Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2021 – 03:30 PM EDT

PDB ID	:	3HAP
Title	:	Crystal structure of bacteriorhodopsin mutant L111A crystallized from bicelles
Authors	:	Joh, N.H.; Yang, D.; Bowie, J.U.
Deposited on	:	2009-05-02
Resolution	:	1.60 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.60 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.
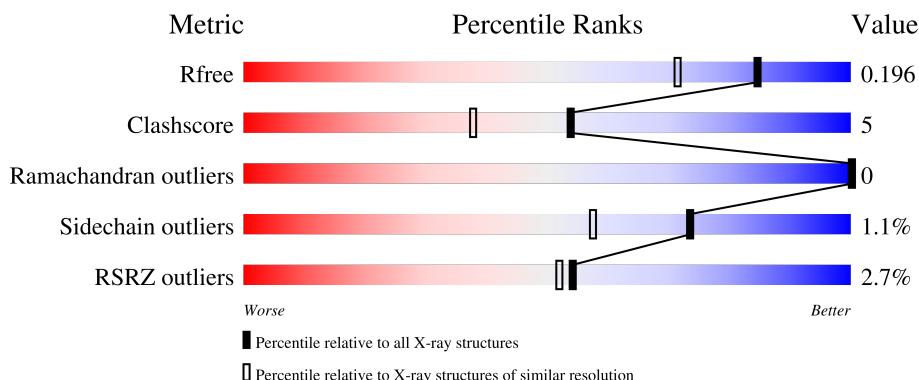
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	2% ▮ 82% 8% 9%
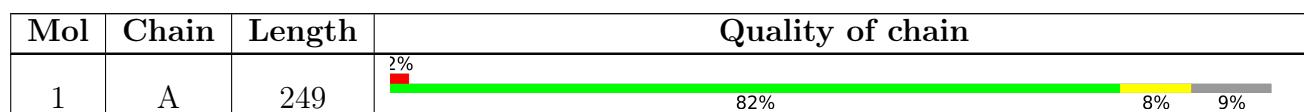
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	D12	A	251	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	D12	A	252	-	X	-	-
3	D12	A	254	-	X	-	-
3	D12	A	255	-	X	-	-
3	D12	A	256	-	X	-	-
3	D12	A	402	-	X	-	-
3	D12	A	403	-	X	-	-
3	D12	A	405	-	X	-	-
5	R16	A	411	-	X	-	-
7	HP6	A	401	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 2283 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	226	Total 1914	C 1305	N 280	O 316	S 13	0	34	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	LEU	engineered mutation	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).

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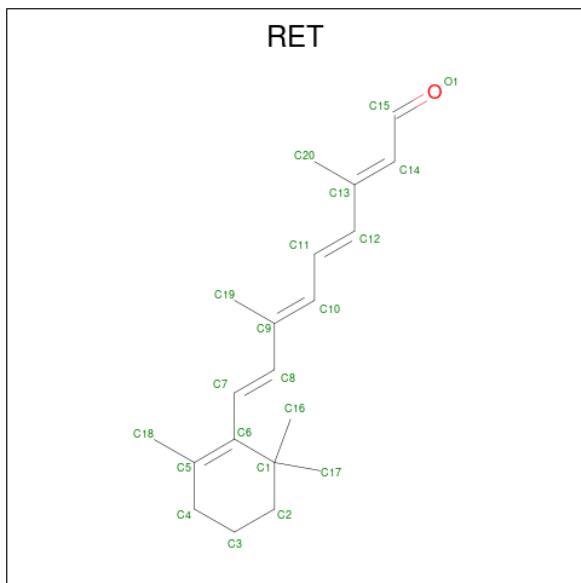
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 20	C 20	0	0

- Molecule 3 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).

D12

C11
C12
C9
C10
C7
C8
C5
C6
C3
C4
C1
C2
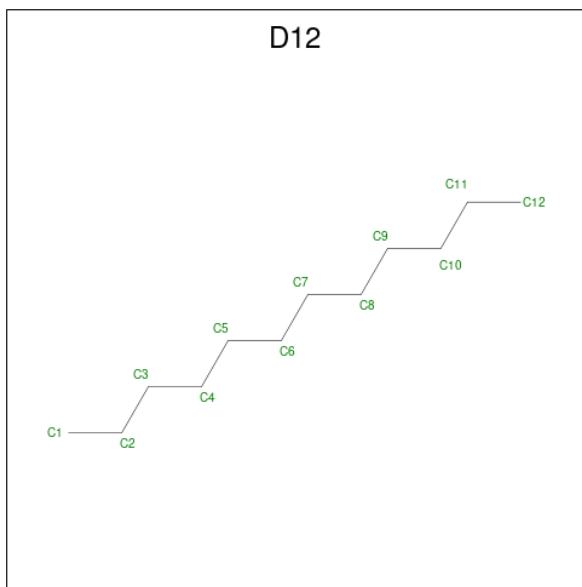
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0
3	A	1	Total 12	C 12	0	0

• Molecule 4 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).

