033:MET:HE2	1:C:1068:LEU:HG	2.00	0.43
1:C:1066:ASP:O	1:C:1070:GLY:N	2.45	0.43
1:C:132:MET:HE2	1:C:132:MET:HB3	1.87	0.43
1:C:130:VAL:CG1	1:C:151:TRP:NE1	2.82	0.43
1:C:332:PHE:C	1:C:332:PHE:CD1	2.97	0.43
1:A:108:ALA:HA	1:A:111:TYR:HB2	2.00	0.43
1:A:160:THR:OG1	1:A:242:SER:HB3	2.18	0.43
1:C:130:VAL:O	1:C:134:THR:HG23	2.18	0.43
1:C:263:LYS:O	1:C:1002:ASP:HB2	2.19	0.43
1:C:103:LYS:HA	1:C:106:GLN:HG3	2.01	0.43
1:C:163:ILE:HG12	1:C:246:PRO:HB2	1.99	0.43
1:A:114:MET:HE3	3:A:1206:CLR:H22	2.00	0.43
1:B:178:GLN:O	1:B:179:ASN:ND2	2.52	0.43
1:C:1061:PHE:O	1:C:1065:PHE:N	2.51	0.43
1:C:113:LEU:HD23	1:C:380:TYR:CZ	2.54	0.43
1:A:213:PHE:CD1	1:A:213:PHE:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HD22	1:C:329:PHE:CD1	2.54	0.43
1:C:184:SER:HB3	1:C:187:ASN:CB	2.49	0.43
1:A:1073:ASP:O	1:A:1077:LYS:N	2.52	0.42
1:B:97:MET:HB3	1:B:97:MET:HE2	1.71	0.42
1:B:323:LYS:O	1:B:327:ILE:HG13	2.19	0.42
1:C:197:ILE:O	1:C:201:THR:HG23	2.19	0.42
1:A:81:THR:HG21	1:A:132:MET:HG3	2.02	0.42
1:A:128:MET:HE3	1:A:370:TYR:CD1	2.54	0.42
1:A:338:PRO:HG3	3:A:1202:CLR:H263	2.01	0.42
1:A:358:ILE:HG13	3:A:1202:CLR:C19	2.49	0.42
1:A:343:ASN:O	1:A:346:ALA:HB3	2.20	0.42
1:C:89:ILE:HD13	1:C:89:ILE:N	2.35	0.42
1:C:71:LEU:O	1:C:75:ASN:HB2	2.20	0.42
1:A:138:GLY:O	1:A:139:TYR:HB2	2.18	0.42
1:A:360:ALA:O	1:A:363:ASN:HB2	2.20	0.42
1:C:142:PRO:HG2	1:C:143:LEU:HD12	2.01	0.42
1:B:133:LEU:HD12	1:B:133:LEU:O	2.19	0.42
1:A:122:LEU:HB3	1:A:158:PHE:CZ	2.54	0.41
1:B:151:TRP:CH2	2:B:1201:7LD:C18	3.03	0.41
1:B:167:CYS:SG	1:B:249:ILE:HG21	2.60	0.41
1:A:1009:THR:O	1:A:1013:ASN:HB3	2.20	0.41
1:C:1098:ARG:HG3	1:C:1098:ARG:HH21	1.84	0.41
1:C:331:LEU:HD13	1:C:375:VAL:CG1	2.50	0.41
4:A:1203:OLA:H31	4:A:1203:OLA:H61	1.49	0.41
1:B:153:TYR:O	1:B:156:VAL:HG22	2.20	0.41
1:A:121:MET:O	1:A:124:GLY:N	2.54	0.41
1:C:1017:ILE:HD11	1:C:1030:LEU:HD22	2.01	0.41
1:B:133:LEU:HG	1:B:142:PRO:HG3	2.03	0.41
1:C:208:MET:N	1:C:209:PRO:HD2	2.36	0.41
1:A:366:VAL:HG22	1:A:370:TYR:CD2	2.56	0.41
1:B:361:LEU:HB3	1:B:365:PHE:CD2	2.56	0.41
1:C:231:ASP:O	1:C:232:ASP:C	2.63	0.41
1:A:74:LYS:O	1:A:78:ALA:N	2.54	0.41
1:B:157:LEU:HD11	1:B:204:VAL:HG22	2.03	0.41
1:B:391:PHE:O	1:B:395:ILE:HG13	2.20	0.41
1:B:128:MET:HG2	1:B:370:TYR:CD2	2.56	0.41
1:B:152:ILE:HD12	1:B:221:VAL:HG23	2.02	0.41
1:A:163:ILE:HG12	1:A:246:PRO:HB2	2.02	0.40
1:C:331:LEU:HA	1:C:331:LEU:HD23	1.84	0.40
1:A:353:CYS:HA	3:A:1202:CLR:H22	2.03	0.40
1:C:119:ALA:HB2	1:C:200:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:O	1:A:162:SER:N	2.48	0.40
1:B:94:LEU:HD13	1:B:391:PHE:HB3	2.03	0.40
1:A:88:THR:O	1:A:92:ASN:HB3	2.21	0.40
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.68	0.40
1:C:166:LEU:HD22	1:C:329:PHE:HD1	1.87	0.40
1:A:110:ASN:HA	1:A:113:LEU:HD12	2.03	0.40
1:B:109:THR:O	1:B:113:LEU:HD13	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLY:N	1:B:351:GLU:O[3_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	365/448 (82%)	350 (96%)	15 (4%)	0	100	100
1	B	346/448 (77%)	339 (98%)	7 (2%)	0	100	100
1	C	366/448 (82%)	361 (99%)	5 (1%)	0	100	100
All	All	1077/1344 (80%)	1050 (98%)	27 (2%)	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	247/390 (63%)	247 (100%)	0	100	100
1	B	216/390 (55%)	216 (100%)	0	100	100
1	C	249/390 (64%)	249 (100%)	0	100	100
All	All	712/1170 (61%)	712 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	ASN
1	A	317	ASN
1	A	319	GLN
1	B	92	ASN
1	B	179	ASN
1	B	384	ASN
1	C	1041	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	CLR	A	1206	-	31,31,31	0.69	0	48,48,48	1.83	13 (27%)
2	7LD	B	1201	-	26,27,27	6.04	12 (46%)	35,40,40	2.60	11 (31%)
5	PEG	A	1205	-	6,6,6	0.45	0	5,5,5	0.29	0
5	PEG	C	1202	-	6,6,6	0.16	0	5,5,5	0.24	0
6	PO4	C	1203	-	4,4,4	0.79	0	6,6,6	0.63	0
3	CLR	A	1202	-	31,31,31	0.76	1 (3%)	48,48,48	2.05	19 (39%)
6	PO4	B	1203	-	4,4,4	0.90	0	6,6,6	0.65	0
7	1PE	C	1204	-	15,15,15	0.58	0	14,14,14	0.54	0
6	PO4	B	1204	-	4,4,4	0.81	0	6,6,6	0.55	0
4	OLA	B	1202	-	9,9,19	1.04	1 (11%)	8,8,19	0.37	0
2	7LD	A	1201	-	26,27,27	6.10	14 (53%)	35,40,40	2.59	12 (34%)
2	7LD	C	1201	-	26,27,27	6.38	13 (50%)	35,40,40	4.12	16 (45%)
4	OLA	A	1203	-	16,16,19	0.93	1 (6%)	15,15,19	0.95	1 (6%)
4	OLA	A	1204	-	19,19,19	0.84	1 (5%)	19,19,19	0.93	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	CLR	A	1206	-	-	10/10/68/68	0/4/4/4
2	7LD	B	1201	-	-	1/12/36/36	0/4/4/4
5	PEG	A	1205	-	-	2/4/4/4	-
5	PEG	C	1202	-	-	2/4/4/4	-
3	CLR	A	1202	-	-	7/10/68/68	0/4/4/4
7	1PE	C	1204	-	-	7/13/13/13	-
4	OLA	B	1202	-	-	2/7/7/17	-
2	7LD	A	1201	-	-	2/12/36/36	0/4/4/4
2	7LD	C	1201	-	-	5/12/36/36	0/4/4/4
4	OLA	A	1203	-	-	9/14/14/17	-
4	OLA	A	1204	-	-	13/17/17/17	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	7LD	C10-C9	22.89	1.57	1.33
2	A	1201	7LD	C10-C9	21.55	1.56	1.33
2	B	1201	7LD	C10-C9	20.32	1.54	1.33
2	B	1201	7LD	C13-N2	-11.39	1.30	1.47
2	C	1201	7LD	C13-C14	11.03	1.66	1.53
2	C	1201	7LD	C16-N3	10.30	1.49	1.35
2	A	1201	7LD	C13-N2	-9.98	1.32	1.47
2	A	1201	7LD	C11-N2	9.79	1.62	1.48
2	A	1201	7LD	C13-C14	9.58	1.64	1.53
2	B	1201	7LD	C13-C14	9.04	1.64	1.53
2	C	1201	7LD	C11-C9	-8.86	1.41	1.52
2	C	1201	7LD	C13-N2	-8.53	1.34	1.47
2	B	1201	7LD	C16-N3	8.50	1.47	1.35
2	B	1201	7LD	C11-N2	8.42	1.60	1.48
2	B	1201	7LD	C11-C9	-8.20	1.42	1.52
2	A	1201	7LD	C16-N3	7.83	1.46	1.35
2	C	1201	7LD	C11-N2	7.65	1.59	1.48
2	A	1201	7LD	C11-C9	-6.81	1.44	1.52
2	B	1201	7LD	C14-C10	-5.76	1.39	1.50
2	A	1201	7LD	C14-C10	-5.62	1.39	1.50
2	C	1201	7LD	C3-C1	-4.89	1.33	1.41
2	C	1201	7LD	C14-C10	-4.53	1.42	1.50
2	A	1201	7LD	C6-C9	4.45	1.57	1.48
2	B	1201	7LD	C3-C1	-4.30	1.34	1.41
2	B	1201	7LD	C6-C9	4.21	1.57	1.48
2	B	1201	7LD	C6-C3	-3.85	1.35	1.41
2	A	1201	7LD	C8-C7	3.68	1.42	1.36
2	C	1201	7LD	C3-C7	-3.61	1.35	1.43
2	B	1201	7LD	C3-C7	-3.43	1.35	1.43
4	A	1203	OLA	C10-C9	3.39	1.51	1.31
2	A	1201	7LD	C6-C3	-3.32	1.36	1.41
2	C	1201	7LD	C6-C9	3.27	1.55	1.48
2	C	1201	7LD	C8-C7	3.08	1.41	1.36
2	C	1201	7LD	C6-C3	-3.00	1.36	1.41
4	B	1202	OLA	C10-C9	2.94	1.48	1.31
4	A	1204	OLA	C10-C9	2.94	1.48	1.31
2	A	1201	7LD	C3-C7	-2.86	1.36	1.43
2	A	1201	7LD	C3-C1	-2.81	1.37	1.41
2	B	1201	7LD	C8-C7	2.64	1.40	1.36
2	C	1201	7LD	C1-N1	2.26	1.41	1.37
3	A	1202	CLR	C19-C10	-2.25	1.50	1.54
2	A	1201	7LD	C1-N1	2.05	1.41	1.37
2	A	1201	7LD	C15-C7	2.04	1.53	1.50

