



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:54 pm BST

PDB ID : 1X0I
Title : Crystal Structure of the Acid Blue Form of Bacteriorhodopsin
Authors : Okumura, H.; Murakami, M.; Kouyama, T.
Deposited on : 2005-03-23
Resolution : 2.30 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 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 : 2.11
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) : 2.11

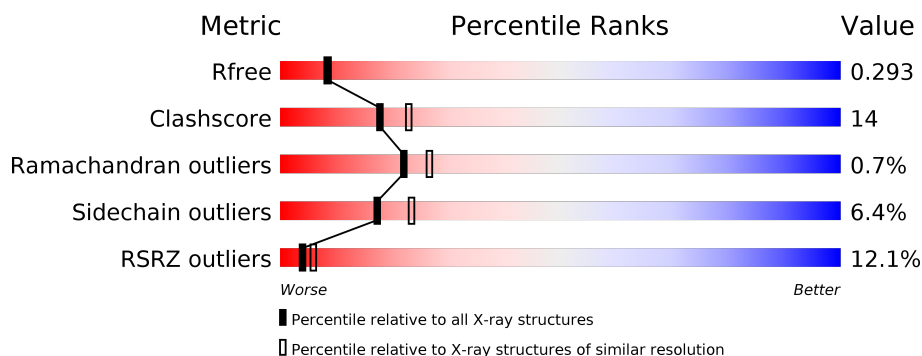
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	1-1	248	
1	2-1	248	

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	SO4	1-1	700	-	-	-	X
2	SO4	2-1	700	-	-	-	X
4	L3P	1-1	260	-	-	-	X
4	L3P	1-1	280	-	-	-	X
4	L3P	1-1	290	-	-	-	X
4	L3P	2-1	260	-	-	-	X
4	L3P	2-1	280	-	-	-	X
4	L3P	2-1	290	-	-	-	X
5	L2P	1-1	270	-	-	-	X
5	L2P	2-1	270	-	-	-	X

2 Entry composition [i](#)

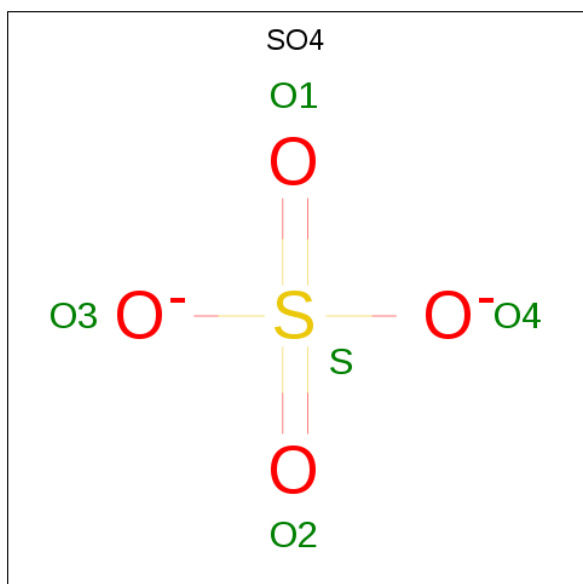
There are 6 unique types of molecules in this entry. The entry contains 3648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

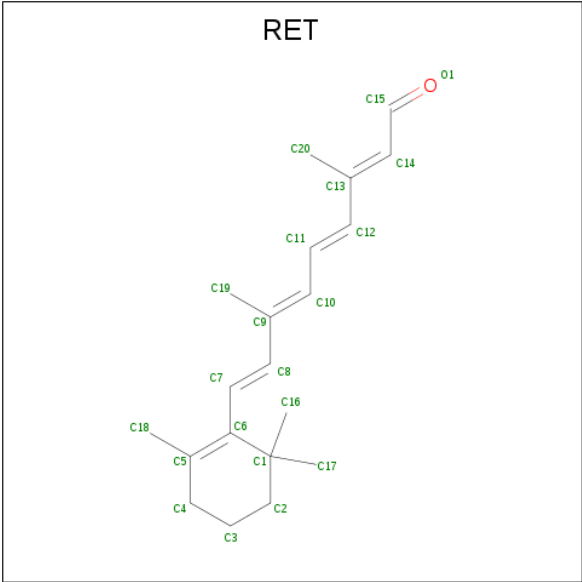
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-1	215	Total	C	N	O	S	0	0	0
			1666	1124	251	283	8			
1	2-1	215	Total	C	N	O	S	0	0	0
			1666	1124	251	283	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



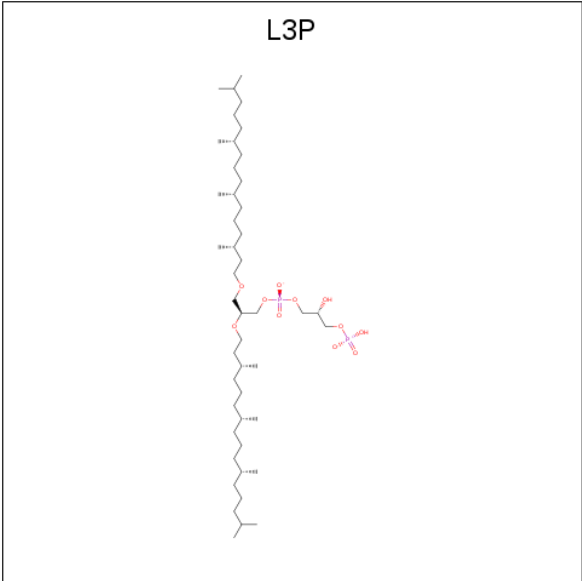
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-1	1	Total	O	S	0	0
			5	4	1		
2	2-1	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-1	1	Total	C	0	0
			20	20		
3	2-1	1	Total	C	0	0
			20	20		

- Molecule 4 is 2,3-DI-O-PHYTANLY-3-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCEROL-1'-PHOSPHATE (three-letter code: L3P) (formula: C₄₆H₉₄O₁₁P₂).