D10
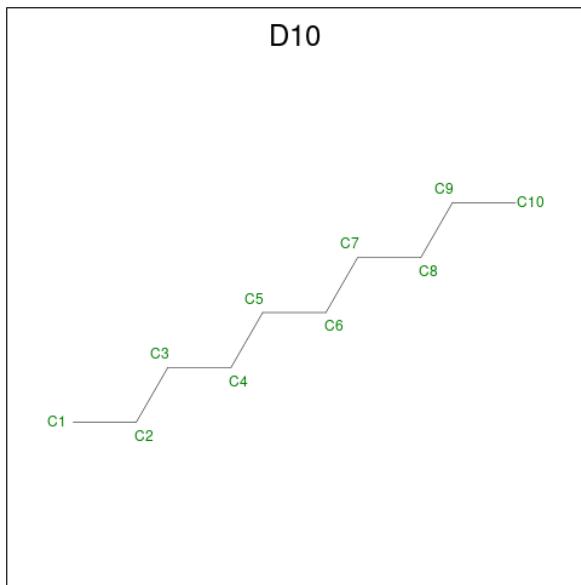
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 10	C 10	0	0
4	A	1	Total 10	C 10	0	0
4	A	1	Total 10	C 10	0	0
4	A	1	Total 10	C 10	0	0

- Molecule 5 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).

R16
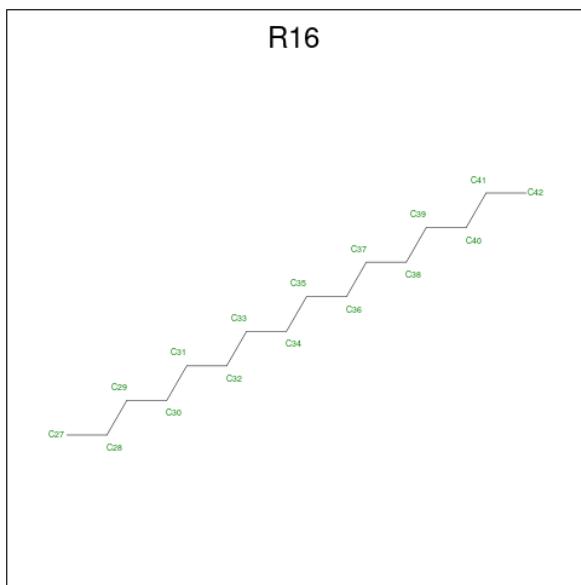
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 16	C 16	0	0

- Molecule 6 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).
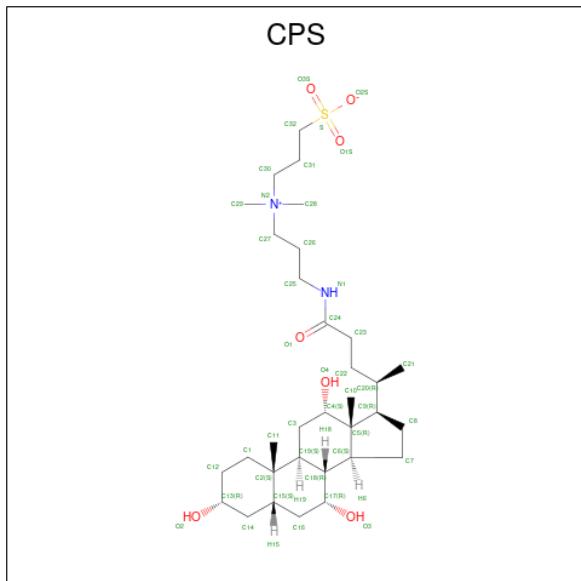
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 27	C 24	O 3	0	0