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	7LD	C12-N2-C11	-14.99	95.81	111.64
2	B	1201	7LD	C14-C10-C9	-8.76	111.57	123.66
2	A	1201	7LD	C6-C9-C10	-7.89	113.96	123.03
2	B	1201	7LD	C6-C9-C10	-7.65	114.23	123.03
2	C	1201	7LD	C6-C9-C10	-7.32	114.61	123.03
2	A	1201	7LD	C12-N2-C11	-7.27	103.95	111.64
2	C	1201	7LD	C7-C8-N1	-6.68	102.98	110.31
2	C	1201	7LD	C3-C7-C8	6.56	111.68	105.93
2	C	1201	7LD	C15-C11-C9	6.43	121.11	113.42
2	C	1201	7LD	C15-C11-N2	-6.43	98.11	110.22
3	A	1202	CLR	C7-C8-C14	-5.28	103.45	110.93
3	A	1202	CLR	C19-C10-C5	-4.71	101.19	108.38
2	C	1201	7LD	C13-N2-C11	4.65	116.25	110.96
3	A	1202	CLR	C16-C17-C13	4.32	108.92	103.84
2	C	1201	7LD	C15-C7-C8	-4.27	130.90	135.09
2	C	1201	7LD	C14-C10-C9	-4.27	117.76	123.66
3	A	1206	CLR	C21-C20-C17	4.10	119.04	112.88
2	A	1201	7LD	C9-C11-N2	4.05	114.07	110.32
3	A	1206	CLR	C15-C14-C8	-4.04	112.66	119.10
3	A	1202	CLR	C15-C14-C13	4.00	108.54	103.84
2	C	1201	7LD	C9-C11-N2	3.93	113.96	110.32
2	B	1201	7LD	C15-C7-C8	-3.79	131.37	135.09
2	B	1201	7LD	C12-N2-C11	-3.77	107.66	111.64
2	A	1201	7LD	O1-C16-N3	-3.74	117.15	121.61
2	A	1201	7LD	C15-C7-C8	-3.72	131.44	135.09
2	C	1201	7LD	O1-C16-N3	-3.70	117.19	121.61
3	A	1206	CLR	C13-C17-C20	3.65	125.13	119.50
2	A	1201	7LD	C6-C9-C11	3.57	120.56	115.00
3	A	1202	CLR	C21-C20-C17	-3.43	107.74	112.88
2	B	1201	7LD	C7-C8-N1	-3.43	106.54	110.31
3	A	1206	CLR	C8-C7-C6	-3.34	108.14	112.76
3	A	1206	CLR	C9-C10-C5	3.32	114.52	109.65
2	C	1201	7LD	C4-C1-N1	3.31	136.04	130.74
2	A	1201	7LD	C15-C7-C3	3.25	122.04	119.05
3	A	1206	CLR	C1-C2-C3	3.03	114.49	110.48
2	B	1201	7LD	C11-C9-C10	-3.02	111.93	121.40
3	A	1206	CLR	C15-C14-C13	3.00	107.37	103.84
3	A	1202	CLR	C18-C13-C12	-2.99	106.20	110.61
2	B	1201	7LD	C15-C7-C3	2.97	121.78	119.05
2	A	1201	7LD	C15-C11-C9	2.93	116.93	113.42
2	B	1201	7LD	C13-N2-C11	-2.80	107.77	110.96
3	A	1202	CLR	C16-C17-C20	-2.74	108.03	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	7LD	C4-C1-N1	2.74	135.12	130.74
3	A	1206	CLR	C3-C4-C5	-2.73	107.71	112.05
3	A	1202	CLR	C1-C10-C9	2.71	112.32	108.74
2	A	1201	7LD	C14-C10-C9	-2.64	120.01	123.66
2	A	1201	7LD	C4-C1-N1	2.61	134.92	130.74
2	C	1201	7LD	C6-C3-C7	2.53	129.49	127.74
3	A	1202	CLR	C12-C13-C17	2.52	120.32	116.60
4	A	1203	OLA	C11-C10-C9	-2.52	105.93	124.83
2	C	1201	7LD	C12-N2-C13	2.51	114.51	109.64
3	A	1202	CLR	C14-C8-C9	-2.50	105.82	109.09
2	C	1201	7LD	C4-C1-C3	-2.49	116.43	121.75
3	A	1202	CLR	C4-C5-C10	2.49	119.61	116.42
2	A	1201	7LD	C7-C8-N1	-2.43	107.64	110.31
4	A	1204	OLA	O2-C1-C2	2.39	121.57	114.00
2	C	1201	7LD	C11-C15-C7	2.35	113.92	110.05
3	A	1202	CLR	C9-C10-C5	2.34	113.08	109.65
2	B	1201	7LD	C6-C9-C11	2.29	118.56	115.00
3	A	1206	CLR	C18-C13-C14	-2.29	107.52	111.68
3	A	1202	CLR	C17-C13-C14	-2.25	97.52	100.10
3	A	1206	CLR	C2-C3-C4	-2.23	107.15	110.29
3	A	1206	CLR	C7-C8-C9	2.22	112.29	109.72
3	A	1202	CLR	C19-C10-C9	-2.21	109.18	111.66
3	A	1206	CLR	C14-C8-C9	-2.20	106.21	109.09
3	A	1202	CLR	C4-C5-C6	-2.19	117.61	120.57
3	A	1202	CLR	C10-C9-C8	-2.15	109.57	112.71
2	A	1201	7LD	C11-C15-C7	2.14	113.57	110.05
2	B	1201	7LD	C1-C3-C7	2.12	111.34	108.01
3	A	1202	CLR	C11-C9-C8	-2.10	108.85	111.78
3	A	1206	CLR	C1-C10-C5	-2.07	105.17	108.74
3	A	1202	CLR	C13-C14-C8	2.07	117.35	114.41
3	A	1202	CLR	C16-C15-C14	-2.06	101.11	105.14

