



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2017 – 05:13 PM EST

PDB ID : 4N6H
Title : 1.8 Å Structure of the human delta opioid 7TM receptor (PSI Community Target)
Authors : Fenalti, G.; Giguere, P.M.; Katritch, V.; Huang, X.-P.; Thompson, A.A.; Han, G.W.; Cherezov, V.; Roth, B.L.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on : unknown
Resolution : 1.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

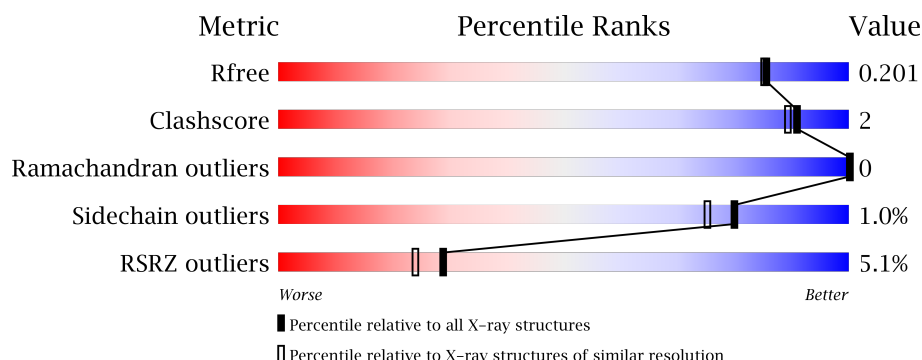
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 ≥ 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	414	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 93%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <div>5% 93% 5% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLA	A	1201	-	-	-	X
2	OLA	A	1202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLA	A	1203	-	-	-	X
2	OLA	A	1204	-	-	-	X
2	OLA	A	1205	-	-	-	X
2	OLA	A	1209	-	-	-	X
2	OLA	A	1210	-	-	-	X
2	OLA	A	1211	-	-	-	X
2	OLA	A	1216	-	-	-	X
2	OLA	A	1217	-	-	-	X
3	OLC	A	1207	-	-	-	X
3	OLC	A	1208	-	-	-	X
3	OLC	A	1223	-	-	-	X
4	PGE	A	1214	-	-	-	X
4	PGE	A	1221	-	-	-	X
5	TLA	A	1218	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3582 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.

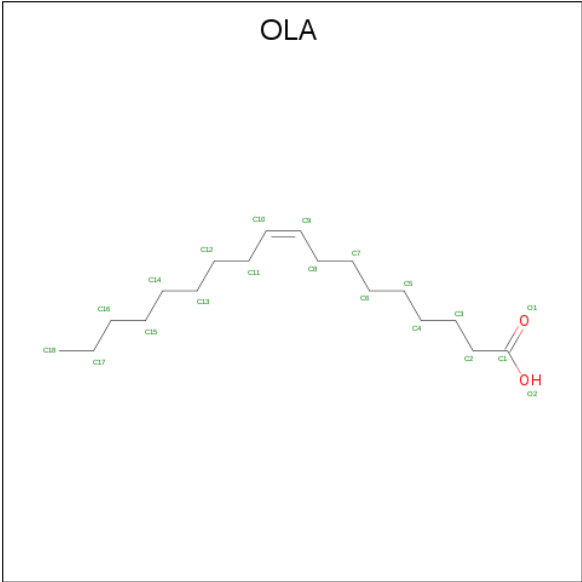
- Molecule 1 is a protein called Soluble cytochrome b562, Delta-type opioid receptor chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	8	0
			3140	2060	511	542	27			

There are 9 discrepancies between the modelled and reference sequences:

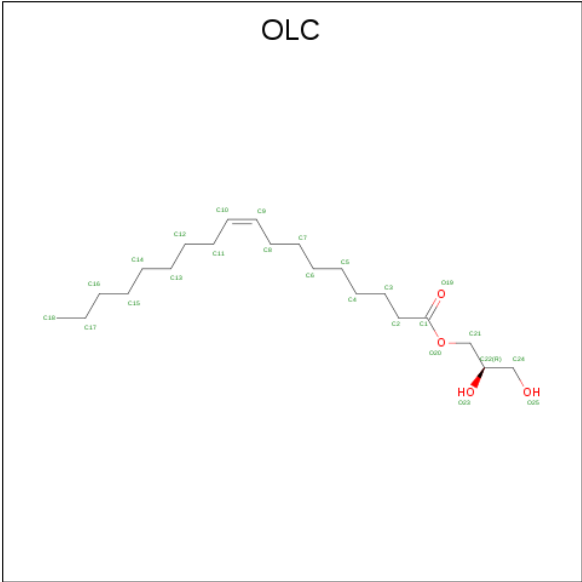
Chain	Residue	Modelled	Actual	Comment	Reference
A	996	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	997	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	998	THR	-	EXPRESSION TAG	UNP P0ABE7
A	999	THR	-	EXPRESSION TAG	UNP P0ABE7
A	1000	MET	-	EXPRESSION TAG	UNP P0ABE7
A	1007	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
A	1102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	1106	LEU	ARG	ENGINEERED MUTATION	UNP P0ABE7
A	37	SER	PRO	ENGINEERED MUTATION	UNP P41143

- Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



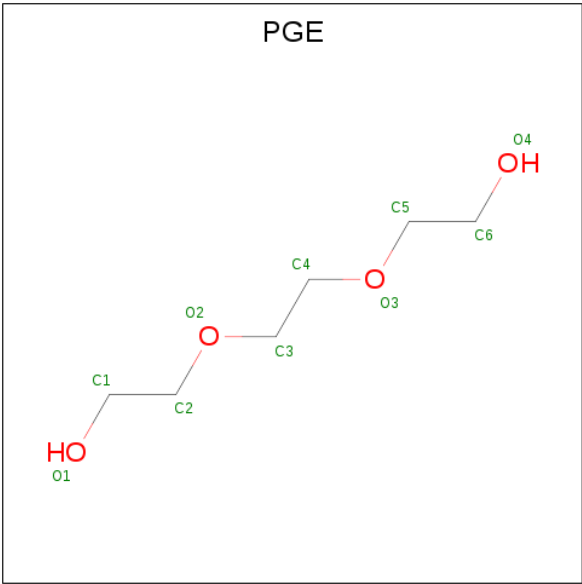
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	17	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			15	13	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			9	7	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			11	9	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			8	6	2		

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



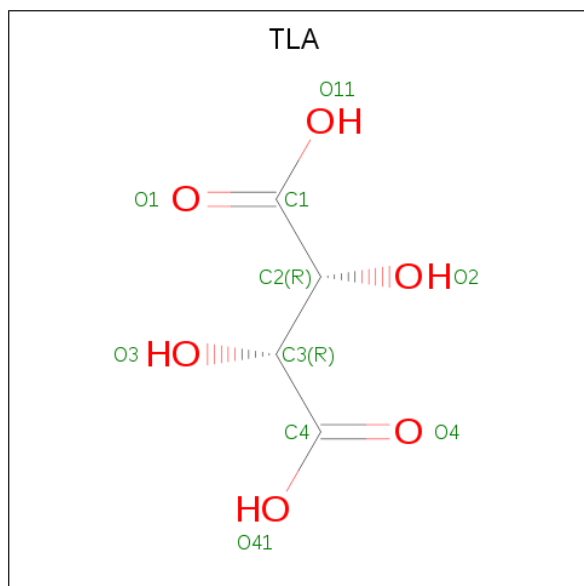
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	9	4		
3	A	1	Total	C	O	0	0
			18	14	4		
3	A	1	Total	C	O	0	0
			16	12	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



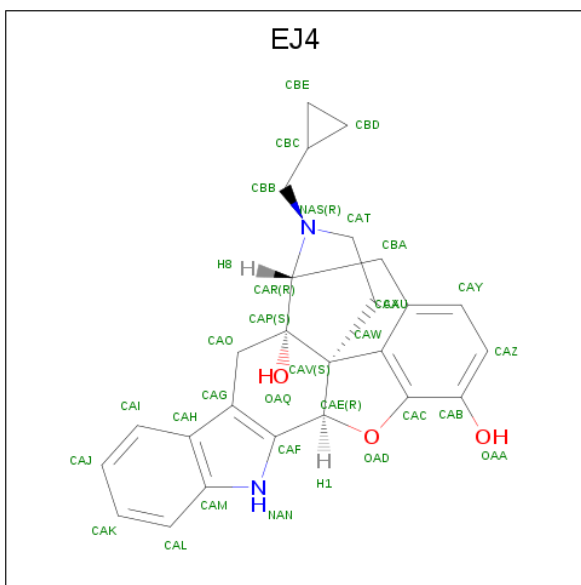
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is (4bS,8R,8aS,14bR)-7-(cyclopropylmethyl)-5,6,7,8,14,14b-hexahydro-4,8-methano[1]benzofuro[2,3-a]pyrido[4,3-b]carbazole-1,8a(9H)-diol (three-letter code: EJ4) (formula: $C_{26}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			31	26	2	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