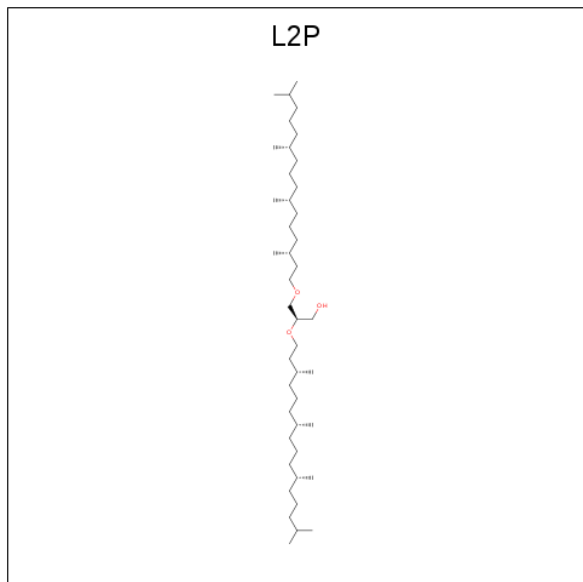
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	1-1	1	Total	C	O	P	0	0
			40	33	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	2-1	1	Total C O P 40 33 6 1	0	0
4	1-1	1	Total C 20 20	0	0
4	2-1	1	Total C 20 20	0	0
4	1-1	1	Total C 20 20	0	0
4	2-1	1	Total C 20 20	0	0

- Molecule 5 is 2,3-DI-PHYTANYL-GLYCEROL (three-letter code: L2P) (formula: $C_{43}H_{88}O_3$).

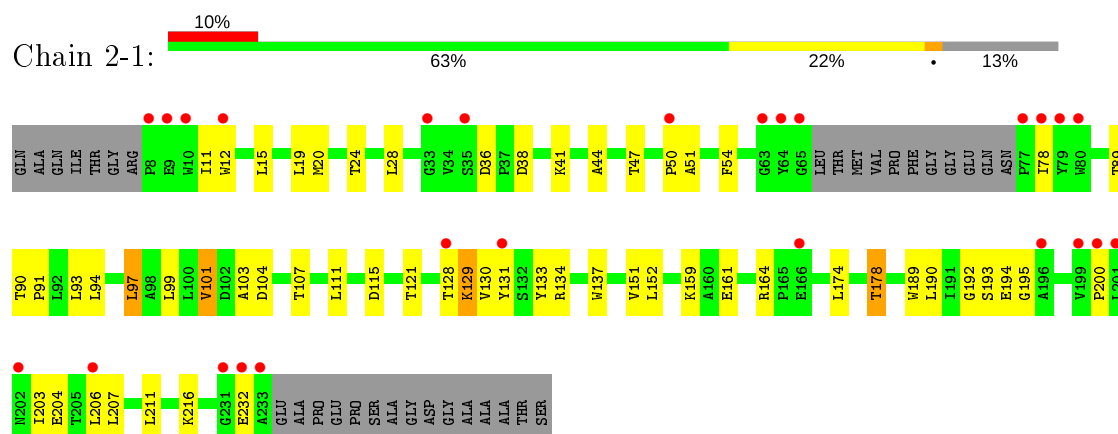


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-1	1	Total C O 28 25 3	0	0
5	2-1	1	Total C O 28 25 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-1	25	Total O 25 25	0	0
6	2-1	25	Total O 25 25	0	0

- Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.64Å 102.64Å 109.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.91 – 2.30 54.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.91-2.30) 99.4 (54.52-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.238 , 0.282 0.246 , 0.293	Depositor DCC
R_{free} test set	767 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3648	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: L2P, RET, L3P, SO4

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	1-1	0.41	0/1711	0.58	1/2335 (0.0%)
1	2-1	0.41	0/1711	0.54	0/2335
All	All	0.41	0/3422	0.56	1/4670 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-1	49	VAL	C-N-CD	5.17	139.25	128.40

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	1-1	1666	0	1724	55	0
1	2-1	1666	0	1724	45	0
2	1-1	5	0	0	0	0
2	2-1	5	0	0	1	0
3	1-1	20	0	27	1	0
3	2-1	20	0	27	1	0
4	1-1	80	0	142	2	0
4	2-1	80	0	142	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-1	28	0	49	0	0
5	2-1	28	0	49	0	0
6	1-1	25	0	0	3	0
6	2-1	25	0	0	1	0
All	All	3648	0	3884	102	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 14.

