



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:48 PM UTC

PDB ID : 3UTY / pdb_00003uty
Title : Crystal structure of bacteriorhodopsin mutant P50A/T46A
Authors : Cao, Z.; Bowie, J.U.
Deposited on : 2011-11-27
Resolution : 2.37 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

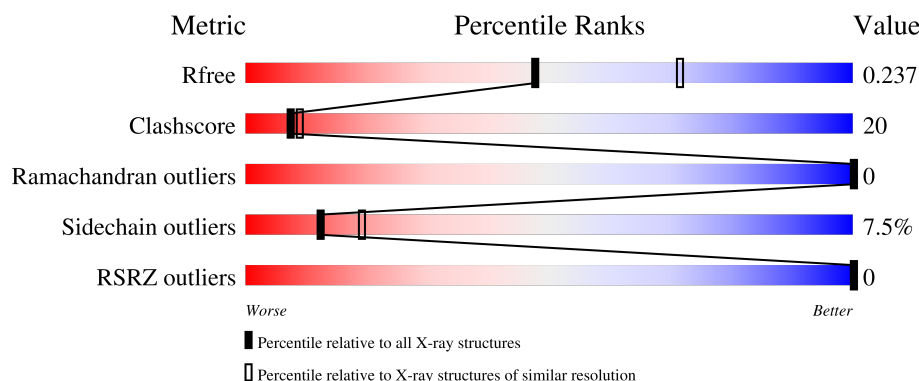
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

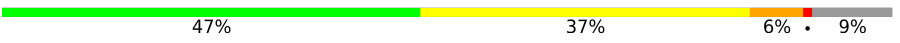
The reported resolution of this entry is 2.37 Å.

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	249	 47% 37% 6% • 9%
1	B	249	 53% 31% 8% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3563 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.

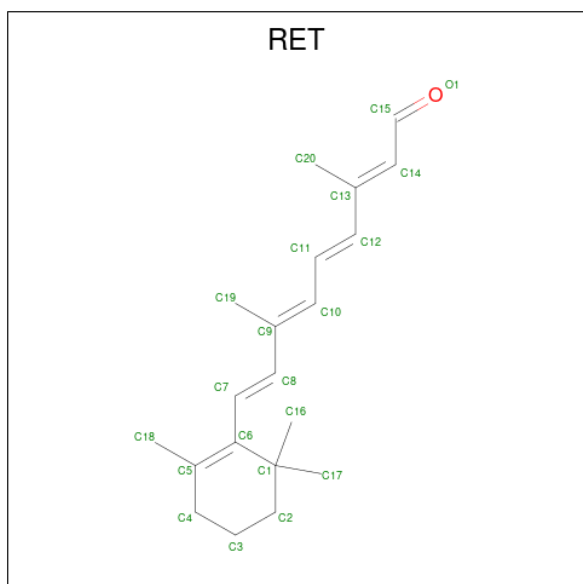
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1752	1177	268	298	9			
1	B	227	Total	C	N	O	S	0	0	0
			1752	1177	268	298	9			

There are 4 discrepancies between the modelled and reference sequences:

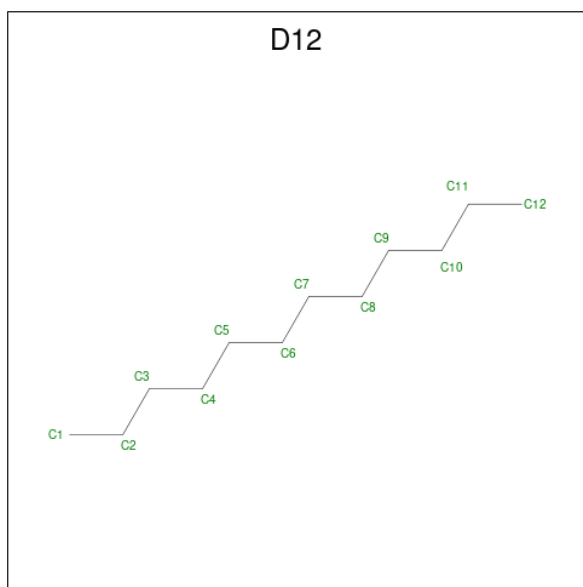
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ALA	THR	engineered mutation	UNP P02945
A	50	ALA	PRO	engineered mutation	UNP P02945
B	46	ALA	THR	engineered mutation	UNP P02945
B	50	ALA	PRO	engineered mutation	UNP P02945

