



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 09:46 PM JST

PDB ID : 7X17
Title : Structure of Pseudomonas NRPS protein, AmbB-TC bound to Ppant-L-Ala
Authors : ChuYuanKee, M.; Bharath, S.R.; Song, H.
Deposited on : 2022-02-23
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

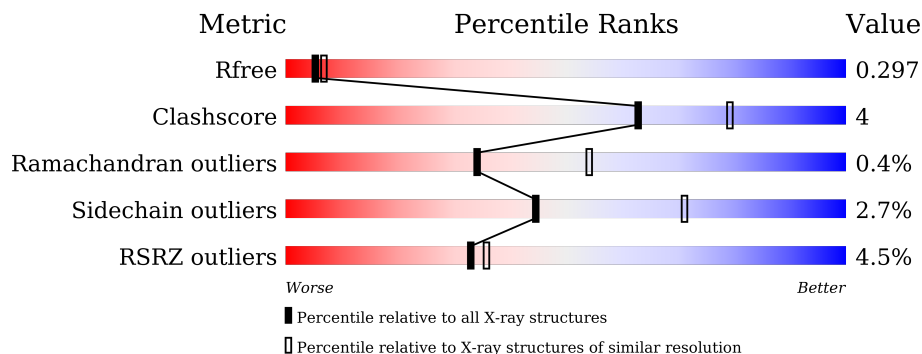
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	523	 4% 70% 7% • 22%
1	B	523	 3% 70% 10% • 20%
1	C	523	 2% 77% 10% 13%
1	D	523	 6% 73% 12% 15%

2 Entry composition [i](#)

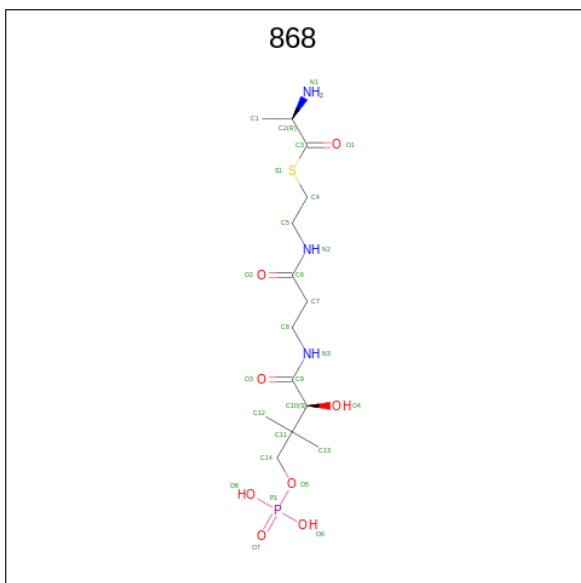
There are 3 unique types of molecules in this entry. The entry contains 13793 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMB antimetabolite synthase AmbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	Total 3161	C 1990	N 606	O 560	S 5	0	0	0
1	B	421	Total 3225	C 2031	N 618	O 571	S 5	0	0	0
1	C	455	Total 3488	C 2196	N 666	O 621	S 5	0	0	0
1	D	443	Total 3399	C 2144	N 650	O 600	S 5	0	0	0

- Molecule 2 is S-[2-[3-[(2S)-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (2R)-2-azanylpropanethioate (three-letter code: 868) (formula: C₁₄H₂₈N₃O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	Total 26	C 14	N 3	O 7	P 1	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	B	1	Total	C	N	O	P	S	0	0
			26	14	3	7	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	14	3	7	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	14	3	7	1	1		

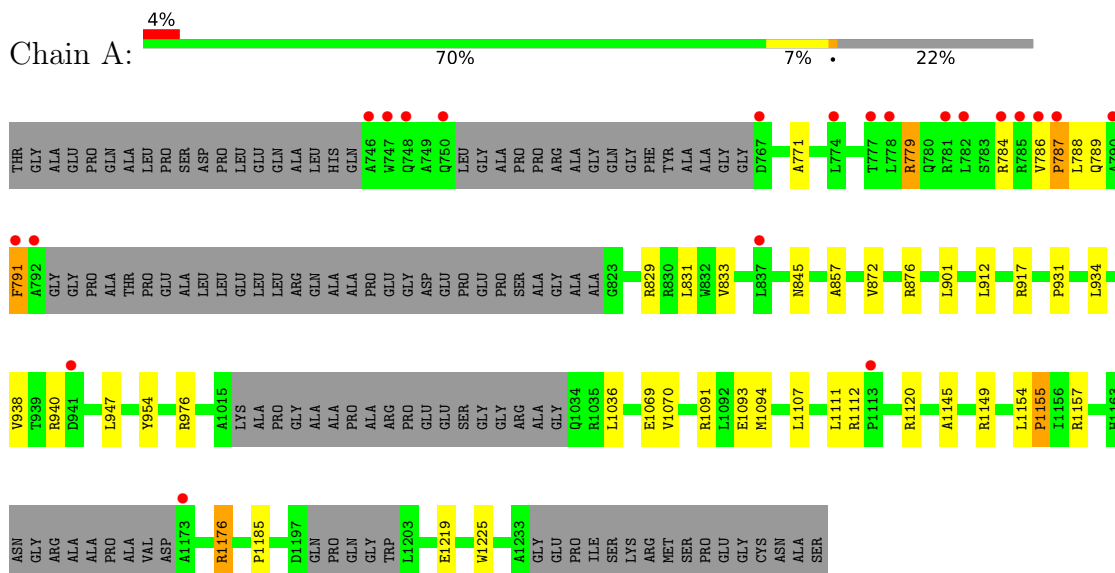
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	122	Total	O	0	0
			122	122		
3	C	113	Total	O	0	0
			113	113		
3	D	91	Total	O	0	0
			91	91		

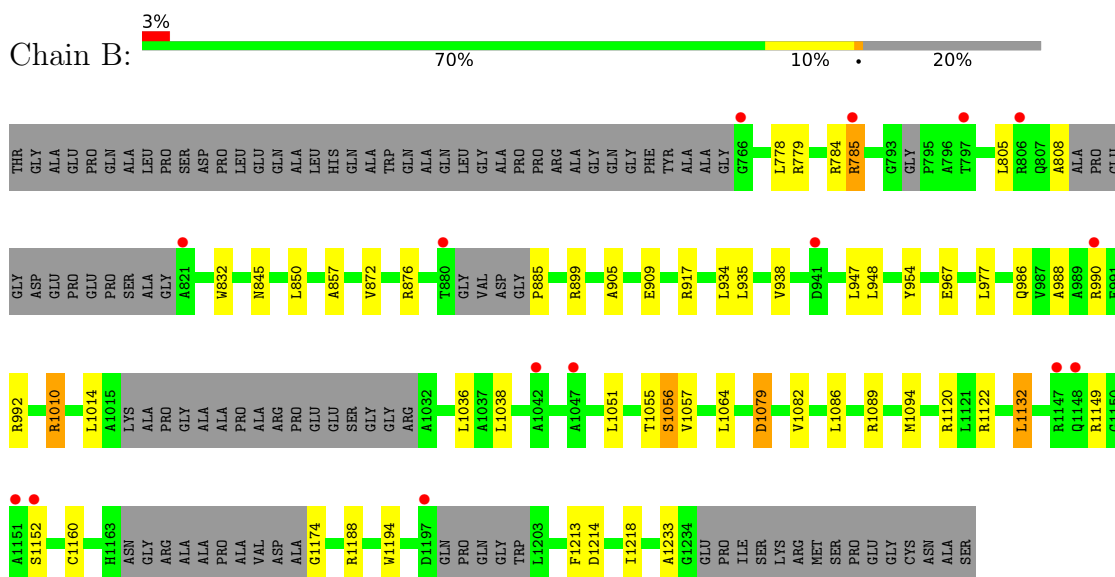
3 Residue-property plots [i](#)

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.