All (102) 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)
1:1:24:THR:HG22	1:1:50:PRO:HG2	1.34	1.08
1:1:89:THR:HG21	1:1:216:LYS:HE3	1.34	1.05
1:1:89:THR:HG21	1:1:216:LYS:HE3	1.36	1.04
1:1:89:THR:HG21	1:1:216:LYS:CE	2.01	0.89
1:1:20:MET:O	1:1:24:THR:HG22	1.74	0.87
1:1:49:VAL:HG13	1:1:89:THR:HG23	1.60	0.83
1:1:47:THR:O	1:1:50:PRO:HD2	1.79	0.82
1:1:24:THR:HG22	1:1:50:PRO:CG	2.11	0.81
1:1:174:LEU:O	1:1:178:THR:HG23	1.82	0.79
1:1:49:VAL:HG13	1:1:89:THR:CG2	2.13	0.79
1:1:121:THR:HG22	1:1:141:SER:HB2	1.67	0.77
1:1:46:THR:O	1:1:50:PRO:HD2	1.87	0.74
1:1:9:GLU:HG2	1:1:202:ASN:HA	1.70	0.73
1:1:104:ASP:HB2	1:1:107:THR:HG22	1.70	0.72
1:1:225:ARG:HH11	1:1:225:ARG:HB3	1.54	0.72
1:1:117:ILE:O	1:1:121:THR:HB	1.90	0.71
1:1:103:ALA:HB1	1:1:107:THR:HG21	1.71	0.71
1:1:44:ALA:HA	4:1:260:L3P:H111	1.73	0.70
1:1:121:THR:HG23	1:1:137:TRP:HE3	1.58	0.69
1:1:104:ASP:O	1:1:107:THR:HG22	1.93	0.69
1:1:21:GLY:O	1:1:25:LEU:HG	1.96	0.65
1:1:104:ASP:HB2	1:1:107:THR:CG2	2.26	0.65
1:1:164:ARG:HH21	1:1:232:GLU:HA	1.61	0.64
1:1:200:PRO:HG2	1:1:203:ILE:HG12	1.79	0.64
1:1:189:TRP:CZ2	1:1:194:GLU:HG2	2.36	0.60
1:1:121:THR:CG2	1:1:141:SER:HB2	2.31	0.60
1:1:41:LYS:HD3	1:1:99:LEU:HD13	1.82	0.60
1:1:192:GLY:O	1:1:197:GLY:HA2	2.03	0.58
1:1:51:ALA:O	1:1:54:PHE:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:ALA:HA	4:1:260:L3P:H111	1.85	0.57
1:1:129:LYS:HB3	1:1:129:LYS:NZ	2.20	0.57
1:1:30:LYS:HE3	1:1:224:LEU:O	2.06	0.54
1:1:20:MET:O	1:1:24:THR:HG23	2.08	0.54
1:1:203:ILE:O	1:1:207:LEU:HG	2.08	0.54
1:1:50:PRO:HD3	6:1:602:HOH:O	2.08	0.54
1:1:191:ILE:HD12	1:1:199:VAL:HG21	1.89	0.54
1:1:50:PRO:O	1:1:54:PHE:N	2.38	0.54
1:1:18:ALA:O	1:1:22:LEU:HG	2.09	0.53
1:1:131:TYR:O	1:1:134:ARG:HB3	2.09	0.53
1:1:11:ILE:O	1:1:15:LEU:HB2	2.09	0.53
1:1:49:VAL:HG21	1:1:93:LEU:HD13	1.90	0.53
1:1:90:THR:OG1	1:1:91:PRO:HD3	2.10	0.52
1:1:104:ASP:O	1:1:107:THR:HG23	2.09	0.52
1:1:121:THR:HG23	1:1:137:TRP:CE3	2.43	0.51
1:1:164:ARG:HE	1:1:232:GLU:HG2	1.74	0.51
1:1:12:TRP:CE3	1:1:206:LEU:HD23	2.44	0.51
1:1:36:ASP:OD2	1:1:38:ASP:HB3	2.10	0.51
1:1:207:LEU:O	1:1:211:LEU:HD22	2.11	0.51
1:1:104:ASP:O	1:1:108:ILE:HG13	2.11	0.51
1:1:90:THR:O	1:1:94:LEU:HD22	2.12	0.50
1:1:204:GLU:HG2	2:1:700:SO4:S	2.52	0.50
1:1:90:THR:HB	1:1:115:ASP:OD2	2.11	0.50
1:1:86:TRP:CD1	3:1:250:RET:H14	2.46	0.50
1:1:49:VAL:HG13	1:1:89:THR:HG21	1.92	0.50
4:1:260:L3P:H2	6:1:634:HOH:O	2.11	0.49
1:1:101:VAL:HG13	1:1:159:LYS:HG2	1.93	0.49
1:1:107:THR:O	1:1:111:LEU:HD13	2.12	0.49
1:1:49:VAL:HG11	1:1:93:LEU:HD11	1.95	0.49
1:1:24:THR:HG22	1:1:50:PRO:CB	2.43	0.49
1:1:103:ALA:HB1	1:1:107:THR:CG2	2.41	0.48
1:1:46:THR:O	1:1:50:PRO:CD	2.57	0.48
1:1:153:PHE:HA	1:1:175:ARG:HD2	1.95	0.47
1:1:136:VAL:HG13	4:1:280:L3P:H201	1.96	0.47
1:1:164:ARG:HG2	1:1:232:GLU:OE2	2.14	0.47
1:1:101:VAL:CG2	1:1:159:LYS:HB3	2.45	0.47
1:1:78:ILE:HA	6:1:609:HOH:O	2.15	0.47
1:1:190:LEU:O	1:1:195:GLY:HA3	2.14	0.46
1:1:12:TRP:CE3	1:1:206:LEU:HD23	2.51	0.46
1:1:164:ARG:HH21	1:1:232:GLU:CA	2.28	0.46
1:1:185:TYR:CZ	1:1:211:LEU:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:VAL:HG13	1:1:159:LYS:HB3	1.98	0.45
3:1:250:RET:H7	3:1:250:RET:H181	1.82	0.45
1:1:47:THR:C	1:1:50:PRO:HD2	2.37	0.45
1:1:77:PRO:HD2	6:1:613:HOH:O	2.16	0.45
1:1:129:LYS:HG2	1:1:129:LYS:H	1.57	0.44
1:1:89:THR:HG21	1:1:216:LYS:HE2	1.92	0.44
1:1:101:VAL:O	1:1:101:VAL:HG13	2.18	0.44
1:1:90:THR:N	1:1:91:PRO:CD	2.81	0.44
1:1:111:LEU:HD11	1:1:151:VAL:HG11	2.00	0.43
1:1:196:ALA:O	1:1:198:ILE:N	2.46	0.43
1:1:129:LYS:HZ3	1:1:129:LYS:HB3	1.84	0.43
1:1:128:THR:HG21	1:1:133:TYR:HB2	2.01	0.43
1:1:49:VAL:HG21	1:1:93:LEU:CD1	2.49	0.43
1:1:107:THR:O	1:1:111:LEU:HD22	2.18	0.43
1:1:199:VAL:HG13	1:1:203:ILE:HB	2.01	0.42
1:1:15:LEU:O	1:1:19:LEU:HG	2.20	0.42
1:1:34:VAL:HG21	1:1:43:TYR:CE1	2.54	0.42
1:1:24:THR:O	1:1:28:LEU:HB2	2.19	0.42
1:1:9:GLU:OE1	1:1:201:LEU:HB3	2.20	0.42
1:1:207:LEU:O	1:1:211:LEU:HD13	2.20	0.42
1:1:90:THR:N	1:1:91:PRO:CD	2.82	0.42
1:1:200:PRO:HG2	1:1:203:ILE:HG12	2.02	0.42
1:1:97:LEU:HD23	1:1:152:LEU:HD13	2.02	0.41
1:1:29:VAL:O	1:1:32:MET:HG3	2.20	0.41
1:1:132:SER:O	1:1:135:PHE:HB3	2.21	0.41
1:1:206:LEU:HD13	1:1:206:LEU:C	2.41	0.41
1:1:101:VAL:HG13	1:1:159:LYS:CG	2.50	0.41
1:1:199:VAL:CG1	1:1:203:ILE:HB	2.52	0.40
1:1:192:GLY:C	1:1:194:GLU:H	2.24	0.40
1:1:9:GLU:CG	1:1:202:ASN:HA	2.45	0.40
1:1:27:PHE:CE2	1:1:50:PRO:HG3	2.57	0.40
1:1:129:LYS:HG3	1:1:130:VAL:N	2.37	0.40