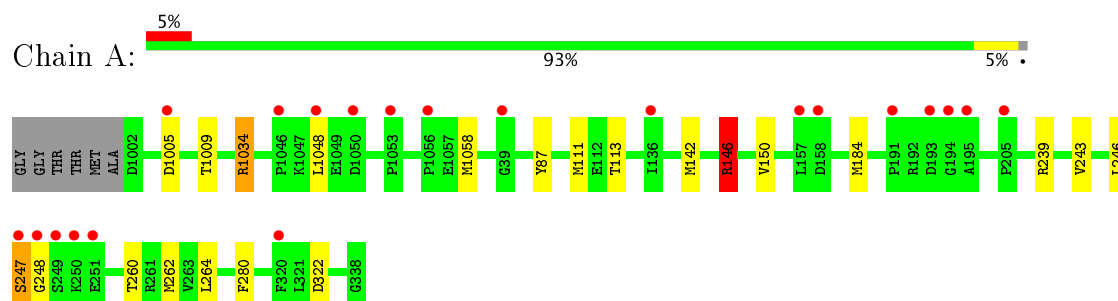
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	101	Total O 101 101	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Soluble cytochrome b562, Delta-type opioid receptor chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.23Å 72.85Å 84.41Å 90.00° 107.48° 90.00°	Depositor
Resolution (Å)	29.70 – 1.80 29.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.70-1.80) 98.3 (29.69-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.190 0.183 , 0.201	Depositor DCC
R_{free} test set	2303 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3582	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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: OLA, OLC, NA, TLA, PGE, EJ4

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	0.56	0/3218	0.68	3/4384 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1034	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	1034	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	146	ARG	NE-CZ-NH1	5.13	122.86	120.30

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	3140	0	3200	14	0
2	A	175	0	245	0	0
3	A	94	0	130	1	0
4	A	30	0	42	0	0
5	A	10	0	4	0	0
6	A	31	0	26	0	0
7	A	1	0	0	0	0
8	A	101	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3582	0	3647	14	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 2.

All (14) 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:247:SER:OG	1:A:248:GLY:N	2.24	0.70
1:A:1034:ARG:HD2	8:A:1335:HOH:O	1.95	0.67
1:A:87:TYR:CB	1:A:142[A]:MET:HG2	2.29	0.63
1:A:87:TYR:HB3	1:A:142[A]:MET:CG	2.30	0.61
1:A:150:VAL:HG12	1:A:239:ARG:HG2	1.85	0.57
1:A:243[A]:VAL:HG21	1:A:246:LEU:HD23	1.88	0.54
1:A:1005:ASP:O	1:A:1009:THR:HG23	2.10	0.51
1:A:184[B]:MET:SD	3:A:1223:OLC:H6A	2.51	0.50
1:A:111:MET:HG2	1:A:113:THR:HG22	1.93	0.50
1:A:243[A]:VAL:CG2	1:A:246:LEU:HD23	2.46	0.45
1:A:262:MET:SD	1:A:322:ASP:HB2	2.57	0.45
1:A:260:THR:O	1:A:264:LEU:HG	2.18	0.44
1:A:146:ARG:HD3	1:A:260:THR:HA	1.99	0.43
1:A:1048:LEU:HD23	1:A:1058:MET:SD	2.61	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	414/414 (100%)	412 (100%)	2 (0%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/348 (93%)	320 (99%)	3 (1%)	82	78