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1201	7LD	C13-C14-C16-N3
2	C	1201	7LD	C13-C14-C16-O1
3	A	1202	CLR	C13-C17-C20-C21
3	A	1202	CLR	C13-C17-C20-C22
3	A	1206	CLR	C16-C17-C20-C21
3	A	1206	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
3	A	1206	CLR	C16-C17-C20-C22
3	A	1202	CLR	C21-C20-C22-C23
3	A	1202	CLR	C16-C17-C20-C21
3	A	1206	CLR	C13-C17-C20-C22
3	A	1202	CLR	C16-C17-C20-C22
4	A	1203	OLA	C3-C4-C5-C6
3	A	1202	CLR	C17-C20-C22-C23
4	A	1204	OLA	C11-C10-C9-C8
4	A	1204	OLA	C11-C12-C13-C14
2	C	1201	7LD	C20-C19-N3-C17
4	A	1204	OLA	C1-C2-C3-C4
3	A	1206	CLR	C20-C22-C23-C24
2	C	1201	7LD	C20-C19-N3-C16
4	A	1203	OLA	C13-C14-C15-C16
7	C	1204	1PE	OH5-C14-C24-OH4
4	A	1204	OLA	C10-C11-C12-C13
4	A	1203	OLA	C7-C8-C9-C10
5	C	1202	PEG	O2-C3-C4-O4
2	A	1201	7LD	C18-C17-N3-C16
4	A	1203	OLA	C4-C5-C6-C7
4	B	1202	OLA	C11-C10-C9-C8
4	A	1203	OLA	C12-C13-C14-C15
4	A	1203	OLA	C6-C7-C8-C9
4	A	1204	OLA	C4-C5-C6-C7
5	A	1205	PEG	C1-C2-O2-C3
4	A	1203	OLA	C5-C6-C7-C8
4	A	1204	OLA	C13-C14-C15-C16
4	A	1204	OLA	C3-C4-C5-C6
5	C	1202	PEG	C4-C3-O2-C2
3	A	1202	CLR	C23-C24-C25-C27
3	A	1206	CLR	C21-C20-C22-C23
4	A	1204	OLA	C15-C16-C17-C18
3	A	1206	CLR	C23-C24-C25-C26
7	C	1204	1PE	C14-C24-OH4-C13
3	A	1206	CLR	C23-C24-C25-C27
7	C	1204	1PE	C24-C14-OH5-C25
4	B	1202	OLA	C9-C10-C11-C12
4	A	1203	OLA	C1-C2-C3-C4
4	A	1203	OLA	C9-C10-C11-C12
7	C	1204	1PE	OH7-C16-C26-OH6
7	C	1204	1PE	OH6-C15-C25-OH5
2	A	1201	7LD	C18-C17-N3-C19