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	1-1	211/248 (85%)	202 (96%)	8 (4%)	1 (0%)	29	35
1	2-1	211/248 (85%)	204 (97%)	5 (2%)	2 (1%)	17	20
All	All	422/496 (85%)	406 (96%)	13 (3%)	3 (1%)	22	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-1	78	ILE
1	2-1	193	SER
1	2-1	78	ILE

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	1-1	172/194 (89%)	157 (91%)	15 (9%)	10	12
1	2-1	172/194 (89%)	165 (96%)	7 (4%)	30	43
All	All	344/388 (89%)	322 (94%)	22 (6%)	17	23

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-1	24	THR
1	1-1	28	LEU
1	1-1	38	ASP
1	1-1	48	LEU
1	1-1	79	TYR
1	1-1	93	LEU
1	1-1	97	LEU
1	1-1	107	THR
1	1-1	111	LEU

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Mol	Chain	Res	Type
1	1-1	121	THR
1	1-1	129	LYS
1	1-1	161	GLU
1	1-1	204	GLU
1	1-1	211	LEU
1	1-1	225	ARG
1	2-1	93	LEU
1	2-1	94	LEU
1	2-1	97	LEU
1	2-1	101	VAL
1	2-1	129	LYS
1	2-1	161	GLU
1	2-1	178	THR

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

Mol	Chain	Res	Type
1	1-1	105	GLN
1	2-1	105	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	RET	2-1	250	1	20,20,21	2.98	6 (30%)	27,27,28	1.46	5 (18%)
4	L3P	1-1	290	-	19,19,58	1.88	5 (26%)	22,22,73	0.73	0
4	L3P	2-1	260	-	39,39,58	1.39	5 (12%)	45,48,73	1.49	6 (13%)
2	SO4	1-1	700	-	4,4,4	0.32	0	6,6,6	0.16	0
5	L2P	2-1	270	-	27,27,45	2.06	9 (33%)	30,31,53	2.11	8 (26%)
4	L3P	2-1	290	-	19,19,58	1.88	5 (26%)	22,22,73	0.73	0
4	L3P	1-1	260	-	39,39,58	1.39	5 (12%)	45,48,73	1.49	6 (13%)
2	SO4	2-1	700	-	4,4,4	0.33	0	6,6,6	0.15	0
3	RET	1-1	250	1	20,20,21	2.63	6 (30%)	27,27,28	1.52	7 (25%)
5	L2P	1-1	270	-	27,27,45	2.06	9 (33%)	30,31,53	2.11	8 (26%)
4	L3P	2-1	280	-	19,19,58	1.45	3 (15%)	22,22,73	0.84	0
4	L3P	1-1	280	-	19,19,58	1.45	3 (15%)	22,22,73	0.84	0