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0

- Molecule 3 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 12 12	0	0

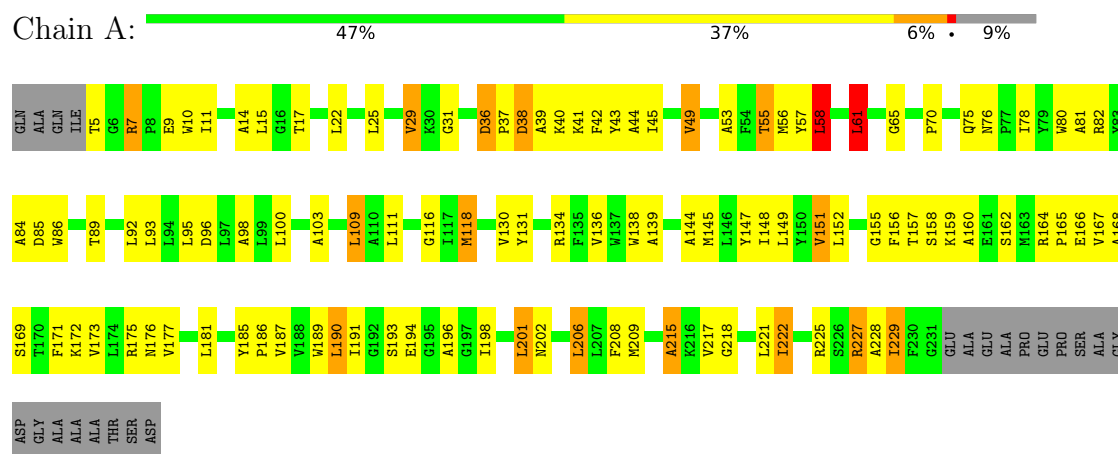
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	2	Total O 2 2	0	0

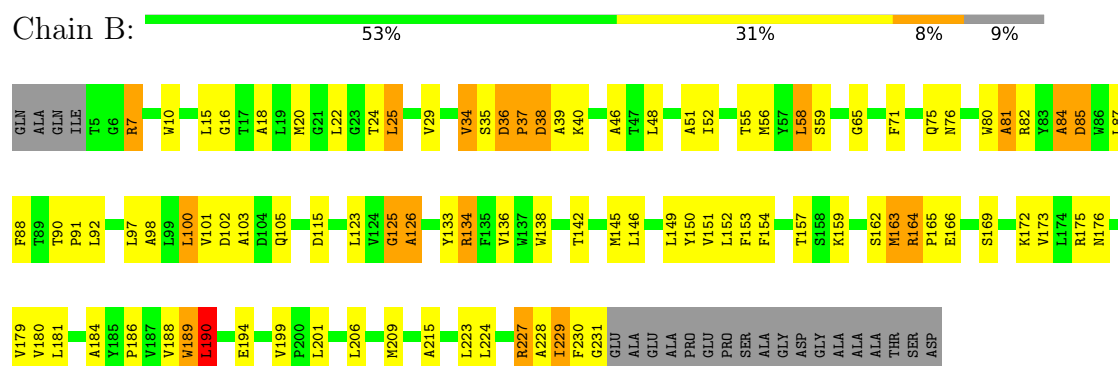
3 Residue-property plots [i](#)

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: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.78Å 116.46Å 57.08Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	90.00 – 2.37 58.23 – 2.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (90.00-2.37) 92.2 (58.23-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.37Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.214 , 0.239 0.216 , 0.237	Depositor DCC
R_{free} test set	1155 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3563	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, D12