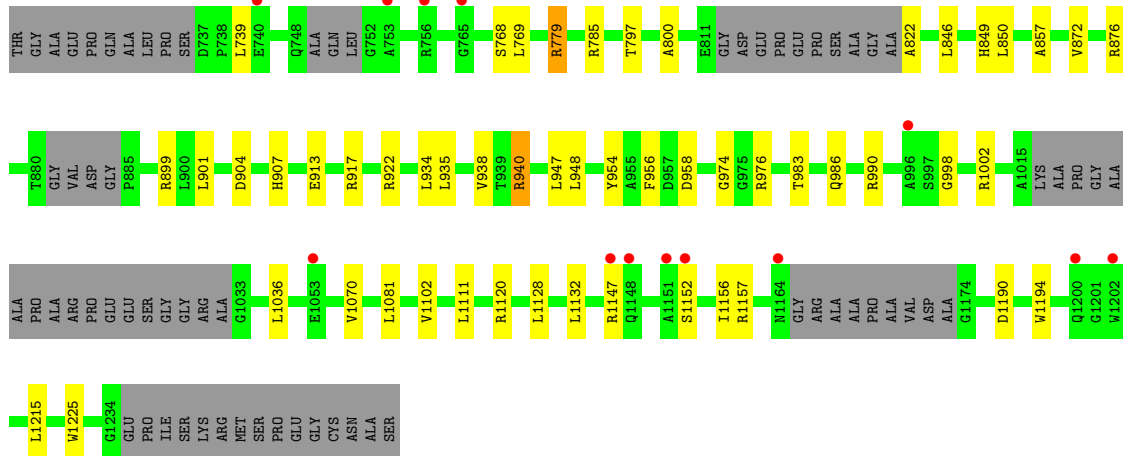
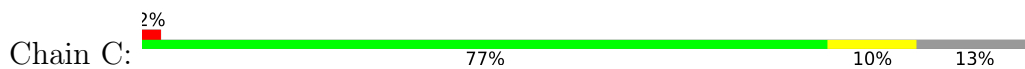
- Molecule 1: AMB antimetabolite synthase AmbB



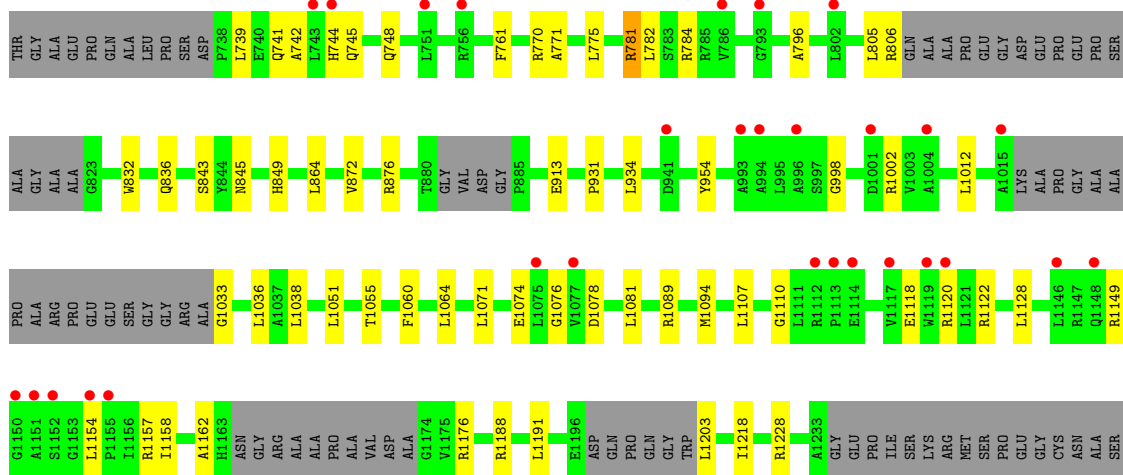
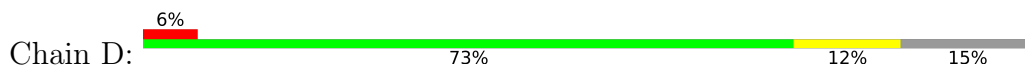
- Molecule 1: AMB antimetabolite synthase AmbB



- Molecule 1: AMB antimetabolite synthase AmbB



● Molecule 1: AMB antimetabolite synthase AmbB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.50Å 71.61Å 173.76Å 90.00° 110.14° 90.00°	Depositor
Resolution (Å)	46.59 – 2.50 48.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.59-2.50) 99.0 (48.83-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20_4459, PHENIX 1.20_4459	Depositor
R, R_{free}	0.246 , 0.299 0.245 , 0.297	Depositor DCC
R_{free} test set	3952 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13793	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: 868

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	0.24	0/3211	0.52	0/4361
1	B	0.24	0/3274	0.52	0/4443
1	C	0.24	0/3550	0.51	0/4825
1	D	0.24	0/3457	0.52	0/4695
All	All	0.24	0/13492	0.52	0/18324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3161	0	3231	23	0
1	B	3225	0	3310	33	0
1	C	3488	0	3540	32	0
1	D	3399	0	3476	34	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	3	0
2	D	26	0	0	1	0
3	A	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	122	0	0	3	0
3	C	113	0	0	3	0
3	D	91	0	0	2	0
All	All	13793	0	13557	117	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 4.