- Molecule 7 is HEPTANE (three-letter code: HP6) (formula: C_7H_{16}).
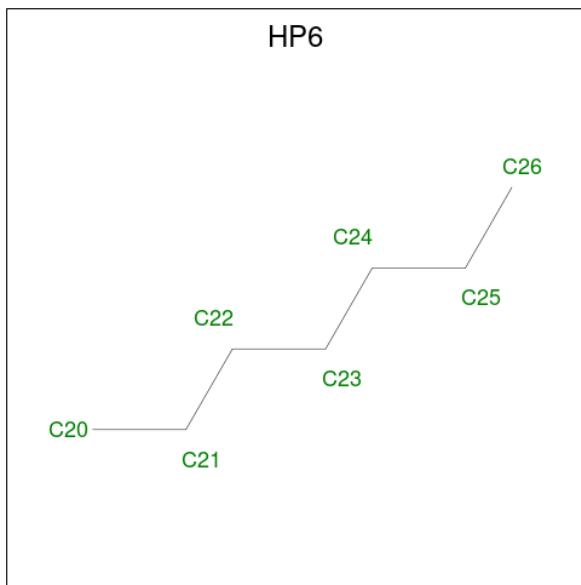
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 7	C 7	0	0

- Molecule 8 is nonane (three-letter code: DD9) (formula: C_9H_{20}).

DD9
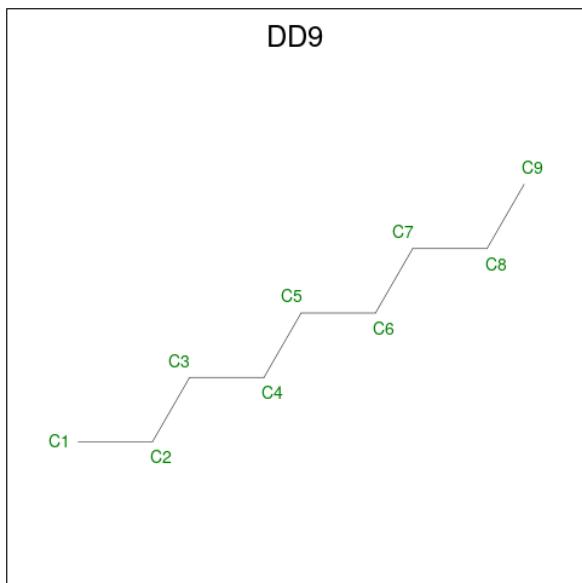
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 9	C 9	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	154	Total 154	O 154	0	0

3 Residue-property plots ⓘ

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

Chain A:
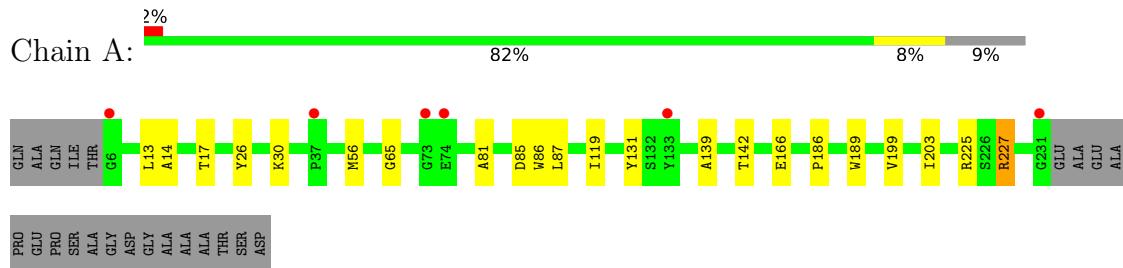
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	44.95Å 102.14Å 128.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.74 – 1.60	Depositor
	21.74 – 1.60	EDS
% Data completeness	93.8 (21.74-1.60)	Depositor
(in resolution range)	93.8 (21.74-1.60)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.167 , 0.192	Depositor
	0.170 , 0.196	DCC
R_{free} test set	2871 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2283	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DD9, D10, RET, CPS, R16, D12, HP6