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	0.76	0/1799	1.52	40/2456 (1.6%)
1	B	0.76	0/1799	1.39	27/2456 (1.1%)
All	All	0.76	0/3598	1.45	67/4912 (1.4%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	N-CA-C	-13.41	96.15	111.03
1	A	36	ASP	CA-C-N	12.70	135.72	119.84
1	A	36	ASP	C-N-CA	12.70	135.72	119.84
1	A	190	LEU	N-CA-C	10.33	124.98	112.38
1	A	158	SER	N-CA-C	-10.20	99.14	111.69
1	A	201	LEU	N-CA-C	8.12	121.05	111.71
1	A	162	SER	N-CA-C	-8.11	102.95	112.92
1	A	193	SER	N-CA-C	7.35	121.16	111.75
1	B	59	SER	N-CA-C	-7.34	103.36	111.36
1	B	201	LEU	N-CA-C	7.33	120.20	111.33
1	A	11	ILE	CB-CA-C	-7.30	102.54	111.88
1	A	42	PHE	N-CA-C	-7.11	104.08	112.89
1	A	139	ALA	N-CA-C	7.04	119.98	111.82
1	A	168	ALA	N-CA-C	-7.00	103.58	111.14
1	B	25	LEU	N-CA-C	6.90	119.39	111.11
1	B	162	SER	N-CA-C	-6.90	104.83	113.18
1	A	58	LEU	CD1-CG-CD2	6.78	125.72	110.80
1	B	230	PHE	N-CA-C	6.67	121.17	109.96
1	A	160	ALA	N-CA-C	-6.54	105.26	113.18
1	A	159	LYS	N-CA-C	6.54	121.09	113.18
1	B	199	VAL	CA-C-N	6.43	126.34	119.85
1	B	199	VAL	C-N-CA	6.43	126.34	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LEU	N-CA-C	6.43	119.10	111.71
1	A	38	ASP	CB-CA-C	6.43	120.91	110.95
1	B	164	ARG	CA-C-N	6.19	125.92	119.05
1	B	164	ARG	C-N-CA	6.19	125.92	119.05
1	A	136	VAL	N-CA-C	-6.10	104.35	111.00
1	A	84	ALA	N-CA-C	-6.08	104.77	111.82
1	B	228	ALA	N-CA-C	-6.07	105.14	112.54
1	B	126	ALA	N-CA-C	-6.04	105.39	112.89
1	B	52	ILE	CB-CA-C	-5.88	104.47	111.81
1	A	130	VAL	N-CA-C	-5.86	99.26	108.23
1	B	189	TRP	N-CA-C	-5.78	104.88	111.07
1	A	206	LEU	CA-CB-CG	-5.77	96.12	116.30
1	A	22	LEU	CA-CB-CG	5.71	136.28	116.30
1	B	84	ALA	N-CA-C	-5.70	104.97	111.07
1	A	61	LEU	N-CA-C	-5.64	104.50	111.33
1	A	196	ALA	N-CA-C	5.58	119.35	112.54
1	A	151	VAL	CA-C-N	5.55	127.66	120.44
1	A	151	VAL	C-N-CA	5.55	127.66	120.44
1	B	37	PRO	CA-C-N	-5.55	113.33	120.65
1	B	37	PRO	C-N-CA	-5.55	113.33	120.65
1	A	7	ARG	CA-C-N	5.54	126.76	119.84
1	A	7	ARG	C-N-CA	5.54	126.76	119.84
1	B	7	ARG	CA-C-N	5.51	125.87	119.47
1	B	7	ARG	C-N-CA	5.51	125.87	119.47
1	B	97	LEU	CD1-CG-CD2	5.49	122.88	110.80
1	B	38	ASP	N-CA-C	-5.48	105.00	110.97
1	B	81	ALA	N-CA-C	-5.46	104.77	111.75
1	A	76	ASN	CA-C-N	5.42	127.84	120.79
1	A	76	ASN	C-N-CA	5.42	127.84	120.79
1	A	44	ALA	N-CA-C	-5.39	105.06	111.69
1	B	24	THR	N-CA-C	-5.36	105.33	111.07
1	A	177	VAL	N-CA-C	-5.28	105.57	110.53
1	B	36	ASP	CA-C-N	-5.27	113.60	119.19
1	B	36	ASP	C-N-CA	-5.27	113.60	119.19
1	B	76	ASN	N-CA-C	5.24	117.52	110.29
1	B	125	GLY	N-CA-C	-5.19	108.22	114.66
1	A	109	LEU	N-CA-C	-5.18	105.55	111.14
1	A	76	ASN	N-CA-C	5.16	116.15	109.65
1	A	222	ILE	CB-CA-C	-5.16	105.10	112.22
1	A	116	GLY	N-CA-C	-5.15	106.17	112.77
1	B	190	LEU	N-CA-C	5.14	117.55	111.33
1	A	134	ARG	N-CA-C	-5.13	104.95	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ALA	N-CA-C	-5.12	105.88	111.82
1	A	215	ALA	N-CA-C	5.01	119.03	113.01
1	A	22	LEU	N-CA-CB	-5.01	102.74	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	1808	75	0
1	B	1752	0	1809	73	0
2	A	20	0	27	2	0
2	B	20	0	27	1	0
3	A	12	0	26	0	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
All	All	3563	0	3697	148	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 20.