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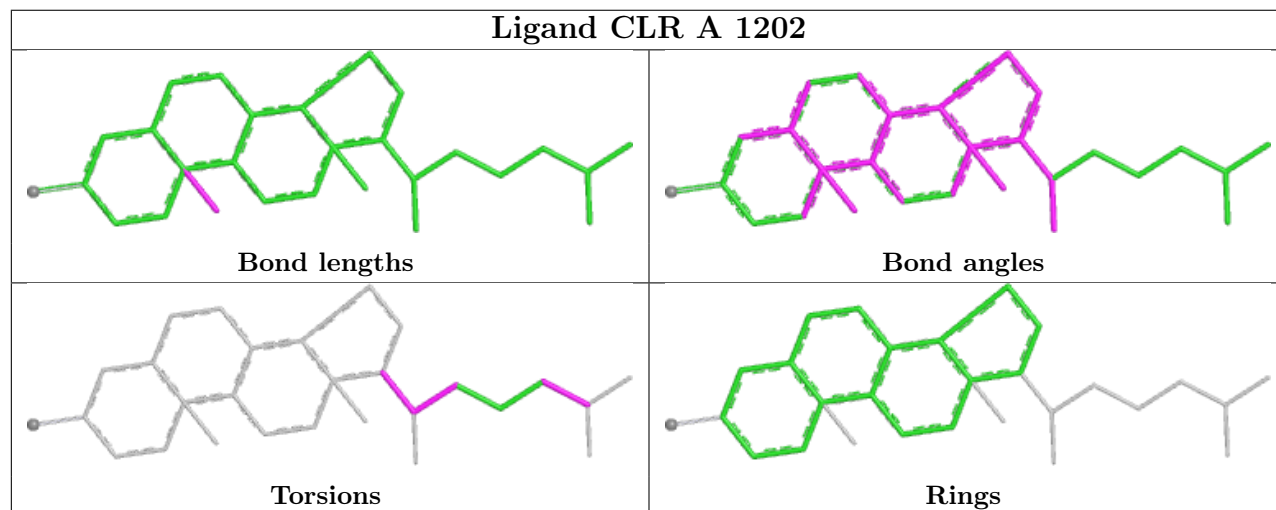
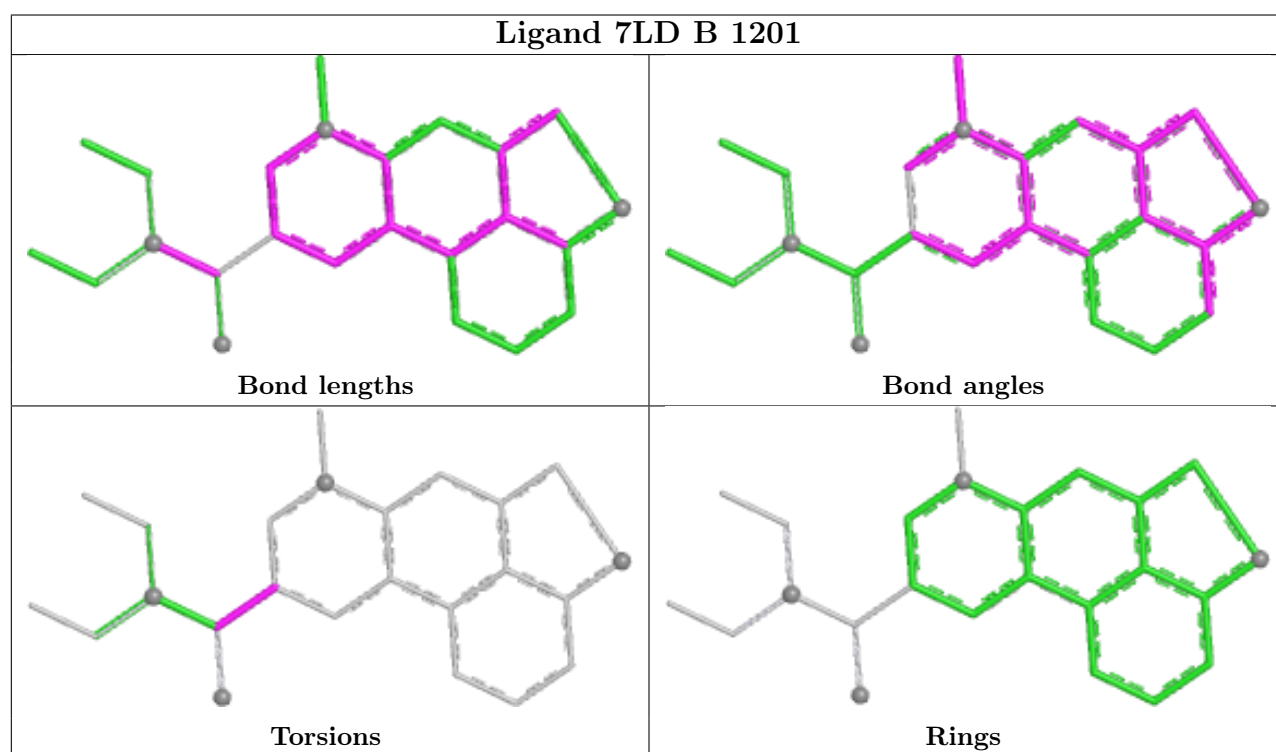
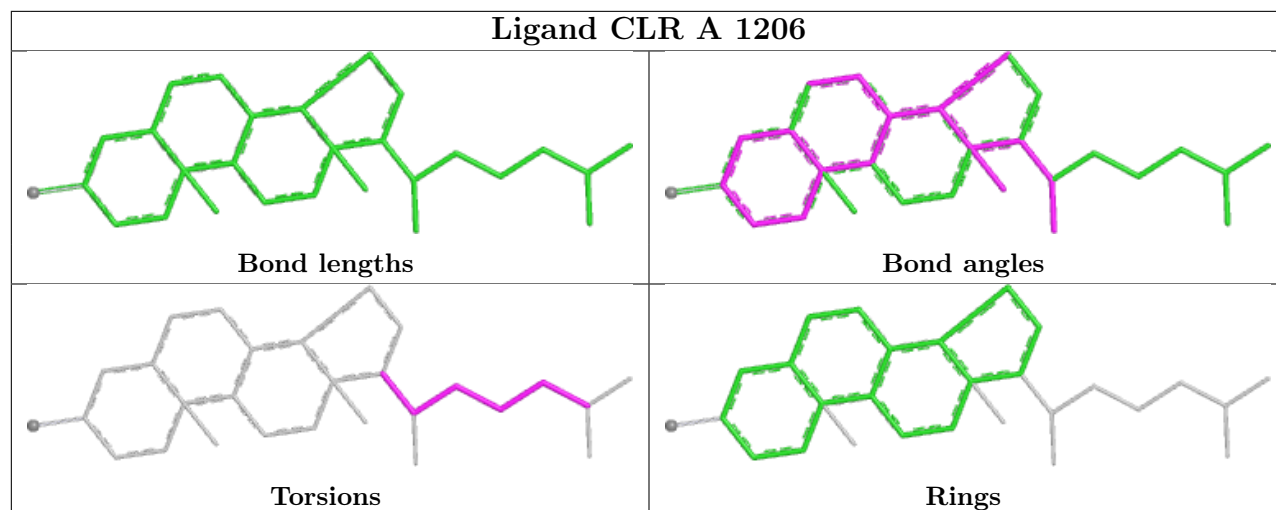
Mol	Chain	Res	Type	Atoms
2	B	1201	7LD	C10-C14-C16-O1
2	C	1201	7LD	C10-C14-C16-O1
3	A	1206	CLR	C17-C20-C22-C23
7	C	1204	1PE	C23-C13-OH4-C24
5	A	1205	PEG	C4-C3-O2-C2
7	C	1204	1PE	C16-C26-OH6-C15
4	A	1204	OLA	C5-C6-C7-C8
4	A	1204	OLA	O2-C1-C2-C3
4	A	1204	OLA	C12-C13-C14-C15
4	A	1204	OLA	C6-C7-C8-C9
4	A	1204	OLA	O1-C1-C2-C3
3	A	1206	CLR	C22-C23-C24-C25