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	RET	2-1	250	1	-	0/13/30/31	0/1/1/1
4	L3P	1-1	290	-	-	9/20/20/67	-
4	L3P	2-1	260	-	-	20/43/43/67	-
4	L3P	1-1	280	-	-	14/20/20/67	-
5	L2P	2-1	270	-	-	12/30/30/51	-
4	L3P	2-1	290	-	-	9/20/20/67	-
4	L3P	1-1	260	-	-	20/43/43/67	-
3	RET	1-1	250	1	-	0/13/30/31	0/1/1/1
5	L2P	1-1	270	-	-	12/30/30/51	-
4	L3P	2-1	280	-	-	14/20/20/67	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-1	250	RET	C14-C13	7.57	1.39	1.33
3	2-1	250	RET	C1-C6	7.01	1.63	1.53
3	1-1	250	RET	C1-C6	6.45	1.62	1.53
3	1-1	250	RET	C14-C13	6.23	1.38	1.33
3	2-1	250	RET	C5-C6	5.51	1.44	1.34
3	1-1	250	RET	C5-C6	5.34	1.43	1.34
4	1-1	290	L3P	C26-C25	4.45	1.71	1.52
4	2-1	290	L3P	C26-C25	4.45	1.71	1.52
5	1-1	270	L2P	O2-C41	4.10	1.54	1.43
5	2-1	270	L2P	O2-C41	4.10	1.54	1.43
5	1-1	270	L2P	O2-C2	4.03	1.54	1.43
5	2-1	270	L2P	O2-C2	4.03	1.54	1.43
4	1-1	290	L3P	C25-C23	3.84	1.72	1.52
4	2-1	290	L3P	C25-C23	3.84	1.72	1.52
4	2-1	260	L3P	P1-O3	3.65	1.72	1.60
4	1-1	260	L3P	P1-O3	3.65	1.72	1.60
5	1-1	270	L2P	C42-C41	3.59	1.63	1.50
5	2-1	270	L2P	C42-C41	3.59	1.63	1.50
3	2-1	250	RET	C7-C6	3.49	1.57	1.45
4	2-1	260	L3P	O2-C41	3.48	1.52	1.43
4	1-1	260	L3P	O2-C41	3.48	1.52	1.43
4	2-1	260	L3P	P1-O2P	3.47	1.68	1.54
4	1-1	260	L3P	P1-O2P	3.47	1.68	1.54
5	1-1	270	L2P	C3-C2	3.12	1.58	1.51
5	2-1	270	L2P	C3-C2	3.12	1.58	1.51
5	1-1	270	L2P	C1-C2	3.12	1.60	1.50
5	2-1	270	L2P	C1-C2	3.12	1.60	1.50
3	1-1	250	RET	C7-C6	3.00	1.55	1.45
4	2-1	260	L3P	O2-C2	2.92	1.51	1.43
4	1-1	260	L3P	O2-C2	2.92	1.51	1.43
5	1-1	270	L2P	O1-C1	2.84	1.49	1.42
5	2-1	270	L2P	O1-C1	2.84	1.49	1.42
4	1-1	290	L3P	C22-C23	2.73	1.66	1.52
4	2-1	290	L3P	C22-C23	2.73	1.66	1.52
5	1-1	270	L2P	C47-C48	2.73	1.66	1.52
5	2-1	270	L2P	C47-C48	2.73	1.66	1.52
3	1-1	250	RET	C2-C1	2.72	1.60	1.54
4	2-1	260	L3P	C42-C41	2.66	1.60	1.50
4	1-1	260	L3P	C42-C41	2.66	1.60	1.50
4	1-1	290	L3P	C26-C27	2.59	1.63	1.52
4	2-1	290	L3P	C26-C27	2.59	1.63	1.52
4	1-1	280	L3P	C17-C18	2.54	1.65	1.52
4	2-1	280	L3P	C17-C18	2.54	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-1	250	RET	C2-C1	2.49	1.59	1.54
5	1-1	270	L2P	C50-C48	2.39	1.65	1.52
5	2-1	270	L2P	C50-C48	2.39	1.65	1.52
3	1-1	250	RET	C2-C3	-2.31	1.46	1.52
3	2-1	250	RET	C2-C3	-2.28	1.46	1.52
4	1-1	280	L3P	C26-C27	2.16	1.61	1.52
4	2-1	280	L3P	C26-C27	2.16	1.61	1.52
4	1-1	290	L3P	C21-C22	2.10	1.61	1.52
4	2-1	290	L3P	C21-C22	2.10	1.61	1.52
4	1-1	280	L3P	C20-C18	2.06	1.63	1.52
4	2-1	280	L3P	C20-C18	2.06	1.63	1.52
5	1-1	270	L2P	C56-C57	2.02	1.60	1.52
5	2-1	270	L2P	C56-C57	2.02	1.60	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-1	270	L2P	O1-C1-C2	7.19	126.36	109.44
5	2-1	270	L2P	O1-C1-C2	7.19	126.36	109.44
4	2-1	260	L3P	C41-O2-C2	5.13	127.20	115.40
4	1-1	260	L3P	C41-O2-C2	5.13	127.20	115.40
4	2-1	260	L3P	P1-O3-C3	4.29	130.12	118.30
4	1-1	260	L3P	P1-O3-C3	4.29	130.12	118.30
5	1-1	270	L2P	C54-C53-C52	-3.97	96.90	111.29
5	2-1	270	L2P	C54-C53-C52	-3.97	96.90	111.29
5	1-1	270	L2P	C41-O2-C2	3.90	124.37	115.40
5	2-1	270	L2P	C41-O2-C2	3.90	124.37	115.40
5	1-1	270	L2P	O3-C3-C2	3.59	121.30	111.78
5	2-1	270	L2P	O3-C3-C2	3.59	121.30	111.78
4	2-1	260	L3P	O2-C41-C42	3.34	115.77	108.77
4	1-1	260	L3P	O2-C41-C42	3.34	115.77	108.77
3	1-1	250	RET	C1-C6-C7	3.33	125.21	115.78
5	1-1	270	L2P	C51-C52-C53	3.16	126.14	115.92
5	2-1	270	L2P	C51-C52-C53	3.16	126.14	115.92
3	1-1	250	RET	C1-C6-C5	-3.05	118.32	122.61
3	1-1	250	RET	C8-C9-C10	-2.90	114.49	118.94
3	2-1	250	RET	C18-C5-C6	-2.83	121.34	124.53
3	1-1	250	RET	C11-C10-C9	2.80	131.31	127.31
3	2-1	250	RET	C20-C13-C14	-2.73	115.65	123.71
4	2-1	260	L3P	C46-C45-C43	-2.68	107.24	115.92
4	1-1	260	L3P	C46-C45-C43	-2.68	107.24	115.92
3	2-1	250	RET	C11-C10-C9	-2.68	123.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-1	250	RET	C1-C6-C5	-2.61	118.94	122.61
4	2-1	260	L3P	C26-C25-C23	-2.50	107.84	115.92
4	1-1	260	L3P	C26-C25-C23	-2.50	107.84	115.92
3	2-1	250	RET	C1-C6-C7	2.41	122.59	115.78
5	1-1	270	L2P	C52-C51-C50	-2.37	102.37	113.24
5	2-1	270	L2P	C52-C51-C50	-2.37	102.37	113.24
5	1-1	270	L2P	C46-C47-C48	2.22	123.09	115.92
5	2-1	270	L2P	C46-C47-C48	2.22	123.09	115.92
4	2-1	260	L3P	O2P-P1-O3	2.19	112.56	106.73
4	1-1	260	L3P	O2P-P1-O3	2.19	112.56	106.73
3	1-1	250	RET	C19-C9-C8	2.14	121.44	118.08
3	1-1	250	RET	C2-C1-C6	2.10	113.72	110.48
3	1-1	250	RET	C7-C6-C5	-2.06	116.47	121.46
5	1-1	270	L2P	C51-C50-C48	2.06	122.57	115.92
5	2-1	270	L2P	C51-C50-C48	2.06	122.57	115.92