All (117) 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:1213:PHE:HB3	1:B:1218:ILE:HD11	1.58	0.85
1:D:1071:LEU:HD11	1:D:1191:LEU:HD23	1.70	0.74
1:C:1081:LEU:HD11	1:C:1156:ILE:HG12	1.69	0.72
1:A:787:PRO:O	1:A:789:GLN:N	2.25	0.69
1:D:781:ARG:HG3	1:D:782:LEU:HD12	1.77	0.66
1:A:1091:ARG:HG2	1:A:1094:MET:HG3	1.78	0.66
1:D:782:LEU:HB3	1:D:784:ARG:HG3	1.79	0.64
1:C:904:ASP:OD1	1:C:907:HIS:ND1	2.31	0.63
1:B:1120:ARG:NH2	3:B:1401:HOH:O	2.30	0.63
1:C:917:ARG:NH2	1:D:845:ASN:O	2.26	0.62
1:B:1014:LEU:HD21	1:B:1079:ASP:HB3	1.86	0.58
1:B:986:GLN:O	1:B:990:ARG:HG3	2.04	0.57
1:D:864:LEU:HD13	1:D:934:LEU:HD23	1.86	0.57
1:D:843:SER:OG	1:D:1188:ARG:NH2	2.37	0.56
1:A:1069:GLU:OE2	1:A:1120:ARG:NH1	2.38	0.56
1:D:1033:GLY:N	3:D:1404:HOH:O	2.38	0.56
1:C:797:THR:HG23	1:C:800:ALA:H	1.71	0.56
1:B:1086:LEU:HD22	1:B:1132:LEU:HD13	1.89	0.54
1:C:983:THR:HG23	1:C:986:GLN:H	1.72	0.54
1:A:1185:PRO:HD3	1:B:917:ARG:HG2	1.90	0.54
1:C:822:ALA:N	3:C:1406:HOH:O	2.40	0.54
1:C:934:LEU:HD22	1:C:947:LEU:HD11	1.91	0.53
1:B:779:ARG:HD2	1:B:785:ARG:HD3	1.90	0.53
1:B:935:LEU:HB3	1:B:948:LEU:HB3	1.90	0.53
1:D:1012:LEU:HD11	1:D:1149:ARG:HD2	1.91	0.53
1:C:922:ARG:HH11	1:C:922:ARG:HG3	1.75	0.52
1:D:1064:LEU:HD21	1:D:1107:LEU:HD22	1.92	0.52
1:D:1071:LEU:HD13	1:D:1158:ILE:HD12	1.92	0.52
1:A:1155:PRO:HB2	1:A:1157:ARG:NH1	2.25	0.51
1:A:901:LEU:HD21	1:A:940:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1056:SER:O	1:B:1056:SER:OG	2.22	0.51
1:C:1036:LEU:HD13	1:C:1215:LEU:HD11	1.93	0.51
1:D:741:GLN:O	1:D:745:GLN:HG3	2.11	0.51
1:C:1102:VAL:HG11	2:C:1514:868:S1	2.51	0.51
1:D:1118:GLU:O	1:D:1122:ARG:HG3	2.11	0.51
1:B:1089:ARG:HA	1:B:1094:MET:HE2	1.94	0.51
1:D:1051:LEU:O	1:D:1055:THR:OG1	2.25	0.50
1:D:1203:LEU:N	3:D:1410:HOH:O	2.44	0.50
1:B:905:ALA:O	1:B:909:GLU:HG3	2.12	0.50
1:C:1194:TRP:HH2	2:C:1514:868:N2	2.10	0.49
1:B:934:LEU:HD22	1:B:947:LEU:HD11	1.93	0.49
1:B:1055:THR:HG23	1:B:1122:ARG:HG3	1.94	0.49
1:A:1091:ARG:HE	1:A:1093:GLU:HG2	1.78	0.49
1:D:872:VAL:O	1:D:876:ARG:HG3	2.13	0.49
1:A:1070:VAL:HG21	1:A:1225:TRP:HA	1.94	0.48
1:D:761:PHE:N	1:D:796:ALA:O	2.44	0.48
1:B:967:GLU:HG2	1:B:977:LEU:HD22	1.95	0.48
1:B:1214:ASP:O	1:B:1218:ILE:HG12	2.13	0.48
1:C:899:ARG:NH2	3:C:1413:HOH:O	2.47	0.48
1:B:1064:LEU:HD11	1:B:1082:VAL:HG11	1.95	0.48
1:C:913:GLU:OE1	1:D:849:HIS:ND1	2.47	0.48
1:D:998:GLY:O	1:D:1002:ARG:HG3	2.13	0.48
1:C:998:GLY:O	1:C:1002:ARG:HG3	2.13	0.48
1:C:940:ARG:NH1	3:C:1408:HOH:O	2.44	0.48
2:C:1514:868:O4	2:C:1514:868:O5	2.32	0.48
1:C:1070:VAL:HG21	1:C:1225:TRP:HA	1.96	0.47
1:C:1111:LEU:HA	1:C:1120:ARG:HH21	1.79	0.47
1:D:876:ARG:O	1:D:931:PRO:HD3	2.14	0.47
1:A:872:VAL:O	1:A:876:ARG:HG3	2.14	0.47
1:A:1176:ARG:HA	1:A:1176:ARG:NE	2.29	0.47
1:B:988:ALA:O	1:B:992:ARG:HG3	2.15	0.46
1:C:850:LEU:HB2	1:C:947:LEU:HB3	1.98	0.46
1:A:917:ARG:NH2	1:B:845:ASN:O	2.35	0.46
1:C:849:HIS:ND1	1:D:913:GLU:OE2	2.48	0.46
1:D:832:TRP:O	1:D:836:GLN:HG2	2.16	0.46
1:B:872:VAL:O	1:B:876:ARG:HG3	2.16	0.45
1:B:857:ALA:HB2	1:B:938:VAL:HG21	1.98	0.45
1:B:1036:LEU:HD23	1:B:1218:ILE:HG22	1.99	0.45
1:D:1060:PHE:HD2	1:D:1128:LEU:HD21	1.80	0.45
1:D:1081:LEU:HD21	1:D:1154:LEU:HG	1.98	0.45
1:C:1147:ARG:NE	1:C:1152:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:LEU:HB2	1:B:947:LEU:HB3	1.99	0.45
1:B:1174:GLY:N	3:B:1408:HOH:O	2.50	0.45
1:A:845:ASN:O	1:B:917:ARG:NH2	2.35	0.44
1:A:829:ARG:NH1	1:A:833:VAL:HG11	2.32	0.44
1:A:1176:ARG:HA	1:A:1176:ARG:HE	1.82	0.44
1:B:778:LEU:HD13	1:B:805:LEU:HD11	2.00	0.44
1:A:857:ALA:HB2	1:A:938:VAL:HG11	2.00	0.44
1:D:1074:GLU:C	1:D:1076:GLY:H	2.20	0.44
1:D:739:LEU:HD11	1:D:784:ARG:NH1	2.33	0.43
1:C:872:VAL:O	1:C:876:ARG:HG3	2.19	0.43
1:C:846:LEU:HD12	1:C:956:PHE:HB3	2.00	0.43
1:D:1089:ARG:HA	1:D:1094:MET:HE2	2.00	0.43
1:C:922:ARG:HG3	1:C:922:ARG:NH1	2.32	0.43
1:D:744:HIS:CE1	1:D:748:GLN:HE21	2.37	0.43
1:B:1055:THR:HG22	1:B:1057:VAL:HG13	2.01	0.43
1:B:1010:ARG:NH1	1:B:1079:ASP:OD2	2.45	0.43
1:B:1036:LEU:HD21	1:B:1038:LEU:HD11	2.01	0.43
1:A:976:ARG:HH11	1:A:976:ARG:HG2	1.84	0.42
1:C:899:ARG:NH1	1:C:901:LEU:HB2	2.33	0.42
1:A:1069:GLU:HA	1:A:1111:LEU:HD21	2.02	0.42
1:C:974:GLY:O	1:C:976:ARG:NH1	2.52	0.42
1:C:1081:LEU:HD12	1:C:1156:ILE:HA	2.00	0.42
1:A:771:ALA:HB1	1:A:791:PHE:HE2	1.85	0.42
1:B:784:ARG:NH1	1:B:808:ALA:O	2.53	0.42
1:A:1036:LEU:HD21	1:A:1219:GLU:HG3	2.01	0.42
1:B:1051:LEU:HD13	1:B:1233:ALA:HA	2.02	0.42
1:C:779:ARG:NH1	1:C:785:ARG:HB2	2.33	0.42
1:C:857:ALA:HB2	1:C:938:VAL:HG21	2.01	0.42
1:D:1162:ALA:O	2:D:1492:868:N3	2.52	0.42
1:B:1149:ARG:HE	1:B:1149:ARG:HB3	1.71	0.41
1:D:1036:LEU:HD23	1:D:1218:ILE:HG22	2.02	0.41
1:A:876:ARG:O	1:A:931:PRO:HD3	2.19	0.41
1:C:739:LEU:HD23	1:C:739:LEU:HA	1.87	0.41
1:D:1110:GLY:O	1:D:1120:ARG:HD2	2.21	0.41
1:A:779:ARG:O	1:A:779:ARG:NH1	2.50	0.41
1:A:934:LEU:HD22	1:A:947:LEU:HD11	2.02	0.41
1:D:1158:ILE:HD13	1:D:1191:LEU:HB3	2.01	0.41
1:D:742:ALA:CB	1:D:782:LEU:HD11	2.50	0.41
1:C:935:LEU:HB3	1:C:948:LEU:HB3	2.02	0.41
1:D:1012:LEU:CD1	1:D:1149:ARG:HD2	2.50	0.41
1:B:832:TRP:CZ3	1:B:885:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1157:ARG:HD2	1:C:1190:ASP:OD2	2.20	0.41
1:B:1188:ARG:NH2	3:B:1412:HOH:O	2.52	0.41
1:D:771:ALA:O	1:D:775:LEU:HG	2.21	0.40
1:C:769:LEU:HD12	1:C:769:LEU:HA	1.80	0.40
1:A:1145:ALA:O	1:A:1149:ARG:HD2	2.21	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	398/523 (76%)	387 (97%)	5 (1%)	6 (2%)	10	18
1	B	407/523 (78%)	401 (98%)	6 (2%)	0	100	100
1	C	443/523 (85%)	434 (98%)	9 (2%)	0	100	100
1	D	431/523 (82%)	424 (98%)	7 (2%)	0	100	100
All	All	1679/2092 (80%)	1646 (98%)	27 (2%)	6 (0%)	34	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	788	LEU
1	A	791	PHE
1	A	786	VAL
1	A	784	ARG
1	A	787	PRO
1	A	1155	PRO