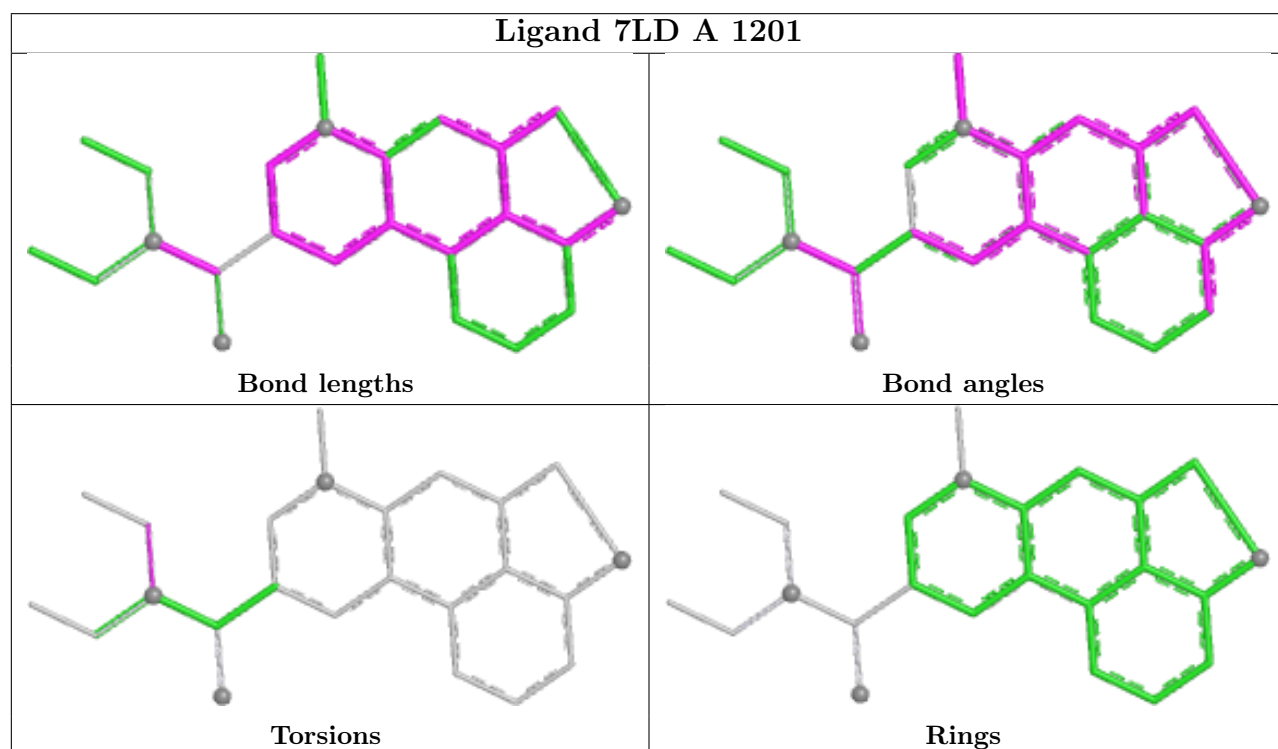
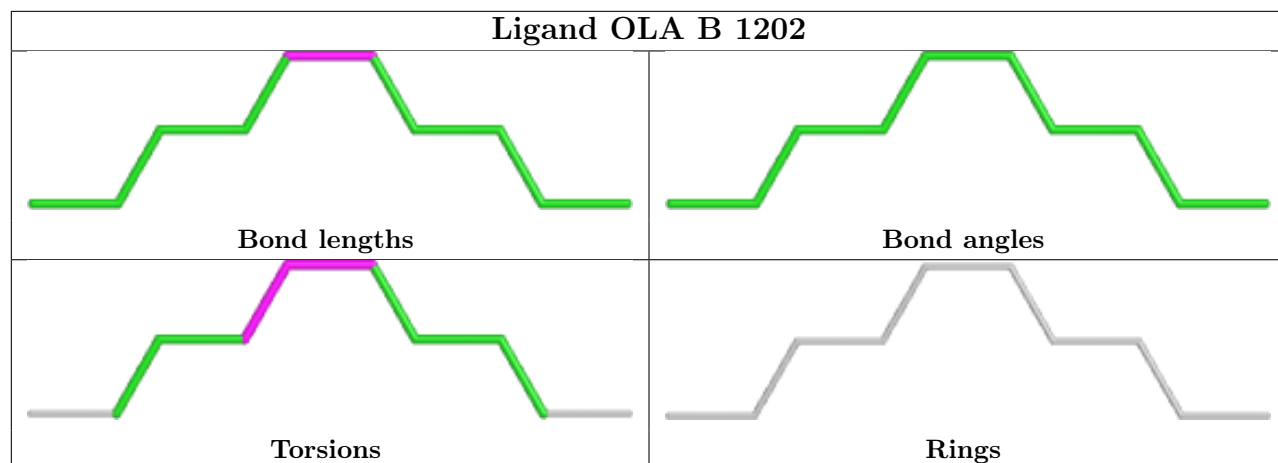
There are no ring outliers.