All (148) 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:B:164:ARG:CG	1:B:165:PRO:HD2	1.74	1.17
1:B:164:ARG:HG3	1:B:165:PRO:CD	1.79	1.12
1:A:206:LEU:HG	1:A:206:LEU:O	1.57	0.96
1:B:175:ARG:HH21	1:B:176:ASN:HD21	1.03	0.96
1:B:169:SER:O	1:B:172:LYS:HG2	1.66	0.95
1:A:186:PRO:HB3	2:A:301:RET:H183	1.50	0.91
1:A:164:ARG:HG3	1:A:165:PRO:HD2	1.53	0.90
1:A:41:LYS:O	1:A:45:ILE:HG13	1.72	0.88
1:B:35:SER:O	1:B:37:PRO:HD3	1.74	0.88
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD12	1:B:58:LEU:O	1.74	0.86
1:B:7:ARG:O	1:B:10:TRP:HD1	1.57	0.86
1:B:223:LEU:O	1:B:229:ILE:HD13	1.78	0.82
1:B:145:MET:HE3	1:B:149:LEU:HD11	1.62	0.82
1:A:221:LEU:O	1:A:225:ARG:HB2	1.80	0.82
1:B:56:MET:HG3	1:B:85:ASP:CB	2.10	0.81
1:B:56:MET:HG3	1:B:85:ASP:HB3	1.61	0.81
1:A:169:SER:O	1:A:172:LYS:HG2	1.81	0.79
1:A:25:LEU:O	1:A:29:VAL:HG13	1.86	0.76
1:A:175:ARG:HH21	1:A:176:ASN:HD21	1.34	0.76
1:B:175:ARG:HH21	1:B:176:ASN:ND2	1.81	0.76
1:A:5:THR:HG22	1:A:7:ARG:HG3	1.68	0.75
1:A:9:GLU:HB3	1:A:202:ASN:HA	1.68	0.75
1:A:70:PRO:HB3	1:A:75:GLN:HE22	1.53	0.73
1:A:111:LEU:HD22	1:A:148:ILE:HG23	1.69	0.72
1:B:186:PRO:HB3	2:B:301:RET:H183	1.70	0.72
1:B:7:ARG:O	1:B:10:TRP:CD1	2.43	0.69
1:B:164:ARG:HG3	1:B:165:PRO:HD2	0.82	0.68
1:A:55:THR:OG1	1:A:56:MET:HE2	1.93	0.68
1:A:167:VAL:HG22	1:A:228:ALA:HB1	1.76	0.68
1:B:223:LEU:O	1:B:229:ILE:CD1	2.42	0.67
1:B:184:ALA:O	1:B:188:VAL:HG23	1.95	0.66
1:B:181:LEU:HD13	1:B:215:ALA:HB2	1.76	0.66
1:A:7:ARG:O	1:A:10:TRP:HD1	1.78	0.65
1:A:36:ASP:O	1:A:40:LYS:HB2	1.98	0.64
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.80	0.64
1:A:39:ALA:HB2	1:A:229:ILE:O	1.98	0.64
1:B:166:GLU:HG2	1:B:227:ARG:HG2	1.81	0.63
1:B:223:LEU:CD1	1:B:229:ILE:HD11	2.29	0.63
1:B:56:MET:HG3	1:B:85:ASP:HB2	1.82	0.62
1:A:70:PRO:HB3	1:A:75:GLN:NE2	2.15	0.61
1:A:187:VAL:O	1:A:191:ILE:HG12	2.00	0.60
1:B:15:LEU:HD23	1:B:209:MET:HE1	1.82	0.60
1:A:31:GLY:O	1:A:40:LYS:HE3	2.02	0.60
1:A:61:LEU:HD12	1:A:61:LEU:O	2.03	0.59
1:B:172:LYS:CG	1:B:173:VAL:N	2.65	0.59
1:B:223:LEU:HD12	1:B:229:ILE:HD11	1.86	0.58
1:A:118:MET:SD	1:A:145:MET:HB2	2.44	0.58
1:A:58:LEU:O	1:A:61:LEU:HB3	2.05	0.57
1:A:175:ARG:HH21	1:A:176:ASN:ND2	2.01	0.56
1:B:48:LEU:HD12	1:B:48:LEU:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD23	1:A:209:MET:HE1	1.87	0.55
1:A:218:GLY:O	1:A:222:ILE:HD12	2.06	0.55
1:A:49:VAL:HG11	1:A:93:LEU:HD21	1.89	0.55
1:B:34:VAL:O	1:B:34:VAL:HG12	2.06	0.55
1:B:175:ARG:NH2	1:B:176:ASN:HD21	1.88	0.55
1:B:39:ALA:HA	1:B:229:ILE:HG23	1.88	0.54
1:B:88:PHE:O	1:B:92:LEU:HD12	2.07	0.54
1:B:90:THR:N	1:B:91:PRO:HD2	2.21	0.54
1:A:169:SER:O	1:A:172:LYS:HE2	2.08	0.54
1:A:172:LYS:CG	1:A:173:VAL:N	2.69	0.54
1:B:165:PRO:HG2	1:B:166:GLU:H	1.72	0.53
1:A:165:PRO:O	1:A:169:SER:CB	2.57	0.53
1:B:84:ALA:O	1:B:87:LEU:HB3	2.09	0.52
1:B:100:LEU:O	1:B:163:MET:HE2	2.08	0.52
1:A:185:TYR:CD2	1:A:208:PHE:HE1	2.26	0.52
1:B:58:LEU:HD12	1:B:58:LEU:C	2.35	0.52
1:B:7:ARG:HH11	1:B:7:ARG:HB3	1.74	0.52
1:B:169:SER:HB2	1:B:172:LYS:NZ	2.24	0.52
1:A:172:LYS:HG3	1:A:173:VAL:N	2.24	0.51
1:A:7:ARG:O	1:A:10:TRP:CD1	2.62	0.51
1:A:9:GLU:CB	1:A:202:ASN:HA	2.39	0.51
1:A:86:TRP:CD1	2:A:301:RET:H14	2.45	0.51
1:B:51:ALA:O	1:B:55:THR:HG23	2.10	0.51