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

Mol	Chain	Res	Type
1	A	146	ARG
1	A	247	SER
1	A	280	PHE

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](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLA	A	1201	-	15,18,19	0.31	0	14,18,19	0.37	0
2	OLA	A	1202	-	16,19,19	0.31	0	15,19,19	0.39	0
2	OLA	A	1203	-	11,14,19	0.28	0	10,14,19	0.47	0
2	OLA	A	1204	-	16,19,19	0.24	0	15,19,19	0.54	0
2	OLA	A	1205	-	16,19,19	0.28	0	15,19,19	0.50	0
2	OLA	A	1206	-	5,8,19	0.21	0	4,8,19	0.53	0
3	OLC	A	1207	-	12,12,24	1.36	1 (8%)	13,13,25	1.19	1 (7%)
3	OLC	A	1208	-	17,17,24	1.23	1 (5%)	18,18,25	1.13	2 (11%)
2	OLA	A	1209	-	9,12,19	0.38	0	8,12,19	0.50	0
2	OLA	A	1210	-	7,10,19	0.23	0	6,10,19	0.59	0
2	OLA	A	1211	-	9,12,19	0.36	0	8,12,19	0.63	0
3	OLC	A	1212	-	15,15,24	1.08	1 (6%)	16,16,25	0.98	1 (6%)
4	PGE	A	1213	-	9,9,9	0.44	0	8,8,8	0.29	0
4	PGE	A	1214	-	9,9,9	0.47	0	8,8,8	0.35	0
2	OLA	A	1215	-	10,13,19	0.35	0	9,13,19	0.58	0
2	OLA	A	1216	-	9,12,19	0.30	0	8,12,19	0.78	0
2	OLA	A	1217	-	4,7,19	0.26	0	3,7,19	0.35	0
5	TLA	A	1218	-	3,9,9	0.34	0	6,12,12	0.52	0
6	EJ4	A	1219	-	36,38,38	3.10	13 (36%)	51,63,63	2.12	14 (27%)
4	PGE	A	1221	-	9,9,9	0.56	0	8,8,8	0.22	0
3	OLC	A	1222	-	21,21,24	0.80	1 (4%)	22,22,25	0.88	1 (4%)
3	OLC	A	1223	-	24,24,24	0.94	1 (4%)	25,25,25	0.88	1 (4%)