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	318/390 (82%)	310 (98%)	8 (2%)	47 73
1	B	323/390 (83%)	313 (97%)	10 (3%)	40 67
1	C	347/390 (89%)	339 (98%)	8 (2%)	50 76
1	D	339/390 (87%)	329 (97%)	10 (3%)	42 69
All	All	1327/1560 (85%)	1291 (97%)	36 (3%)	44 71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	779	ARG
1	A	831	LEU
1	A	912	LEU
1	A	954	TYR
1	A	1107	LEU
1	A	1112	ARG
1	A	1154	LEU
1	A	1176	ARG
1	B	785	ARG
1	B	899	ARG
1	B	954	TYR
1	B	1010	ARG
1	B	1056	SER
1	B	1079	ASP
1	B	1132	LEU
1	B	1152	SER
1	B	1160	CYS
1	B	1194	TRP
1	C	768	SER
1	C	779	ARG
1	C	940	ARG
1	C	954	TYR
1	C	958	ASP
1	C	990	ARG

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Mol	Chain	Res	Type
1	C	1128	LEU
1	C	1132	LEU
1	D	770	ARG
1	D	781	ARG
1	D	805	LEU
1	D	806	ARG
1	D	954	TYR
1	D	1038	LEU
1	D	1078	ASP
1	D	1157	ARG
1	D	1176	ARG
1	D	1228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	744	HIS
1	D	745	GLN
1	D	862	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	868	D	1492	1	18,25,26	2.19	6 (33%)	22,33,36	1.63	7 (31%)
2	868	C	1514	1	18,25,26	2.22	5 (27%)	22,33,36	1.77	7 (31%)
2	868	A	1301	1	18,25,26	1.92	3 (16%)	22,33,36	1.37	5 (22%)
2	868	B	1527	1	18,25,26	2.17	6 (33%)	22,33,36	1.15	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	868	D	1492	1	-	12/30/33/34	-
2	868	C	1514	1	-	15/30/33/34	-
2	868	A	1301	1	-	10/30/33/34	-
2	868	B	1527	1	-	16/30/33/34	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1514	868	C9-N3	5.82	1.46	1.33
2	D	1492	868	C9-N3	5.72	1.46	1.33
2	B	1527	868	C9-N3	5.65	1.45	1.33
2	C	1514	868	C6-N2	5.62	1.46	1.33
2	D	1492	868	C6-N2	5.48	1.45	1.33
2	B	1527	868	C6-N2	5.42	1.45	1.33
2	A	1301	868	C9-N3	4.90	1.44	1.33
2	A	1301	868	C6-N2	4.84	1.44	1.33
2	C	1514	868	C3-S1	2.28	1.82	1.75
2	D	1492	868	O3-C9	-2.22	1.19	1.23
2	B	1527	868	C3-S1	2.22	1.82	1.75
2	B	1527	868	O3-C9	-2.17	1.19	1.23
2	C	1514	868	O3-C9	-2.17	1.19	1.23
2	D	1492	868	C3-S1	2.16	1.82	1.75
2	D	1492	868	O2-C6	-2.12	1.18	1.23
2	C	1514	868	O2-C6	-2.11	1.19	1.23
2	A	1301	868	C3-S1	2.10	1.81	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1527	868	O5-C14	-2.08	1.39	1.44
2	B	1527	868	O2-C6	-2.06	1.19	1.23
2	D	1492	868	O5-C14	-2.03	1.39	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1514	868	C4-S1-C3	4.20	114.40	101.75
2	C	1514	868	O1-C3-S1	-3.13	119.59	123.80
2	D	1492	868	C4-S1-C3	3.01	110.81	101.75
2	A	1301	868	O1-C3-S1	-3.00	119.76	123.80
2	D	1492	868	C7-C6-N2	2.88	121.27	116.42
2	D	1492	868	O1-C3-S1	-2.85	119.97	123.80
2	B	1527	868	C4-S1-C3	2.76	110.06	101.75
2	C	1514	868	C8-C7-C6	2.73	116.91	112.36
2	C	1514	868	C10-C9-N3	2.71	121.98	116.58
2	D	1492	868	O3-C9-N3	-2.66	117.28	122.99
2	D	1492	868	C5-N2-C6	-2.60	118.01	122.84
2	C	1514	868	C7-C6-N2	2.58	120.77	116.42
2	B	1527	868	O1-C3-S1	-2.50	120.44	123.80
2	D	1492	868	C10-C9-N3	2.35	121.26	116.58
2	A	1301	868	C8-C7-C6	-2.29	108.55	112.36
2	C	1514	868	O3-C9-N3	-2.26	118.15	122.99
2	A	1301	868	O2-C6-N2	-2.18	118.89	123.01
2	A	1301	868	C4-C5-N2	-2.18	107.83	112.42
2	C	1514	868	C13-C11-C10	2.11	112.48	108.82
2	D	1492	868	O2-C6-N2	-2.07	119.11	123.01
2	A	1301	868	O3-C9-N3	-2.05	118.60	122.99