1:A:111:LEU:HD21	1:A:151:VAL:HG11	1.92	0.51
1:A:39:ALA:CA	1:A:229:ILE:O	2.58	0.50
1:B:25:LEU:O	1:B:29:VAL:HG23	2.11	0.50
1:B:98:ALA:HB1	1:B:103:ALA:HB3	1.93	0.50
1:A:89:THR:O	1:A:93:LEU:HG	2.12	0.50
1:B:172:LYS:HG3	1:B:173:VAL:N	2.26	0.50
1:A:185:TYR:CD2	1:A:208:PHE:CE1	3.00	0.49
1:B:46:ALA:CB	1:B:224:LEU:HD11	2.42	0.49
1:B:150:TYR:CE1	1:B:154:PHE:CE2	3.00	0.49
1:B:38:ASP:HB3	1:B:231:GLY:N	2.28	0.49
1:B:165:PRO:HG2	1:B:166:GLU:N	2.27	0.48
1:A:157:THR:O	1:A:157:THR:HG22	2.13	0.48
1:B:125:GLY:O	1:B:134:ARG:NH1	2.46	0.48
1:A:138:TRP:CZ2	1:A:190:LEU:HD13	2.48	0.48
1:A:166:GLU:O	1:A:166:GLU:CD	2.57	0.48
1:A:151:VAL:O	1:A:155:GLY:N	2.45	0.48
1:B:71:PHE:CE2	1:B:134:ARG:NH2	2.81	0.48
1:A:190:LEU:C	1:A:190:LEU:HD23	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:CB	1:A:229:ILE:O	2.63	0.47
1:A:78:ILE:HD12	1:A:194:GLU:HG3	1.95	0.47
1:B:145:MET:HE3	1:B:149:LEU:CD1	2.39	0.47
1:A:144:ALA:O	1:A:148:ILE:HG13	2.15	0.47
1:B:16:GLY:O	1:B:20:MET:HG2	2.15	0.46
1:B:126:ALA:C	1:B:134:ARG:HH12	2.23	0.46
1:B:157:THR:OG1	1:B:175:ARG:NH1	2.46	0.46
1:A:157:THR:O	1:A:157:THR:CG2	2.63	0.46
1:A:82:ARG:O	1:A:85:ASP:HB3	2.16	0.45
1:A:38:ASP:O	1:A:41:LYS:HG2	2.16	0.45
1:B:169:SER:HA	1:B:172:LYS:HD3	1.97	0.45
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.51	0.45
1:A:57:TYR:OH	1:A:209:MET:HA	2.17	0.45
1:A:98:ALA:HB1	1:A:103:ALA:HB3	1.99	0.45
1:A:17:THR:HG23	1:A:58:LEU:HB2	1.99	0.45
1:B:101:VAL:O	1:B:102:ASP:HB3	2.17	0.45
1:A:14:ALA:HA	1:A:61:LEU:HD22	1.98	0.45
1:A:93:LEU:O	1:A:96:ASP:HB2	2.16	0.45
1:A:217:VAL:O	1:A:221:LEU:HG	2.17	0.45
1:B:133:TYR:O	1:B:136:VAL:HB	2.17	0.45
1:A:167:VAL:HG22	1:A:228:ALA:CB	2.44	0.44
1:B:172:LYS:HG2	1:B:173:VAL:H	1.82	0.44
1:B:91:PRO:HD3	1:B:115:ASP:OD1	2.17	0.44
1:B:102:ASP:O	1:B:103:ALA:C	2.61	0.44
1:A:39:ALA:O	1:A:43:TYR:HD2	2.00	0.43
1:B:142:THR:O	1:B:146:LEU:HG	2.18	0.43
1:B:34:VAL:O	1:B:34:VAL:CG1	2.67	0.43
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.56	0.43
1:A:166:GLU:HG2	1:A:227:ARG:HB2	2.01	0.43
1:B:153:PHE:O	1:B:157:THR:HB	2.19	0.43
1:B:138:TRP:CZ2	1:B:190:LEU:HD13	2.53	0.43
1:B:166:GLU:OE2	1:B:166:GLU:O	2.37	0.43
1:A:92:LEU:O	1:A:95:LEU:HB3	2.18	0.43
1:A:181:LEU:HD13	1:A:215:ALA:HB2	2.01	0.43
1:B:101:VAL:O	1:B:102:ASP:CB	2.64	0.43
1:A:165:PRO:O	1:A:169:SER:HB3	2.18	0.42
1:B:189:TRP:CE2	1:B:194:GLU:HB3	2.53	0.42
1:A:61:LEU:HD12	1:A:61:LEU:C	2.44	0.42
1:B:150:TYR:CE1	1:B:154:PHE:CD2	3.07	0.41
1:A:7:ARG:HH21	1:A:201:LEU:HD21	1.84	0.41
1:A:144:ALA:O	1:A:147:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:CG	1:A:165:PRO:HD2	2.37	0.41
1:B:227:ARG:H	1:B:227:ARG:HD3	1.86	0.41
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.80	0.41
1:A:131:TYR:O	1:A:131:TYR:HD1	2.04	0.41
1:B:18:ALA:O	1:B:22:LEU:HG	2.21	0.41
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.86	0.41
1:B:164:ARG:CB	1:B:165:PRO:HD2	2.47	0.41
1:A:80:TRP:C	1:A:82:ARG:N	2.77	0.41
1:B:15:LEU:HD23	1:B:209:MET:CE	2.49	0.41
1:B:123:LEU:HD12	1:B:123:LEU:O	2.21	0.41
1:A:138:TRP:HB2	1:A:189:TRP:CZ3	2.56	0.40
1:B:36:ASP:O	1:B:40:LYS:HB2	2.20	0.40
1:B:159:LYS:O	1:B:159:LYS:HG2	2.21	0.40
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.88	0.40
1:B:80:TRP:C	1:B:82:ARG:N	2.74	0.40