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	0.49	0/2067	0.55	0/2817

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1914	0	2097	20	0
2	A	20	0	27	6	0
3	A	96	0	109	1	0
4	A	40	0	88	2	0
5	A	16	0	6	0	0
6	A	27	0	39	1	0
7	A	7	0	10	0	0
8	A	9	0	20	0	0
9	A	154	0	0	1	0
All	All	2283	0	2396	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (24) 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:227[A]:ARG:HD3	1:A:227[A]:ARG:H	1.29	0.94
2:A:301:RET:H8	2:A:301:RET:H171	1.65	0.78
1:A:227[A]:ARG:H	1:A:227[A]:ARG:CD	1.98	0.75
1:A:225[A]:ARG:HG3	9:A:343:HOH:O	1.93	0.68
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.90	0.53
1:A:203[B]:ILE:HD13	4:A:257:D10:H82	1.91	0.53
1:A:186:PRO:HB3	2:A:301:RET:H183	1.91	0.53
1:A:199:VAL:HG22	3:A:254:D12:H51	1.90	0.53
2:A:301:RET:H171	2:A:301:RET:C8	2.34	0.52
1:A:14:ALA:O	1:A:17[B]:THR:OG1	2.26	0.50
1:A:13:LEU:O	1:A:17[B]:THR:HG23	2.11	0.49
1:A:189:TRP:CD1	2:A:301:RET:H22	2.49	0.48
4:A:406:D10:H102	6:A:501:CPS:H12A	1.97	0.47
2:A:301:RET:H7	2:A:301:RET:H181	1.68	0.46
1:A:26:TYR:CE1	1:A:30:LYS:HE3	2.51	0.45
1:A:56[B]:MET:HG3	1:A:85:ASP:HB2	1.99	0.43
1:A:139:ALA:HA	1:A:142[B]:THR:HG22	2.01	0.43
1:A:166[A]:GLU:OE2	1:A:227[A]:ARG:NH1	2.52	0.43
1:A:87[B]:LEU:HG	1:A:119:ILE:HG21	2.01	0.42
1:A:139:ALA:O	1:A:142[B]:THR:HG22	2.20	0.42
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.89	0.42
1:A:86:TRP:CD1	2:A:301:RET:H14	2.55	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	259/249 (104%)	258 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/194 (111%)	212 (99%)	3 (1%)	67	47

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

Mol	Chain	Res	Type
1	A	131	TYR
1	A	227[A]	ARG
1	A	227[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	105	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	405	-	11,11,11	3.16	6 (54%)	10,10,10	6.13	4 (40%)
3	D12	A	254	-	11,11,11	3.41	6 (54%)	10,10,10	6.99	4 (40%)
4	D10	A	406	-	9,9,9	0.20	0	8,8,8	0.59	0
4	D10	A	257	-	9,9,9	0.21	0	8,8,8	0.58	0
4	D10	A	409	-	9,9,9	0.22	0	8,8,8	0.54	0
6	CPS	A	501	-	30,30,45	0.45	0	47,48,70	1.11	3 (6%)
4	D10	A	250	-	9,9,9	0.24	0	8,8,8	0.51	0
3	D12	A	251	-	11,11,11	3.30	6 (54%)	10,10,10	6.51	4 (40%)
8	DD9	A	253	-	8,8,8	0.22	0	7,7,7	0.51	0
3	D12	A	256	-	11,11,11	3.17	6 (54%)	10,10,10	6.27	4 (40%)
5	R16	A	411	-	15,15,15	7.28	15 (100%)	14,14,14	11.83	14 (100%)
3	D12	A	403	-	11,11,11	3.27	6 (54%)	10,10,10	6.35	4 (40%)
3	D12	A	255	-	11,11,11	3.24	6 (54%)	10,10,10	6.20	4 (40%)
3	D12	A	252	-	11,11,11	3.23	6 (54%)	10,10,10	6.41	4 (40%)
2	RET	A	301	1	20,20,21	1.06	1 (5%)	27,27,28	3.24	10 (37%)
7	HP6	A	401	-	6,6,6	3.13	3 (50%)	5,5,5	6.58	3 (60%)
3	D12	A	402	-	11,11,11	3.21	6 (54%)	10,10,10	6.43	4 (40%)