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	868	C10-C9-N3-C8
2	A	1301	868	C6-C7-C8-N3
2	A	1301	868	O1-C3-S1-C4
2	A	1301	868	C2-C3-S1-C4
2	B	1527	868	C5-C4-S1-C3
2	B	1527	868	C6-C7-C8-N3
2	B	1527	868	O4-C10-C11-C13
2	B	1527	868	O4-C10-C11-C14
2	B	1527	868	O4-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	B	1527	868	C9-C10-C11-C13
2	B	1527	868	C9-C10-C11-C14
2	B	1527	868	C9-C10-C11-C12
2	B	1527	868	C10-C11-C14-O5
2	B	1527	868	O1-C3-S1-C4
2	B	1527	868	C2-C3-S1-C4
2	B	1527	868	C1-C2-C3-O1
2	C	1514	868	C10-C9-N3-C8
2	C	1514	868	C5-C4-S1-C3
2	C	1514	868	C6-C7-C8-N3
2	C	1514	868	O4-C10-C11-C13
2	C	1514	868	O4-C10-C11-C14
2	C	1514	868	O4-C10-C11-C12
2	C	1514	868	C9-C10-C11-C13
2	C	1514	868	C9-C10-C11-C14
2	C	1514	868	C9-C10-C11-C12
2	C	1514	868	O1-C3-S1-C4
2	C	1514	868	C2-C3-S1-C4
2	D	1492	868	C10-C9-N3-C8
2	D	1492	868	C6-C7-C8-N3
2	D	1492	868	O4-C10-C9-O3
2	D	1492	868	O1-C3-S1-C4
2	D	1492	868	C2-C3-S1-C4
2	A	1301	868	O3-C9-N3-C8
2	C	1514	868	O3-C9-N3-C8
2	D	1492	868	O3-C9-N3-C8
2	B	1527	868	C13-C11-C14-O5
2	B	1527	868	C12-C11-C14-O5
2	A	1301	868	O4-C10-C9-N3
2	D	1492	868	O4-C10-C9-N3
2	A	1301	868	O4-C10-C9-O3
2	C	1514	868	C13-C11-C14-O5
2	C	1514	868	C1-C2-C3-S1
2	D	1492	868	C1-C2-C3-S1
2	D	1492	868	C11-C10-C9-O3
2	B	1527	868	S1-C4-C5-N2
2	A	1301	868	C4-C5-N2-C6
2	B	1527	868	N1-C2-C3-O1
2	D	1492	868	C11-C10-C9-N3
2	A	1301	868	C5-C4-S1-C3
2	D	1492	868	C5-C4-S1-C3
2	C	1514	868	C1-C2-C3-O1

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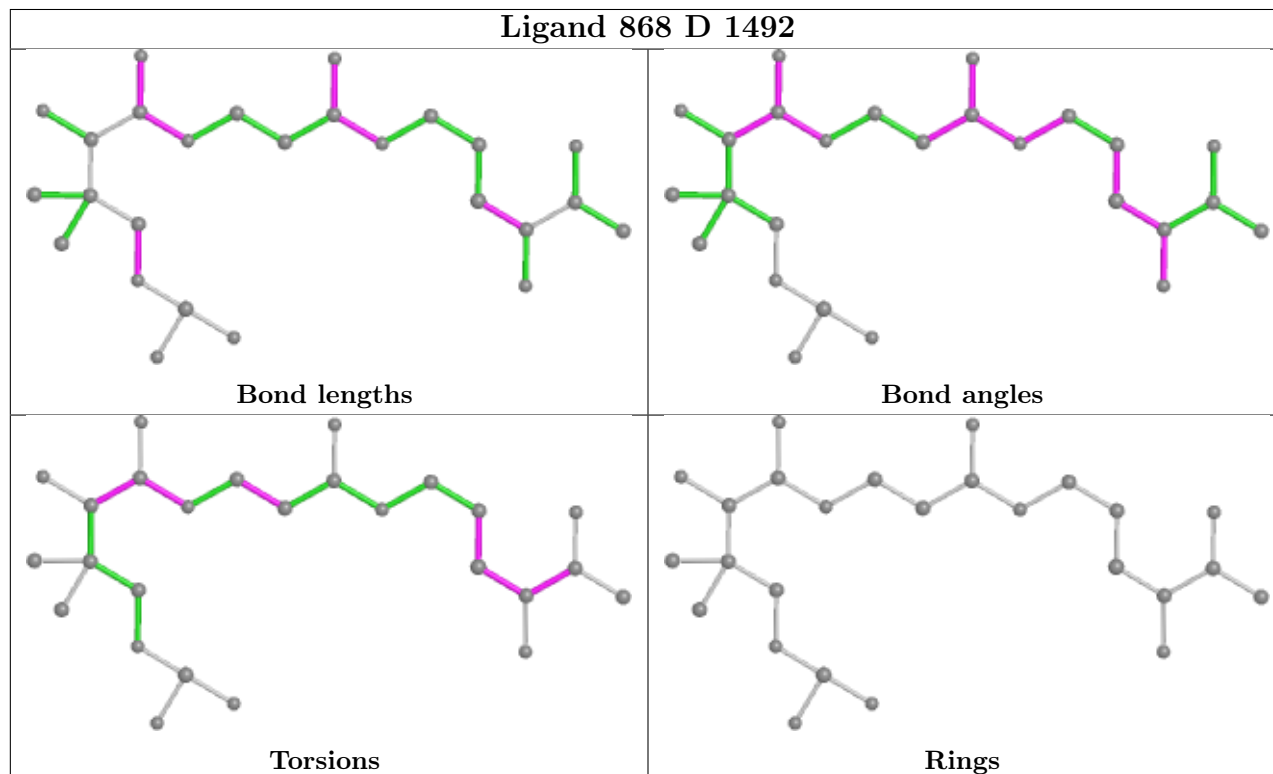
Mol	Chain	Res	Type	Atoms
2	D	1492	868	C1-C2-C3-O1
2	A	1301	868	C11-C10-C9-O3