There are no symmetry-related clashes.

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	225/249 (90%)	219 (97%)	6 (3%)	0	100	100
1	B	225/249 (90%)	219 (97%)	6 (3%)	0	100	100
All	All	450/498 (90%)	438 (97%)	12 (3%)	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	180/193 (93%)	169 (94%)	11 (6%)	17	27
1	B	180/193 (93%)	164 (91%)	16 (9%)	9	13
All	All	360/386 (93%)	333 (92%)	27 (8%)	12	19

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	49	VAL
1	A	55	THR
1	A	58	LEU
1	A	61	LEU
1	A	109	LEU
1	A	118	MET
1	A	152	LEU
1	A	198	ILE
1	A	227	ARG
1	A	229	ILE
1	B	34	VAL
1	B	58	LEU
1	B	75	GLN
1	B	85	ASP
1	B	100	LEU
1	B	105	GLN
1	B	134	ARG
1	B	151	VAL
1	B	152	LEU
1	B	163	MET
1	B	179	VAL
1	B	180	VAL
1	B	190	LEU
1	B	206	LEU
1	B	227	ARG
1	B	229	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	176	ASN
1	B	76	ASN
1	B	176	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	D12	A	501	-	11,11,11	0.22	0	10,10,10	1.03	1 (10%)
2	RET	A	301	1	20,20,21	2.48	6 (30%)	27,27,28	2.70	12 (44%)
2	RET	B	301	1	20,20,21	2.17	6 (30%)	27,27,28	2.71	12 (44%)