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	405	-	-	2/9/9/9	-
3	D12	A	254	-	-	6/9/9/9	-
4	D10	A	406	-	-	4/7/7/7	-
4	D10	A	257	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D10	A	409	-	-	2/7/7/7	-
6	CPS	A	501	-	-	1/7/72/90	0/4/4/4
4	D10	A	250	-	-	2/7/7/7	
3	D12	A	251	-	-	5/9/9/9	-
8	DD9	A	253	-	-	2/6/6/6	-
3	D12	A	256	-	-	6/9/9/9	-
5	R16	A	411	-	-	9/13/13/13	-
3	D12	A	403	-	-	3/9/9/9	-
3	D12	A	255	-	-	7/9/9/9	-
3	D12	A	252	-	-	2/9/9/9	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
7	HP6	A	401	-	-	2/4/4/4	-
3	D12	A	402	-	-	6/9/9/9	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	411	R16	C38-C37	15.35	2.37	1.51
5	A	411	R16	C40-C39	15.25	2.37	1.51
5	A	411	R16	C39-C38	-5.79	1.19	1.51
3	A	254	D12	C8-C7	-5.78	1.19	1.51
3	A	252	D12	C8-C7	-5.74	1.19	1.51
3	A	254	D12	C9-C8	-5.73	1.19	1.51
5	A	411	R16	C32-C31	-5.70	1.19	1.51
5	A	411	R16	C31-C30	-5.66	1.19	1.51
5	A	411	R16	C30-C29	-5.62	1.20	1.51
3	A	403	D12	C9-C8	-5.61	1.20	1.51
3	A	403	D12	C8-C7	-5.56	1.20	1.51
3	A	256	D12	C8-C7	-5.55	1.20	1.51
3	A	402	D12	C9-C8	-5.55	1.20	1.51
3	A	251	D12	C9-C8	-5.54	1.20	1.51
7	A	401	HP6	C24-C23	-5.53	1.20	1.51
5	A	411	R16	C36-C35	-5.51	1.20	1.51
3	A	405	D12	C9-C8	-5.50	1.20	1.51
3	A	256	D12	C9-C8	-5.49	1.20	1.51
3	A	255	D12	C8-C7	-5.49	1.20	1.51
3	A	251	D12	C8-C7	-5.48	1.20	1.51
5	A	411	R16	C37-C36	-5.40	1.21	1.51
5	A	411	R16	C33-C32	-5.37	1.21	1.51
3	A	402	D12	C8-C7	-5.36	1.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	D12	C8-C7	-5.34	1.21	1.51
3	A	255	D12	C9-C8	-5.31	1.21	1.51
5	A	411	R16	C35-C34	-5.18	1.22	1.51
3	A	252	D12	C9-C8	-5.18	1.22	1.51
5	A	411	R16	C34-C33	-4.99	1.23	1.51
5	A	411	R16	C41-C40	-4.60	1.19	1.51
5	A	411	R16	C28-C29	-4.55	1.19	1.51
3	A	254	D12	C7-C6	-4.51	1.26	1.51
3	A	252	D12	C7-C6	-4.50	1.26	1.51
7	A	401	HP6	C25-C24	-4.48	1.19	1.51
3	A	254	D12	C10-C9	-4.42	1.26	1.51
3	A	251	D12	C7-C6	-4.41	1.26	1.51
3	A	402	D12	C7-C6	-4.41	1.26	1.51
3	A	251	D12	C10-C9	-4.37	1.27	1.51
3	A	255	D12	C7-C6	-4.33	1.27	1.51
3	A	256	D12	C7-C6	-4.29	1.27	1.51
3	A	403	D12	C10-C9	-4.26	1.27	1.51
3	A	255	D12	C10-C9	-4.24	1.27	1.51
3	A	402	D12	C10-C9	-4.23	1.27	1.51
3	A	405	D12	C7-C6	-4.16	1.28	1.51
3	A	403	D12	C7-C6	-4.15	1.28	1.51
3	A	405	D12	C10-C9	-4.11	1.28	1.51
3	A	256	D12	C10-C9	-4.09	1.28	1.51
3	A	252	D12	C10-C9	-4.06	1.28	1.51
3	A	254	D12	C11-C10	-3.59	1.26	1.51
2	A	301	RET	C14-C13	3.57	1.36	1.33
3	A	251	D12	C11-C10	-3.55	1.26	1.51
3	A	255	D12	C11-C10	-3.54	1.26	1.51
3	A	403	D12	C11-C10	-3.45	1.27	1.51
3	A	252	D12	C11-C10	-3.36	1.27	1.51
3	A	402	D12	C11-C10	-3.14	1.29	1.51
3	A	405	D12	C11-C10	-3.13	1.29	1.51
3	A	256	D12	C11-C10	-3.06	1.29	1.51
3	A	254	D12	C12-C11	-2.91	1.26	1.49
5	A	411	R16	C42-C41	-2.87	1.26	1.49
3	A	251	D12	C12-C11	-2.79	1.27	1.49
7	A	401	HP6	C26-C25	-2.79	1.27	1.49
3	A	255	D12	C12-C11	-2.78	1.27	1.49
5	A	411	R16	C27-C28	-2.78	1.27	1.49
3	A	403	D12	C12-C11	-2.75	1.27	1.49
3	A	252	D12	C12-C11	-2.60	1.28	1.49
3	A	405	D12	C12-C11	-2.55	1.29	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	D12	C12-C11	-2.47	1.29	1.49
3	A	256	D12	C12-C11	-2.26	1.31	1.49