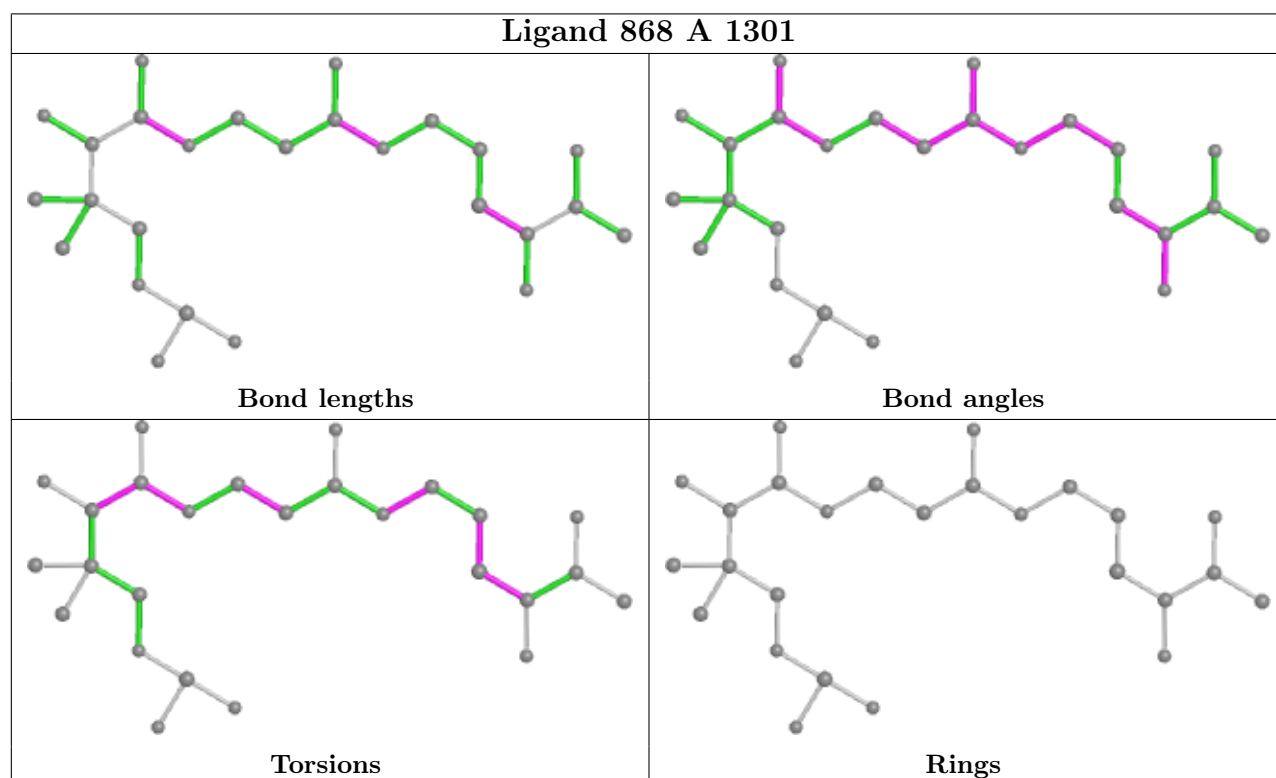
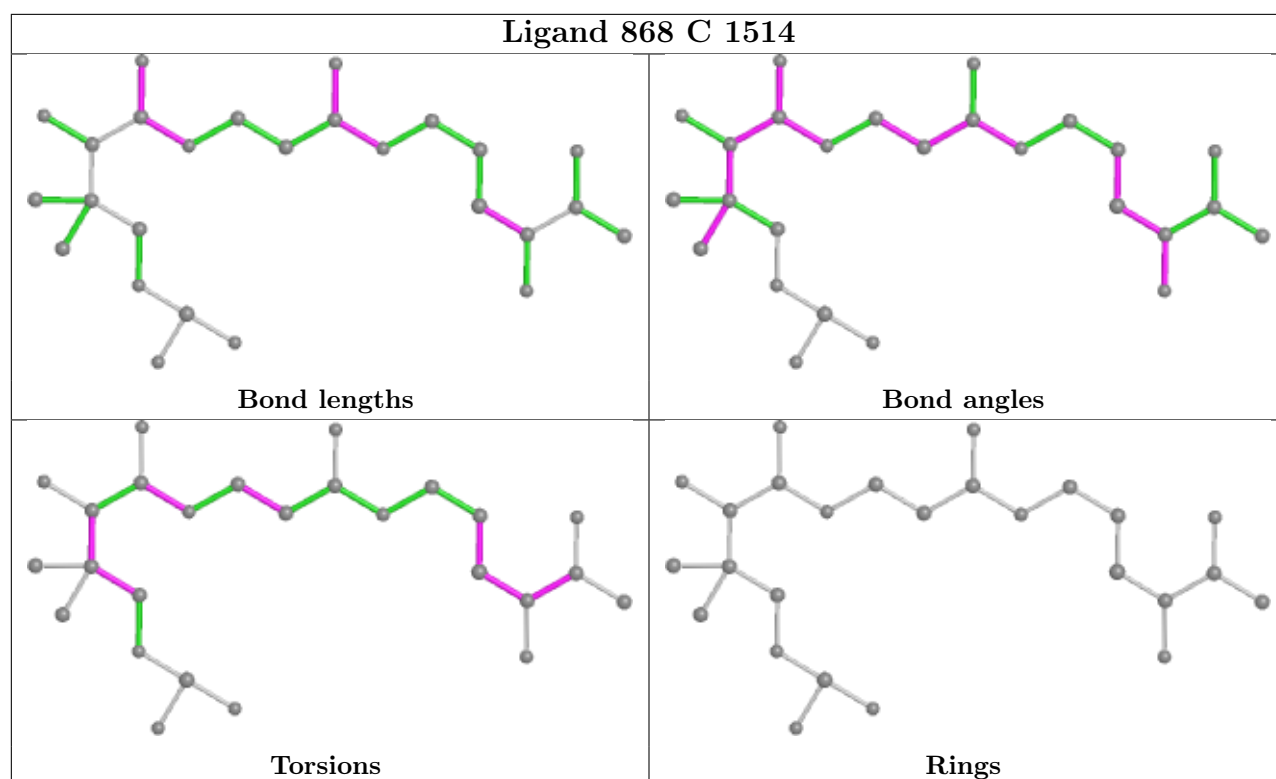
There are no ring outliers.