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	D12	A	501	-	-	0/9/9/9	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
2	RET	B	301	1	-	0/13/30/31	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C1-C6	5.91	1.61	1.53
2	A	301	RET	C14-C13	5.08	1.37	1.33
2	B	301	RET	C1-C6	4.99	1.60	1.53
2	A	301	RET	C5-C6	4.36	1.41	1.34
2	B	301	RET	C14-C13	4.23	1.36	1.33
2	B	301	RET	C5-C6	3.78	1.40	1.34
2	A	301	RET	C17-C1	3.46	1.60	1.53
2	A	301	RET	C4-C5	3.12	1.56	1.51
2	B	301	RET	C4-C5	3.08	1.56	1.51
2	B	301	RET	C17-C1	2.96	1.59	1.53
2	B	301	RET	C16-C1	2.53	1.58	1.53
2	A	301	RET	C16-C1	2.41	1.58	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C18-C5-C6	5.94	130.97	124.48
2	A	301	RET	C18-C5-C6	5.77	130.78	124.48
2	B	301	RET	C8-C9-C10	-5.35	110.59	119.01
2	A	301	RET	C8-C9-C10	-4.87	111.34	119.01
2	A	301	RET	C11-C10-C9	-4.57	120.87	127.28
2	B	301	RET	C11-C10-C9	-4.21	121.38	127.28
2	A	301	RET	C10-C11-C12	-4.00	111.60	123.20
2	B	301	RET	C20-C13-C12	3.97	124.15	118.09
2	B	301	RET	C10-C11-C12	-3.95	111.76	123.20
2	A	301	RET	C20-C13-C12	3.77	123.85	118.09
2	A	301	RET	C12-C13-C14	-3.70	108.73	118.55
2	B	301	RET	C19-C9-C8	3.50	123.44	118.09
2	A	301	RET	C19-C9-C8	3.45	123.36	118.09
2	B	301	RET	C12-C13-C14	-3.44	109.41	118.55
2	A	301	RET	C7-C6-C5	-3.40	113.71	121.56
2	B	301	RET	C7-C6-C5	-3.28	114.00	121.56
2	A	301	RET	C1-C6-C7	3.27	124.53	115.65
2	B	301	RET	C1-C6-C7	3.14	124.16	115.65
2	A	301	RET	C2-C1-C6	2.97	114.75	110.44
2	B	301	RET	C2-C1-C6	2.92	114.69	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	D12	C9-C8-C7	-2.29	102.81	114.37
2	B	301	RET	C17-C1-C6	2.21	113.70	110.24
2	B	301	RET	C18-C5-C4	-2.20	108.90	113.60
2	A	301	RET	C18-C5-C4	-2.16	109.00	113.60
2	A	301	RET	C8-C7-C6	2.09	132.58	127.00

There are no chirality outliers.

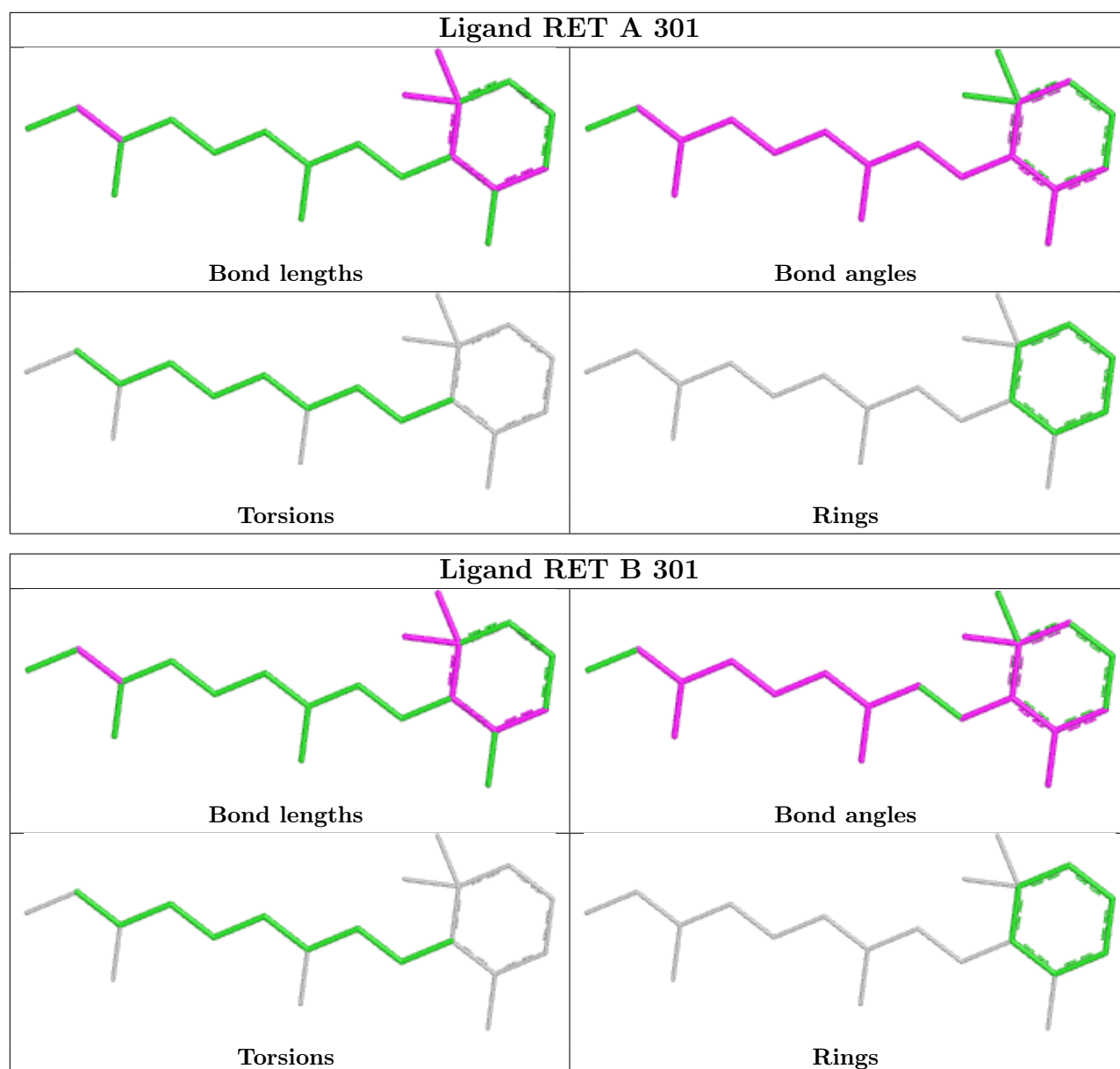
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	2	0
2	B	301	RET	1	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 [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	227/249 (91%)	-1.43	0 100 100	22, 32, 58, 76	0
1	B	227/249 (91%)	-1.42	0 100 100	19, 35, 55, 62	0
All	All	454/498 (91%)	-1.43	0 100 100	19, 34, 57, 76	0