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	411	R16	C40-C39-C38	-22.02	2.66	114.42
5	A	411	R16	C39-C38-C37	-21.34	6.07	114.42
3	A	252	D12	C8-C7-C6	12.16	176.17	114.42
5	A	411	R16	C32-C31-C30	11.92	174.96	114.42
3	A	254	D12	C10-C9-C8	11.81	174.38	114.42
3	A	254	D12	C9-C8-C7	11.80	174.31	114.42
3	A	254	D12	C8-C7-C6	11.62	173.39	114.42
5	A	411	R16	C31-C30-C29	11.58	173.24	114.42
3	A	402	D12	C8-C7-C6	11.26	171.57	114.42
5	A	411	R16	C33-C32-C31	11.20	171.31	114.42
3	A	402	D12	C10-C9-C8	11.13	170.91	114.42
3	A	251	D12	C8-C7-C6	11.06	170.59	114.42
3	A	256	D12	C8-C7-C6	11.05	170.52	114.42
7	A	401	HP6	C24-C23-C22	10.94	169.96	114.42
3	A	255	D12	C8-C7-C6	10.92	169.87	114.42
3	A	251	D12	C10-C9-C8	10.91	169.80	114.42
3	A	256	D12	C9-C8-C7	10.89	169.70	114.42
3	A	403	D12	C10-C9-C8	10.84	169.47	114.42
3	A	403	D12	C9-C8-C7	10.78	169.14	114.42
3	A	251	D12	C9-C8-C7	10.67	168.61	114.42
3	A	252	D12	C9-C8-C7	10.64	168.44	114.42
3	A	402	D12	C9-C8-C7	10.60	168.22	114.42
3	A	405	D12	C10-C9-C8	10.57	168.08	114.42
3	A	256	D12	C10-C9-C8	10.38	167.13	114.42
3	A	403	D12	C8-C7-C6	10.31	166.78	114.42
3	A	405	D12	C9-C8-C7	10.20	166.23	114.42
3	A	255	D12	C10-C9-C8	10.04	165.39	114.42
3	A	255	D12	C9-C8-C7	9.91	164.73	114.42
3	A	405	D12	C8-C7-C6	9.90	164.71	114.42
5	A	411	R16	C34-C33-C32	9.67	163.51	114.42
3	A	252	D12	C10-C9-C8	9.63	163.30	114.42
5	A	411	R16	C36-C35-C34	9.61	163.19	114.42
5	A	411	R16	C37-C36-C35	9.58	163.08	114.42
2	A	301	RET	C17-C1-C6	-8.89	95.89	110.30
5	A	411	R16	C35-C34-C33	8.70	158.59	114.42
3	A	254	D12	C12-C11-C10	8.47	177.69	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	251	D12	C12-C11-C10	8.10	174.90	113.42
5	A	411	R16	C38-C37-C36	8.10	155.53	114.42
3	A	255	D12	C12-C11-C10	7.95	173.76	113.42
5	A	411	R16	C27-C28-C29	7.93	173.63	113.42
7	A	401	HP6	C26-C25-C24	7.83	172.84	113.42
5	A	411	R16	C42-C41-C40	7.82	172.79	113.42
3	A	403	D12	C12-C11-C10	7.72	172.04	113.42
3	A	405	D12	C12-C11-C10	7.59	171.06	113.42
3	A	252	D12	C12-C11-C10	7.32	168.99	113.42
3	A	402	D12	C12-C11-C10	6.90	165.84	113.42
2	A	301	RET	C2-C1-C6	6.82	120.98	110.48
3	A	256	D12	C12-C11-C10	6.54	163.04	113.42
5	A	411	R16	C28-C29-C30	6.31	173.86	115.30
5	A	411	R16	C41-C40-C39	5.98	170.86	115.30
7	A	401	HP6	C25-C24-C23	5.91	170.14	115.30
2	A	301	RET	C17-C1-C16	-5.72	90.98	108.53
2	A	301	RET	C16-C1-C6	5.70	119.54	110.30