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-1	270	L2P	C1-C2-C3-O3
5	1-1	270	L2P	O2-C2-C3-O3
4	2-1	260	L3P	C41-C42-C43-C44
5	2-1	270	L2P	C1-C2-C3-O3
5	2-1	270	L2P	O2-C2-C3-O3
4	1-1	260	L3P	C41-C42-C43-C44
4	1-1	280	L3P	C13-C15-C16-C17
4	2-1	280	L3P	C13-C15-C16-C17
4	2-1	260	L3P	C23-C25-C26-C27
4	1-1	260	L3P	C23-C25-C26-C27
4	1-1	280	L3P	C20-C21-C22-C23
4	2-1	280	L3P	C20-C21-C22-C23
4	2-1	260	L3P	C20-C21-C22-C23
4	2-1	260	L3P	C25-C26-C27-C28
4	1-1	280	L3P	C15-C16-C17-C18
4	1-1	260	L3P	C20-C21-C22-C23
4	1-1	260	L3P	C25-C26-C27-C28
4	2-1	280	L3P	C15-C16-C17-C18
4	2-1	260	L3P	C18-C20-C21-C22
4	1-1	260	L3P	C18-C20-C21-C22
4	2-1	260	L3P	C26-C27-C28-C30
4	1-1	260	L3P	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
5	1-1	270	L2P	C56-C57-C58-C60
5	2-1	270	L2P	C56-C57-C58-C60
4	1-1	280	L3P	C26-C27-C28-C29
4	2-1	280	L3P	C26-C27-C28-C29
5	1-1	270	L2P	C56-C57-C58-C59
4	1-1	280	L3P	C26-C27-C28-C30
5	2-1	270	L2P	C56-C57-C58-C59
4	2-1	280	L3P	C26-C27-C28-C30
4	2-1	260	L3P	C26-C27-C28-C29
4	1-1	260	L3P	C26-C27-C28-C29
4	1-1	290	L3P	C11-C12-C13-C14
4	2-1	290	L3P	C11-C12-C13-C14
4	2-1	260	L3P	C17-C18-C20-C21
4	1-1	260	L3P	C17-C18-C20-C21
4	1-1	290	L3P	C26-C27-C28-C29
4	2-1	290	L3P	C26-C27-C28-C29
5	1-1	270	L2P	C53-C55-C56-C57
5	2-1	270	L2P	C53-C55-C56-C57
4	2-1	260	L3P	C19-C18-C20-C21
4	1-1	260	L3P	C19-C18-C20-C21
4	1-1	290	L3P	C26-C27-C28-C30
4	2-1	290	L3P	C26-C27-C28-C30
4	2-1	260	L3P	C41-C42-C43-C45
4	1-1	260	L3P	C41-C42-C43-C45
4	1-1	280	L3P	C23-C25-C26-C27
4	2-1	280	L3P	C23-C25-C26-C27
4	1-1	290	L3P	C22-C23-C25-C26
4	1-1	280	L3P	C17-C18-C20-C21
4	2-1	290	L3P	C22-C23-C25-C26
4	2-1	280	L3P	C17-C18-C20-C21
4	1-1	290	L3P	C24-C23-C25-C26
4	2-1	260	L3P	C21-C22-C23-C24
4	1-1	280	L3P	C14-C13-C15-C16
4	1-1	280	L3P	C19-C18-C20-C21
4	2-1	290	L3P	C24-C23-C25-C26
4	1-1	260	L3P	C21-C22-C23-C24
4	2-1	280	L3P	C14-C13-C15-C16
4	2-1	280	L3P	C19-C18-C20-C21
5	1-1	270	L2P	C42-C41-O2-C2
5	2-1	270	L2P	C42-C41-O2-C2
4	1-1	290	L3P	C15-C16-C17-C18
4	2-1	290	L3P	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	2-1	260	L3P	C1-C2-C3-O3
4	1-1	260	L3P	C1-C2-C3-O3
5	1-1	270	L2P	C46-C47-C48-C50
4	2-1	260	L3P	C21-C22-C23-C25
4	2-1	260	L3P	C22-C23-C25-C26
4	1-1	280	L3P	C12-C13-C15-C16
4	1-1	280	L3P	C21-C22-C23-C25
5	2-1	270	L2P	C46-C47-C48-C50
4	1-1	260	L3P	C21-C22-C23-C25
4	1-1	260	L3P	C22-C23-C25-C26
4	2-1	280	L3P	C12-C13-C15-C16
4	2-1	280	L3P	C21-C22-C23-C25
5	1-1	270	L2P	C2-C1-O1-C11
5	2-1	270	L2P	C2-C1-O1-C11
5	1-1	270	L2P	C46-C47-C48-C49
4	1-1	280	L3P	C21-C22-C23-C24
5	2-1	270	L2P	C46-C47-C48-C49
4	2-1	280	L3P	C21-C22-C23-C24
4	1-1	290	L3P	C17-C18-C20-C21
4	1-1	280	L3P	C16-C17-C18-C20
4	2-1	290	L3P	C17-C18-C20-C21
4	2-1	280	L3P	C16-C17-C18-C20
4	2-1	260	L3P	C24-C23-C25-C26
4	1-1	280	L3P	C16-C17-C18-C19
4	1-1	260	L3P	C24-C23-C25-C26
4	2-1	280	L3P	C16-C17-C18-C19
4	2-1	260	L3P	C42-C43-C45-C46
4	1-1	260	L3P	C42-C43-C45-C46
5	1-1	270	L2P	C12-C11-O1-C1
5	2-1	270	L2P	C12-C11-O1-C1
4	1-1	290	L3P	C19-C18-C20-C21
4	2-1	290	L3P	C19-C18-C20-C21
4	1-1	290	L3P	C11-C12-C13-C15
4	2-1	290	L3P	C11-C12-C13-C15
4	2-1	260	L3P	O2-C2-C3-O3
4	1-1	260	L3P	O2-C2-C3-O3
4	2-1	260	L3P	C44-C43-C45-C46
4	1-1	260	L3P	C44-C43-C45-C46
5	1-1	270	L2P	O1-C1-C2-C3
5	2-1	270	L2P	O1-C1-C2-C3
4	2-1	260	L3P	C42-C41-O2-C2
4	1-1	260	L3P	C42-C41-O2-C2