There are no RSRZ outliers to report.

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.

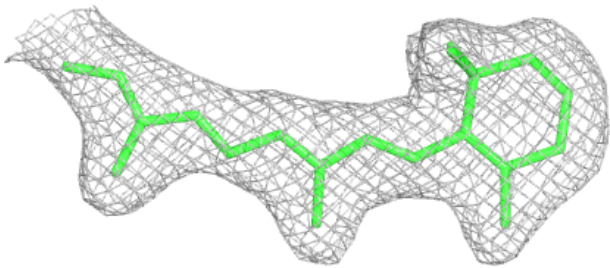
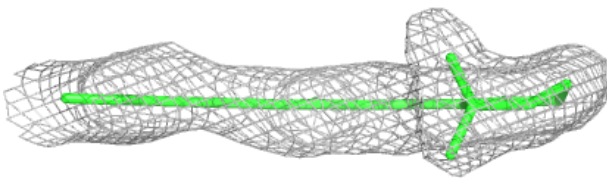
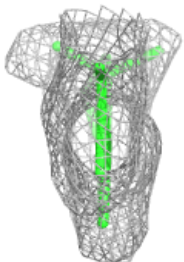
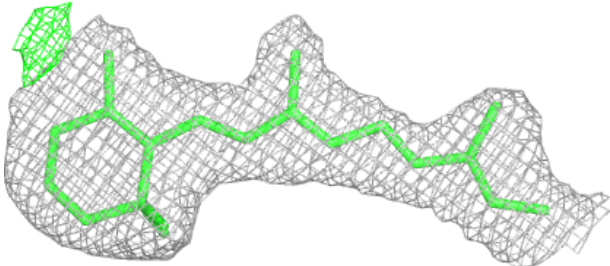
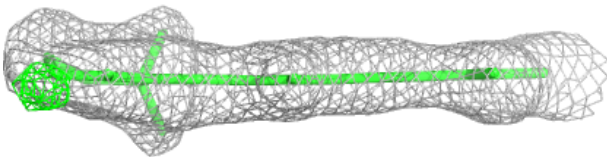
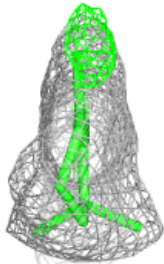
6.4 Ligands [i](#)

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. 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(Å ²)	Q<0.9
2	RET	A	301	20/21	0.99	0.03	20,24,25,27	0
2	RET	B	301	20/21	0.99	0.03	27,29,33,34	0
3	D12	A	501	12/12	0.99	0.06	45,46,47,48	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 RET A 301: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D electron density map of RET A 301. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.
 A 3D electron density map of RET A 301, side view. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.	 A 3D electron density map of RET A 301, top view. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.
Electron density around RET B 301: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D electron density map of RET B 301. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.
 A 3D electron density map of RET B 301, side view. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.	 A 3D electron density map of RET B 301, top view. The map is shown as a gray mesh. The positive density is highlighted in green, showing a complex, branched structure. The negative density is highlighted in purple.

6.5 Other polymers [i](#)

There are no such residues in this entry.