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	OLA	A	1201	-	-	0/14/16/17	0/0/0/0
2	OLA	A	1202	-	-	0/15/17/17	0/0/0/0
2	OLA	A	1203	-	-	0/10/12/17	0/0/0/0
2	OLA	A	1204	-	-	0/15/17/17	0/0/0/0
2	OLA	A	1205	-	-	0/15/17/17	0/0/0/0
2	OLA	A	1206	-	-	0/4/6/17	0/0/0/0
3	OLC	A	1207	-	-	0/12/12/24	0/0/0/0
3	OLC	A	1208	-	-	0/17/17/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1209	-	-	0/8/10/17	0/0/0/0
2	OLA	A	1210	-	-	0/6/8/17	0/0/0/0
2	OLA	A	1211	-	-	0/8/10/17	0/0/0/0
3	OLC	A	1212	-	-	0/15/15/24	0/0/0/0
4	PGE	A	1213	-	-	0/7/7/7	0/0/0/0
4	PGE	A	1214	-	-	0/7/7/7	0/0/0/0
2	OLA	A	1215	-	-	0/9/11/17	0/0/0/0
2	OLA	A	1216	-	-	0/8/10/17	0/0/0/0
2	OLA	A	1217	-	-	0/3/5/17	0/0/0/0
5	TLA	A	1218	-	-	0/4/12/12	0/0/0/0
6	EJ4	A	1219	-	-	0/4/60/60	0/0/8/8
4	PGE	A	1221	-	-	0/7/7/7	0/0/0/0
3	OLC	A	1222	-	-	0/21/21/24	0/0/0/0
3	OLC	A	1223	-	-	0/24/24/24	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1219	EJ4	CBA-CAR	-5.47	1.46	1.55
6	A	1219	EJ4	CAO-CAG	-5.03	1.44	1.51
6	A	1219	EJ4	CBA-CAX	-4.90	1.42	1.51
6	A	1219	EJ4	CAL-CAM	-3.36	1.35	1.41
6	A	1219	EJ4	CAH-CAM	-2.94	1.34	1.42
6	A	1219	EJ4	CAG-CAH	-2.92	1.36	1.41
6	A	1219	EJ4	CAI-CAH	-2.74	1.36	1.42
6	A	1219	EJ4	CAV-CAW	-2.67	1.45	1.50
6	A	1219	EJ4	CAX-CAW	-2.24	1.35	1.39
6	A	1219	EJ4	CAP-CAV	3.06	1.58	1.53
3	A	1222	OLC	O20-C1	3.08	1.42	1.33
3	A	1212	OLC	O20-C1	3.98	1.45	1.33
6	A	1219	EJ4	CAR-NAS	4.04	1.52	1.48
3	A	1223	OLC	O20-C1	4.25	1.45	1.33
6	A	1219	EJ4	OAQ-CAP	4.47	1.51	1.44
3	A	1207	OLC	O20-C1	4.50	1.46	1.33
3	A	1208	OLC	O20-C1	4.66	1.47	1.33
6	A	1219	EJ4	OAD-CAE	11.85	1.63	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1219	EJ4	OAD-CAE-CAV	-7.53	99.57	104.92
6	A	1219	EJ4	CBA-CAR-NAS	-3.70	111.50	115.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1219	EJ4	CAP-CAV-CAE	-3.38	115.28	118.19
6	A	1219	EJ4	CAV-CAW-CAX	-2.93	122.41	126.07
6	A	1219	EJ4	CAT-NAS-CAR	-2.44	106.55	111.05
6	A	1219	EJ4	OAD-CAC-CAW	-2.38	109.93	112.83
6	A	1219	EJ4	CAB-CAC-CAW	-2.29	117.75	120.88
3	A	1222	OLC	O20-C1-O19	-2.18	118.13	123.55
3	A	1208	OLC	O20-C1-O19	-2.16	118.18	123.55
3	A	1212	OLC	O20-C1-C2	2.37	118.79	111.90
6	A	1219	EJ4	CBB-NAS-CAR	2.50	118.64	113.55
3	A	1223	OLC	O20-C1-C2	2.65	119.61	111.90
6	A	1219	EJ4	CAT-CAU-CAV	2.78	114.66	111.72
3	A	1207	OLC	O20-C1-C2	2.94	120.47	111.90
6	A	1219	EJ4	CAV-CAW-CAC	3.13	112.34	109.27
6	A	1219	EJ4	OAD-CAC-CAB	3.29	132.25	126.19
3	A	1208	OLC	O20-C1-C2	3.37	121.71	111.90
6	A	1219	EJ4	CAX-CBA-CAR	4.12	120.72	114.44
6	A	1219	EJ4	CAW-CAV-CAE	4.32	103.00	98.58
6	A	1219	EJ4	CAP-CAR-NAS	4.51	109.19	105.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1223	OLC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	408/414 (98%)	-0.01	21 (5%) 29 24	21, 34, 61, 80	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	GLY	4.4
1	A	158	ASP	4.1
1	A	1005	ASP	3.4
1	A	195	ALA	3.2
1	A	1050	ASP	3.1
1	A	251	GLU	3.1
1	A	194	GLY	2.8
1	A	1056	PRO	2.7
1	A	205	PRO	2.6
1	A	193	ASP	2.5
1	A	1048	LEU	2.5
1	A	320	PHE	2.5
1	A	1046	PRO	2.4
1	A	191	PRO	2.4
1	A	136	ILE	2.4
1	A	39	GLY	2.4
1	A	1053	PRO	2.4
1	A	249	SER	2.2
1	A	250	LYS	2.1
1	A	157	LEU	2.0
1	A	247	SER	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OLA	A	1211	13/20	0.88	0.32	8.43	65,68,77,80	0
2	OLA	A	1209	13/20	0.59	0.26	8.27	65,81,91,92	0
2	OLA	A	1205	20/20	0.77	0.20	4.51	60,69,74,80	0
3	OLC	A	1208	18/25	0.75	0.25	4.02	65,71,75,78	0
2	OLA	A	1203	15/20	0.66	0.23	3.86	69,76,86,88	0
2	OLA	A	1201	19/20	0.70	0.18	3.47	48,57,69,70	0
2	OLA	A	1210	11/20	0.64	0.23	3.30	75,81,89,95	0
3	OLC	A	1207	13/25	0.78	0.21	3.13	50,58,68,74	0
2	OLA	A	1202	20/20	0.62	0.15	2.93	57,62,84,85	0
4	PGE	A	1214	10/10	0.67	0.17	2.79	58,68,80,83	0
3	OLC	A	1223	25/25	0.85	0.15	2.49	49,58,61,62	0
5	TLA	A	1218	10/10	0.79	0.17	2.16	35,50,58,59	0
2	OLA	A	1217	8/20	0.77	0.13	2.15	72,75,85,85	0
4	PGE	A	1221	10/10	0.67	0.20	2.15	59,63,69,71	0
2	OLA	A	1204	20/20	0.85	0.14	2.05	55,63,70,77	0
2	OLA	A	1216	13/20	0.71	0.23	2.05	75,77,88,90	0
3	OLC	A	1212	16/25	0.78	0.13	1.96	56,68,72,76	0
2	OLA	A	1206	9/20	0.79	0.13	1.38	48,59,62,63	0
3	OLC	A	1222	22/25	0.93	0.12	0.90	33,42,53,61	0
6	EJ4	A	1219	31/31	0.94	0.14	0.56	22,25,29,31	0
4	PGE	A	1213	10/10	0.93	0.10	0.40	55,59,62,66	0
7	NA	A	1220	1/1	0.99	0.07	-2.27	26,26,26,26	0
2	OLA	A	1215	14/20	0.67	0.30	-	66,74,83,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.