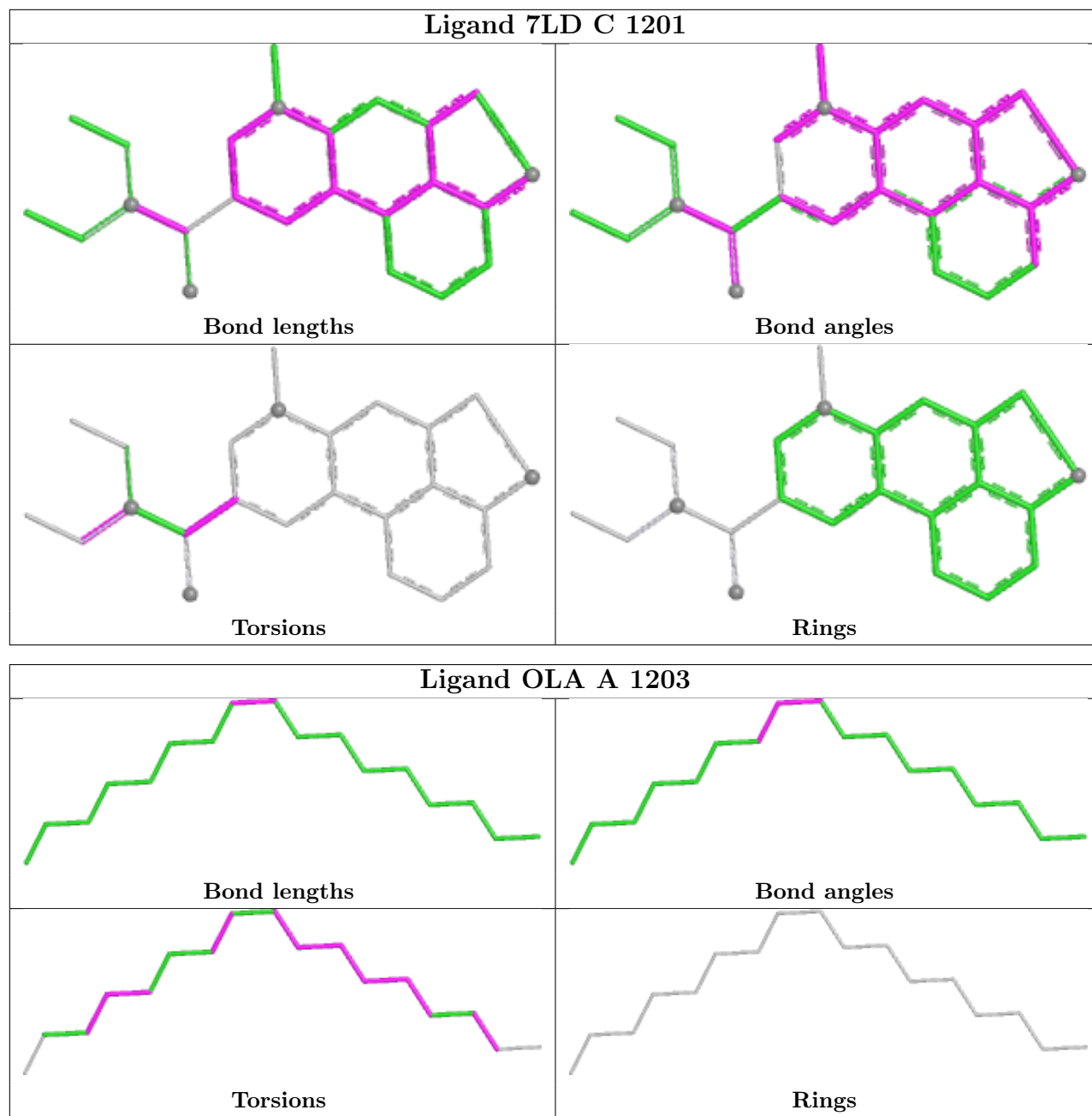
8 monomers are involved in 31 short contacts:

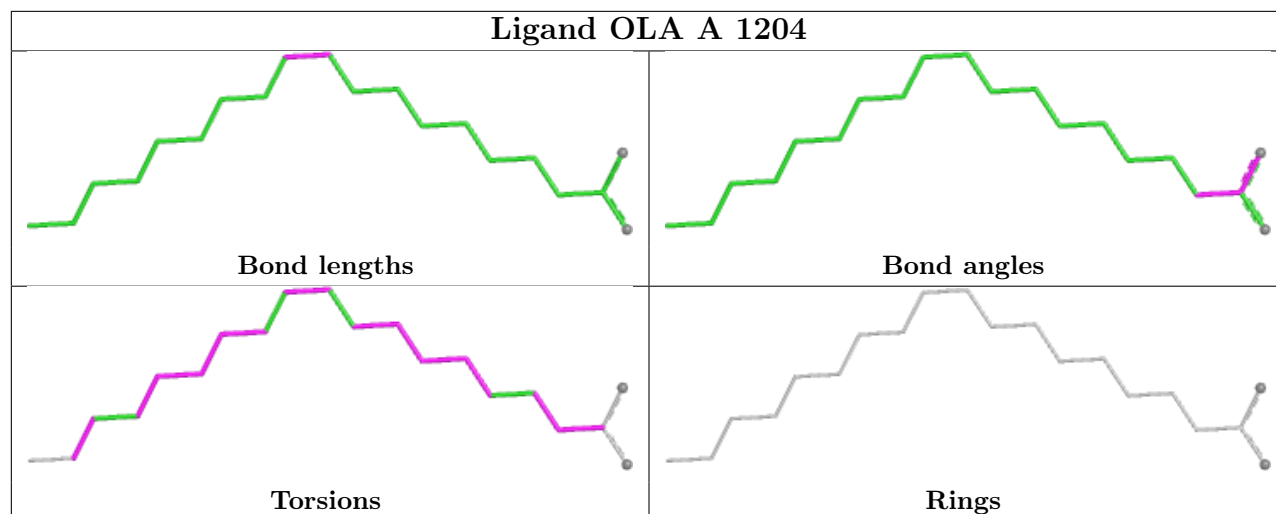
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1206	CLR	10	0
2	B	1201	7LD	1	0
5	A	1205	PEG	1	0
3	A	1202	CLR	8	0
7	C	1204	1PE	3	0
6	B	1204	PO4	1	0
4	A	1203	OLA	3	0
4	A	1204	OLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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, 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	377/448 (84%)	0.34	21 (5%) 30 23	19, 43, 97, 120	0
1	B	358/448 (79%)	0.43	14 (3%) 43 31	22, 56, 106, 126	0
1	C	376/448 (83%)	0.34	20 (5%) 32 24	20, 46, 85, 105	0
All	All	1111/1344 (82%)	0.37	55 (4%) 34 25	19, 48, 100, 126	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1035	ALA	6.4
1	C	176	ALA	4.9
1	A	1054	ASP	4.0
1	B	1036	ALA	4.0
1	B	1039	ASP	3.8
1	C	215	LEU	3.4
1	A	353	CYS	3.4
1	C	254	TYR	3.3
1	C	225	GLY	3.3
1	A	1060	ASP	3.1
1	C	179	ASN	3.1
1	C	1063	HIS	3.0
1	A	108	ALA	2.8
1	C	383	PHE	2.8
1	C	1045	PRO	2.8
1	B	1065	PHE	2.7
1	A	166	LEU	2.7
1	C	318	GLU	2.7
1	A	1029	ALA	2.6
1	C	1092	GLU	2.6
1	C	395	ILE	2.6
1	C	1064	GLY	2.6
1	A	83	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	175	VAL	2.6
1	A	176	ALA	2.6
1	C	224	GLU	2.5
1	A	1046	PRO	2.5
1	B	1066	ASP	2.5
1	B	188	SER	2.4
1	A	1068	LEU	2.4
1	A	179	ASN	2.4
1	C	178	GLN	2.4
1	B	171	LEU	2.3
1	B	215	LEU	2.3
1	A	352	SER	2.3
1	B	1060	ASP	2.3
1	A	1086	GLU	2.3
1	A	1047	LYS	2.3
1	A	226	SER	2.3
1	C	226	SER	2.3
1	B	1038	LEU	2.3
1	A	1050	ASP	2.3
1	A	210	ILE	2.2
1	B	1100	ALA	2.2
1	C	1062	ARG	2.2
1	A	1055	SER	2.2
1	C	227	CYS	2.2
1	C	354	ASN	2.1
1	A	125	PHE	2.1
1	C	206	ILE	2.1
1	B	105	LEU	2.1
1	A	213	PHE	2.1
1	C	183	HIS	2.1
1	A	1025	GLN	2.1
1	B	176	ALA	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 oligosaccharides in this entry.