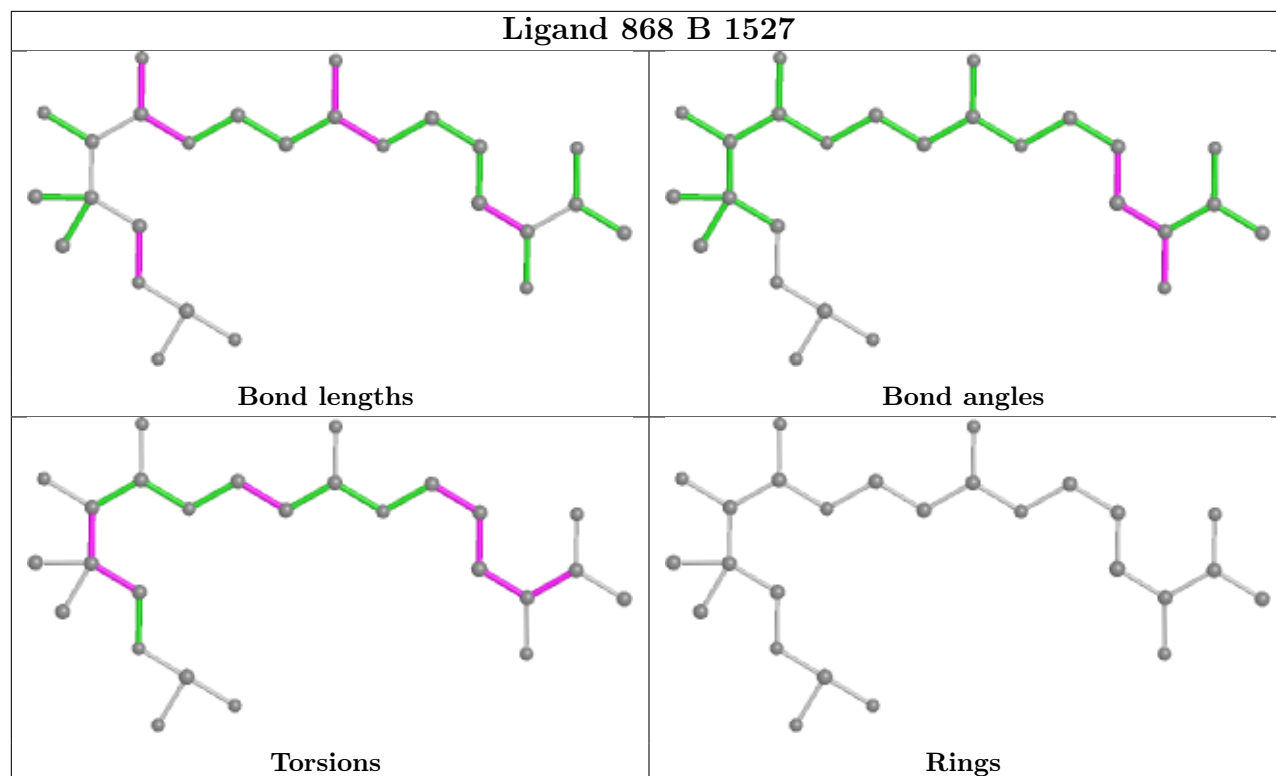
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1492	868	1	0
2	C	1514	868	3	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	410/523 (78%)	0.30	21 (5%) 28 29	9, 25, 56, 68	0
1	B	421/523 (80%)	0.26	15 (3%) 42 46	11, 26, 46, 60	0
1	C	455/523 (86%)	0.27	13 (2%) 51 55	13, 28, 52, 70	0
1	D	443/523 (84%)	0.42	29 (6%) 18 19	12, 33, 53, 74	0
All	All	1729/2092 (82%)	0.31	78 (4%) 33 36	9, 27, 52, 74	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	747	TRP	4.7
1	A	748	GLN	4.6
1	A	786	VAL	4.3
1	A	790	ALA	4.2
1	A	792	ALA	3.9
1	D	1114	GLU	3.8
1	D	1117	VAL	3.8
1	D	793	GLY	3.6
1	B	806	ARG	3.6
1	B	766	GLY	3.5
1	A	785	ARG	3.5
1	C	753	ALA	3.4
1	A	746	ALA	3.4
1	C	1148	GLN	3.3
1	D	1150	GLY	3.2
1	B	880	THR	3.1
1	A	791	PHE	3.0
1	C	1147	ARG	3.0
1	A	778	LEU	2.9
1	C	756	ARG	2.9
1	C	1202	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1152	SER	2.8
1	B	941	ASP	2.8
1	D	1112	ARG	2.8
1	B	797	THR	2.7
1	A	774	LEU	2.7
1	B	785	ARG	2.7
1	B	1147	ARG	2.7
1	D	1154	LEU	2.7
1	B	1148	GLN	2.6
1	A	941	ASP	2.6
1	D	744	HIS	2.6
1	C	1164	ASN	2.6
1	D	1075	LEU	2.6
1	D	1120	ARG	2.6
1	D	1155	PRO	2.6
1	A	1113	PRO	2.6
1	A	784	ARG	2.6
1	B	821	ALA	2.5
1	D	1113	PRO	2.5
1	C	996	ALA	2.5
1	D	1077	VAL	2.5
1	D	1119	TRP	2.5
1	D	1015	ALA	2.5
1	A	782	LEU	2.5
1	C	740	GLU	2.5
1	D	993	ALA	2.4
1	A	767	ASP	2.4
1	D	802	LEU	2.4
1	B	990	ARG	2.4
1	A	787	PRO	2.4
1	D	1001	ASP	2.4
1	B	1151	ALA	2.3
1	D	756	ARG	2.3
1	A	777	THR	2.3
1	D	996	ALA	2.3
1	B	1042	ALA	2.3
1	C	1200	GLN	2.2
1	D	994	ALA	2.2
1	D	1004	ALA	2.2
1	D	1146	LEU	2.2
1	D	1151	ALA	2.2
1	D	1152	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	781	ARG	2.2
1	A	837	LEU	2.2
1	C	765	GLY	2.2
1	D	751	LEU	2.2
1	B	1197	ASP	2.2
1	C	1053	GLU	2.2
1	D	941	ASP	2.1
1	D	743	LEU	2.1
1	D	1148	GLN	2.1
1	A	1173	ALA	2.1
1	C	1152	SER	2.1
1	B	1047	ALA	2.0
1	D	786	VAL	2.0
1	C	1151	ALA	2.0
1	A	750	GLN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