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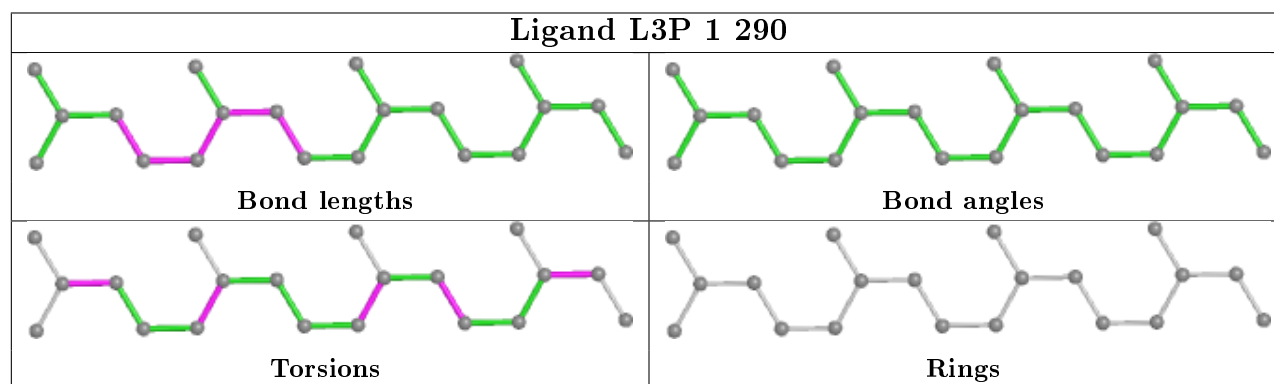
Mol	Chain	Res	Type	Atoms
4	2-1	260	L3P	C12-C11-O1-C1
4	1-1	260	L3P	C12-C11-O1-C1
5	1-1	270	L2P	C43-C45-C46-C47
5	2-1	270	L2P	C43-C45-C46-C47