6.4 Ligands

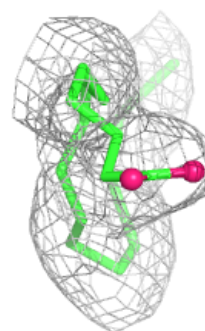
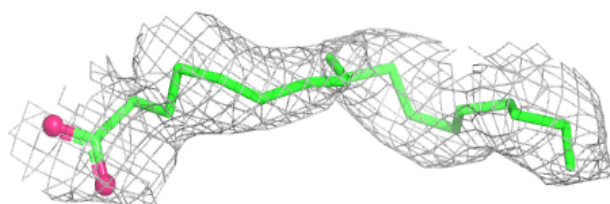
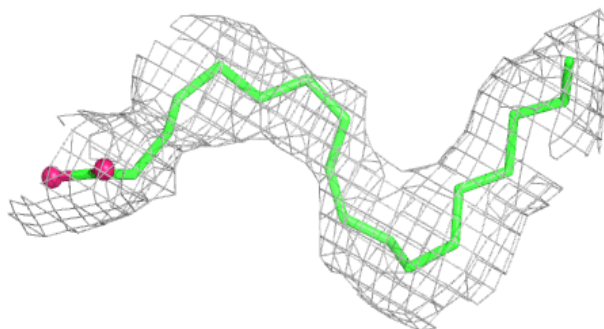
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	C	1203	5/5	0.69	0.13	78,79,93,105	0
5	PEG	C	1202	7/7	0.80	0.23	29,32,41,48	0
4	OLA	A	1204	20/20	0.81	0.16	23,48,74,75	0
3	CLR	A	1202	28/28	0.82	0.17	19,53,62,64	0
4	OLA	B	1202	10/20	0.82	0.22	23,27,35,37	0
4	OLA	A	1203	17/20	0.83	0.23	21,25,33,40	0
3	CLR	A	1206	28/28	0.85	0.16	45,51,63,67	0
2	7LD	C	1201	24/24	0.89	0.18	28,36,55,62	0
2	7LD	B	1201	24/24	0.89	0.18	37,43,57,64	0
6	PO4	B	1203	5/5	0.90	0.23	59,70,86,91	0
5	PEG	A	1205	7/7	0.93	0.12	28,34,41,41	0
2	7LD	A	1201	24/24	0.93	0.13	24,31,35,40	0
7	1PE	C	1204	16/16	0.93	0.14	43,49,76,80	0
6	PO4	B	1204	5/5	0.96	0.19	65,70,89,97	0

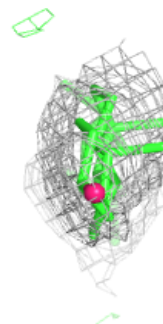
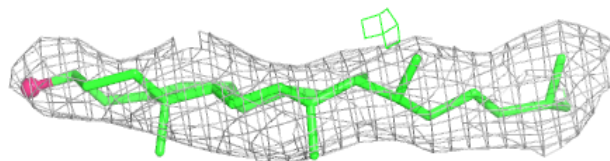
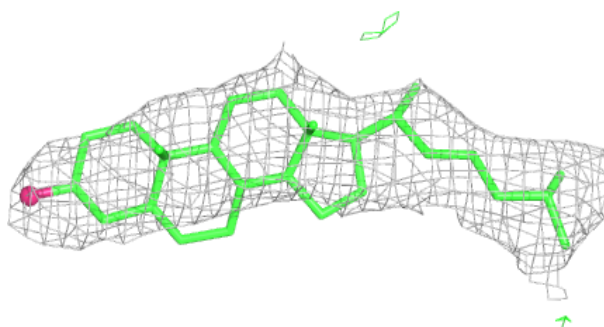
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLA A 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

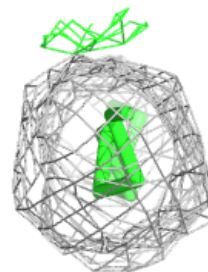
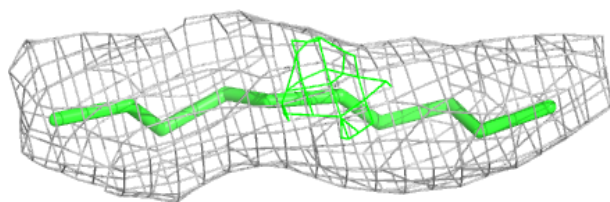
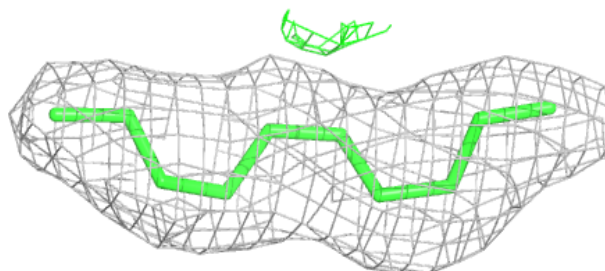
**Electron density around CLR A 1202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