2	A	301	RET	C17-C1-C2	-4.94	89.14	108.91
2	A	301	RET	C1-C6-C5	-4.04	116.92	122.61
2	A	301	RET	C1-C6-C7	3.60	125.97	115.78
6	A	501	CPS	C7-C6-C5	2.99	106.48	103.55
2	A	301	RET	C18-C5-C6	-2.77	121.42	124.53
6	A	501	CPS	C1-C12-C13	2.71	113.95	110.47
2	A	301	RET	C16-C1-C2	2.55	119.11	108.91
2	A	301	RET	C10-C11-C12	-2.40	115.73	123.22
6	A	501	CPS	C16-C15-C14	-2.21	108.65	111.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	D12	C7-C8-C9-C10
3	A	252	D12	C7-C8-C9-C10
3	A	251	D12	C6-C7-C8-C9
5	A	411	R16	C35-C36-C37-C38
3	A	402	D12	C6-C7-C8-C9
3	A	403	D12	C6-C7-C8-C9
5	A	411	R16	C32-C33-C34-C35
3	A	254	D12	C5-C6-C7-C8
3	A	254	D12	C6-C7-C8-C9
5	A	411	R16	C34-C35-C36-C37
5	A	411	R16	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	A	411	R16	C29-C30-C31-C32
3	A	255	D12	C5-C6-C7-C8
3	A	402	D12	C7-C8-C9-C10
5	A	411	R16	C39-C40-C41-C42
3	A	403	D12	C7-C8-C9-C10
6	A	501	CPS	C9-C20-C22-C23
3	A	402	D12	C5-C6-C7-C8
4	A	406	D10	C2-C3-C4-C5
3	A	254	D12	C2-C3-C4-C5
3	A	256	D12	C2-C3-C4-C5
3	A	255	D12	C7-C8-C9-C10
3	A	254	D12	C3-C4-C5-C6
4	A	250	D10	C4-C5-C6-C7
4	A	409	D10	C2-C3-C4-C5
4	A	257	D10	C6-C7-C8-C9
4	A	257	D10	C5-C6-C7-C8
3	A	402	D12	C3-C4-C5-C6
5	A	411	R16	C28-C29-C30-C31
7	A	401	HP6	C23-C24-C25-C26
5	A	411	R16	C27-C28-C29-C30
4	A	250	D10	C6-C7-C8-C9
3	A	255	D12	C6-C7-C8-C9
3	A	255	D12	C2-C3-C4-C5
4	A	406	D10	C3-C4-C5-C6
3	A	254	D12	C4-C5-C6-C7
3	A	251	D12	C4-C5-C6-C7
4	A	257	D10	C4-C5-C6-C7
3	A	256	D12	C6-C7-C8-C9
3	A	255	D12	C1-C2-C3-C4
4	A	257	D10	C7-C8-C9-C10
3	A	256	D12	C3-C4-C5-C6
7	A	401	HP6	C22-C23-C24-C25
3	A	254	D12	C9-C10-C11-C12
4	A	406	D10	C1-C2-C3-C4
5	A	411	R16	C38-C39-C40-C41
3	A	252	D12	C6-C7-C8-C9
3	A	256	D12	C1-C2-C3-C4
3	A	251	D12	C5-C6-C7-C8
3	A	402	D12	C4-C5-C6-C7
3	A	403	D12	C3-C4-C5-C6
3	A	251	D12	C9-C10-C11-C12
4	A	257	D10	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	409	D10	C3-C4-C5-C6
3	A	256	D12	C11-C10-C9-C8
8	A	253	DD9	C2-C3-C4-C5
4	A	406	D10	C6-C7-C8-C9
3	A	402	D12	C11-C10-C9-C8
3	A	255	D12	C11-C10-C9-C8
3	A	256	D12	C7-C8-C9-C10
3	A	251	D12	C2-C3-C4-C5
3	A	405	D12	C1-C2-C3-C4
8	A	253	DD9	C5-C6-C7-C8
3	A	255	D12	C4-C5-C6-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	254	D12	1	0
4	A	406	D10	1	0
4	A	257	D10	1	0
6	A	501	CPS	1	0
2	A	301	RET	6	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 then 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.