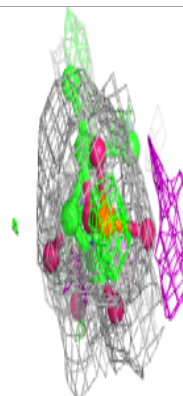
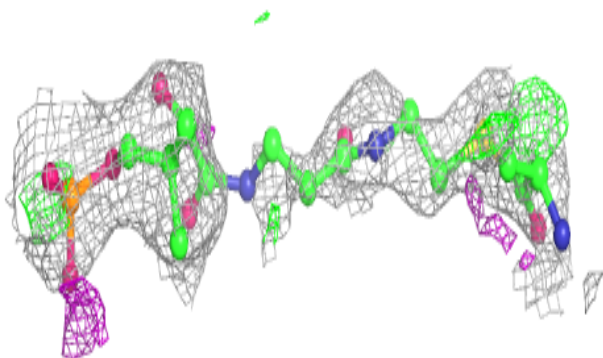
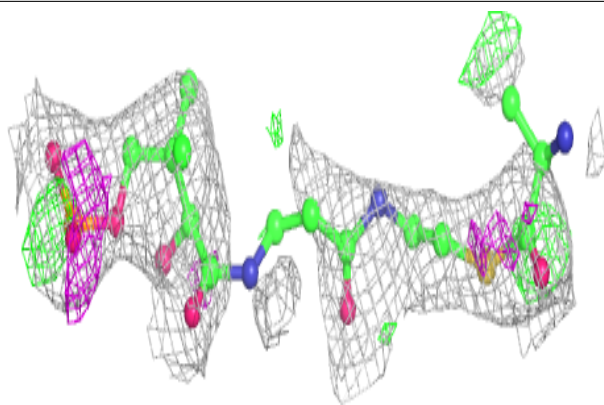
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	868	C	1514	26/27	0.81	0.31	33,47,60,65	0
2	868	A	1301	26/27	0.82	0.29	23,45,60,89	0
2	868	D	1492	26/27	0.83	0.24	34,44,60,67	0
2	868	B	1527	26/27	0.88	0.24	13,38,46,97	0

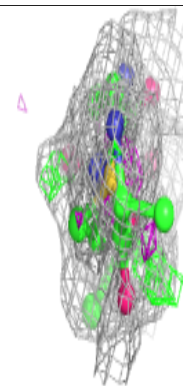
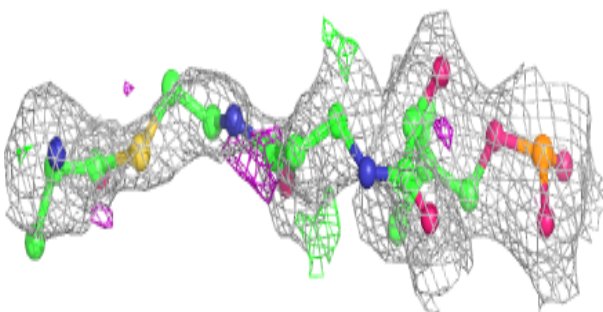
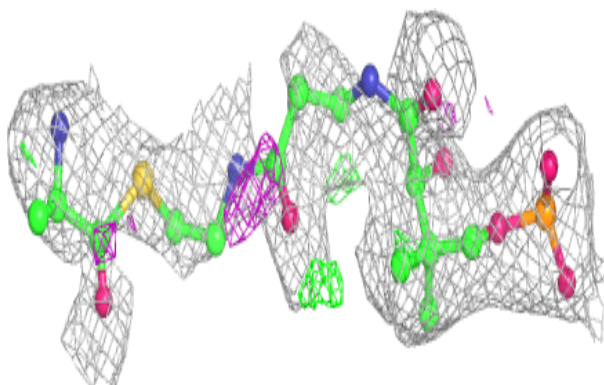
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 868 C 1514:

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

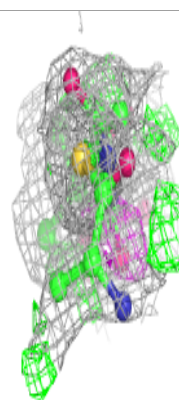
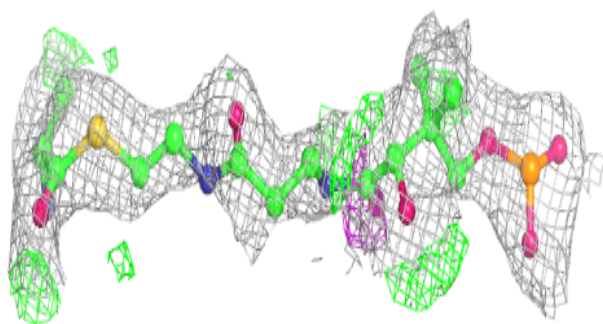
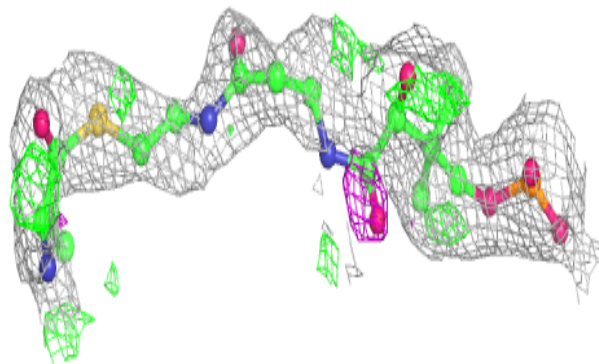
**Electron density around 868 A 1301:**

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

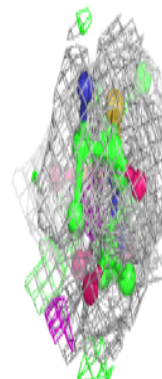
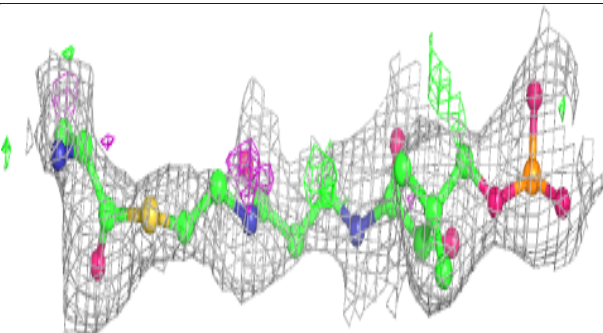
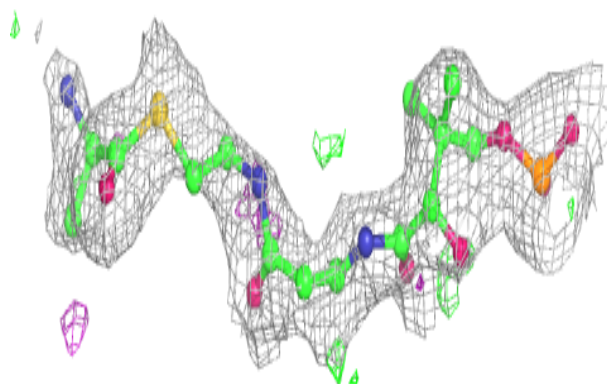


Electron density around 868 D 1492:

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

**Electron density around 868 B 1527:**

$2mF_o-DF_c$ (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.