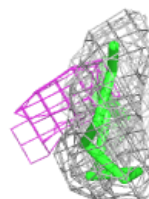
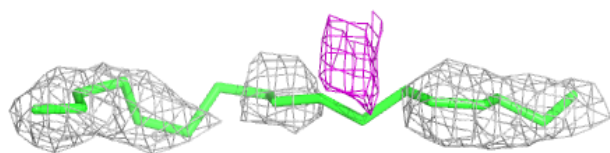
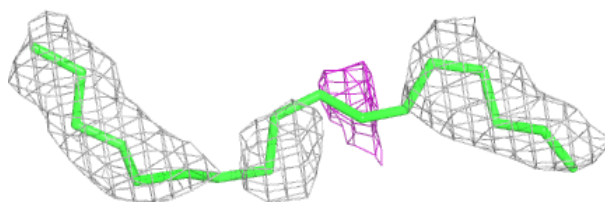


Electron density around OLA B 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

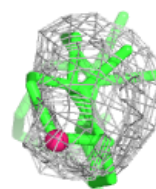
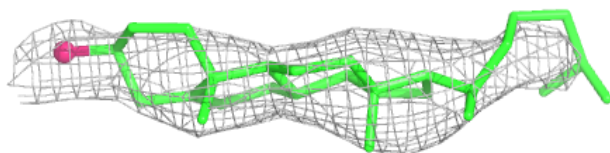
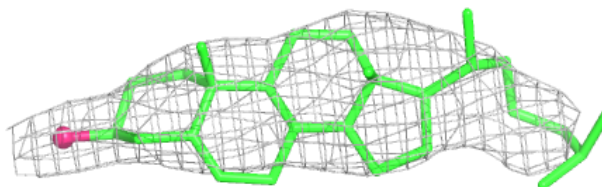
**Electron density around OLA A 1203:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

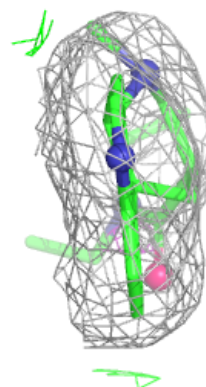
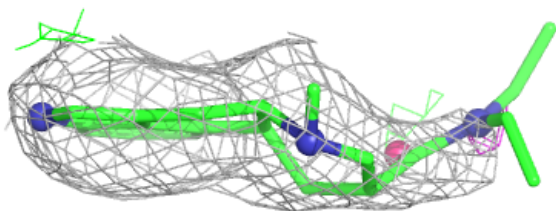
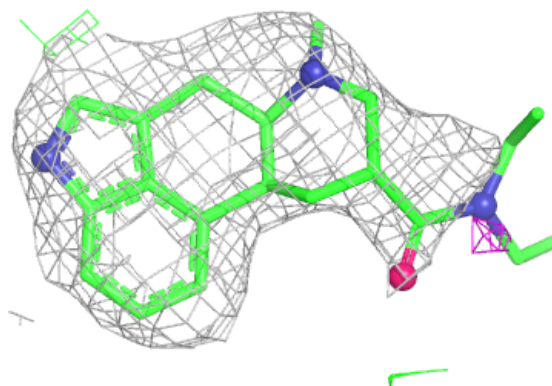


Electron density around CLR A 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

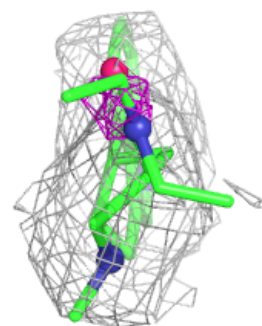
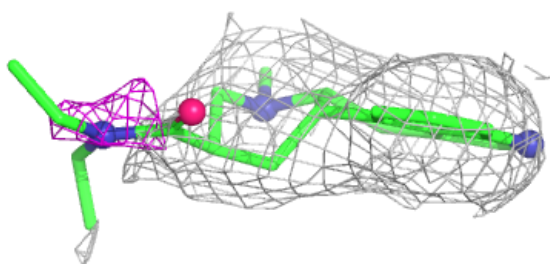
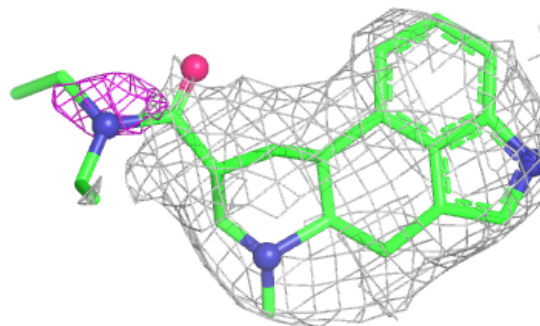
**Electron density around 7LD C 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

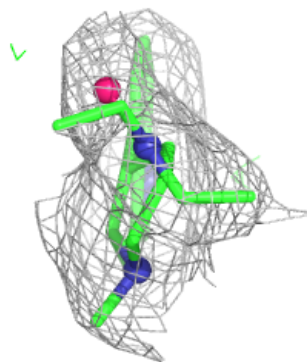
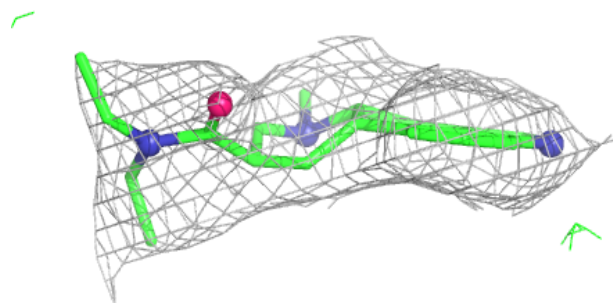
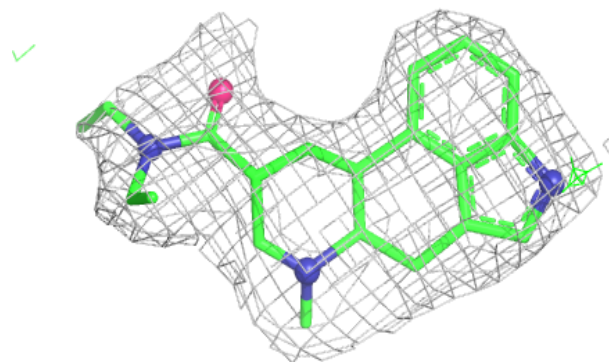


Electron density around 7LD B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 7LD A 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.