Ligand CPS A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 301

Bond lengths

Bond angles

Torsions

Rings
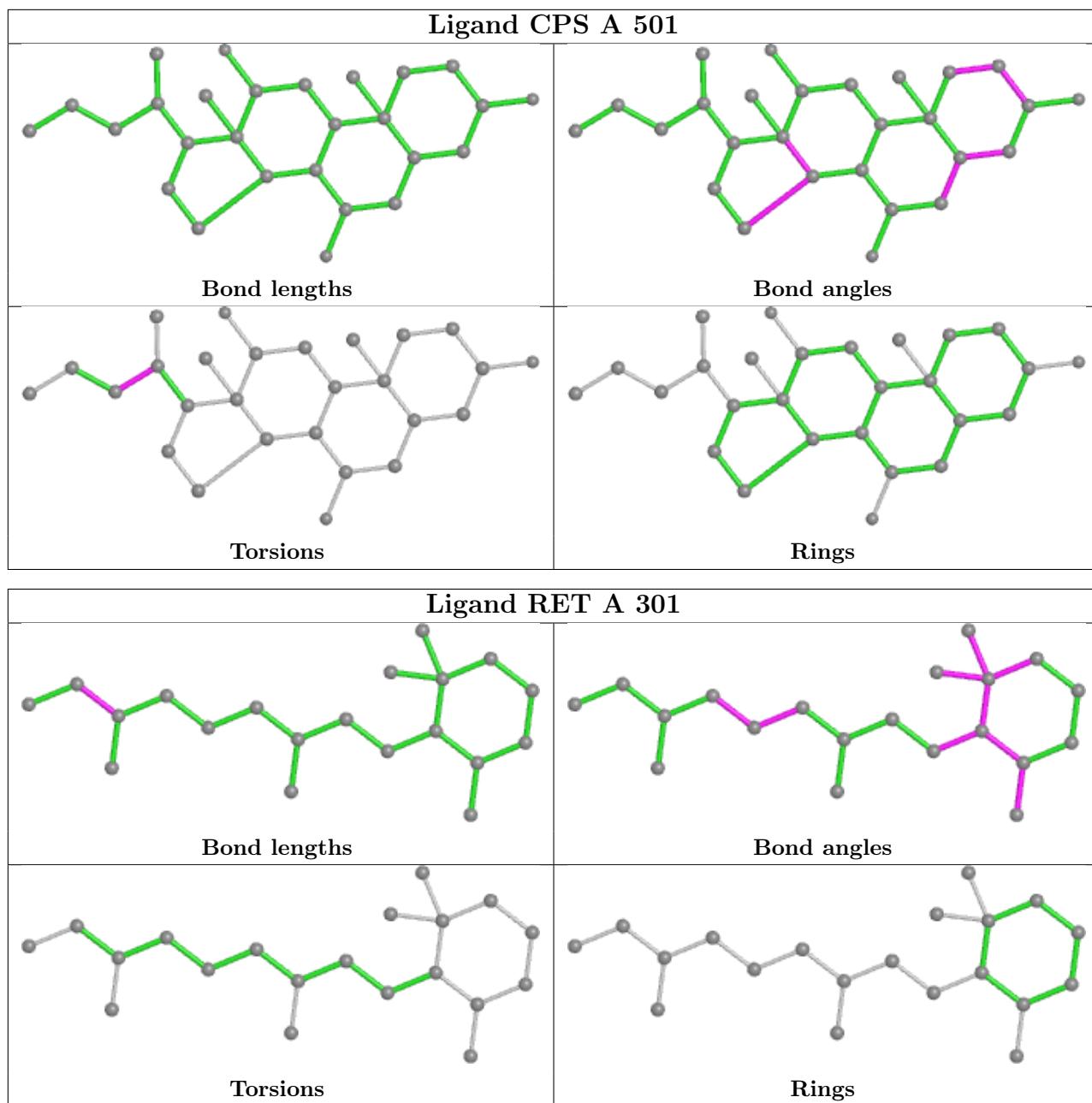
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	226/249 (90%)	-0.33	6 (2%)	54	52	11, 14, 23, 30	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLY	5.8
1	A	73	GLY	3.2
1	A	231	GLY	3.2
1	A	133	TYR	2.8
1	A	37	PRO	2.7
1	A	74	GLU	2.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
4	D10	A	250	10/10	0.47	0.19	52,53,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	D12	A	405	12/12	0.54	0.15	38,41,42,43	0
6	CPS	A	501	27/42	0.54	0.29	42,44,46,46	0
3	D12	A	255	12/12	0.57	0.17	54,55,56,56	0
3	D12	A	254	12/12	0.61	0.17	47,50,53,53	0
3	D12	A	251	12/12	0.63	0.14	50,51,51,52	0
3	D12	A	252	12/12	0.65	0.20	53,54,55,56	0
3	D12	A	402	12/12	0.68	0.18	52,53,53,53	0
4	D10	A	406	10/10	0.76	0.17	33,34,38,38	0
7	HP6	A	401	7/7	0.76	0.13	42,42,43,43	0
3	D12	A	256	12/12	0.79	0.14	51,52,53,53	0
4	D10	A	257	10/10	0.79	0.15	47,47,48,48	0
5	R16	A	411	16/16	0.81	0.14	25,31,41,41	0
4	D10	A	409	10/10	0.83	0.14	43,43,43,43	0
3	D12	A	403	12/12	0.83	0.12	36,37,40,40	0
8	DD9	A	253	9/9	0.86	0.11	37,38,40,41	0
2	RET	A	301	20/21	0.91	0.12	12,13,20,20	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 CPS A 501:

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

Electron density around 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.