There are no ring outliers.

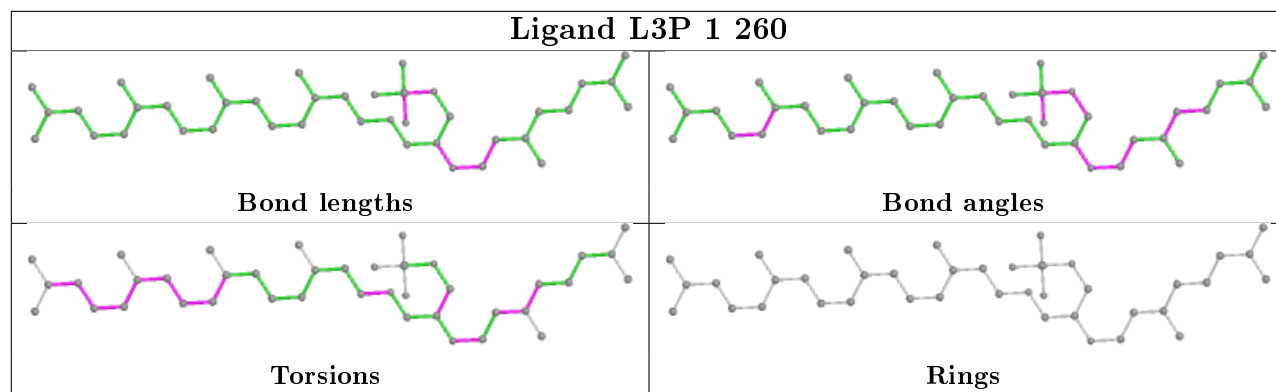
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2-1	250	RET	1	0
4	2-1	260	L3P	2	0
4	1-1	260	L3P	1	0
2	2-1	700	SO4	1	0
3	1-1	250	RET	1	0
4	1-1	280	L3P	1	0

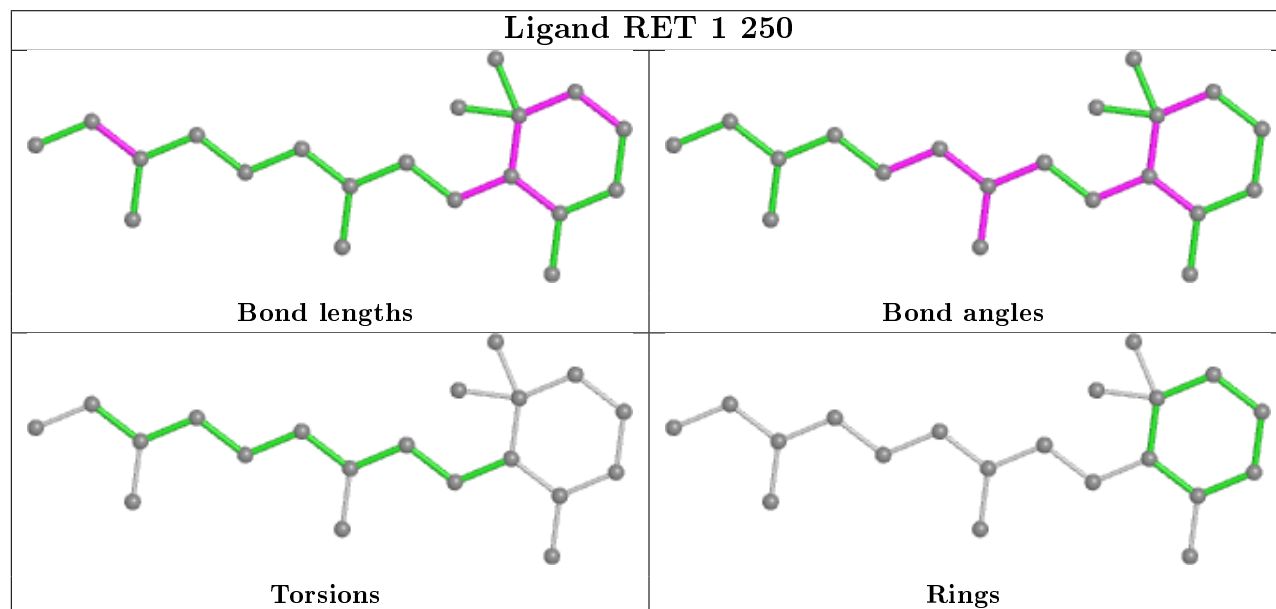
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



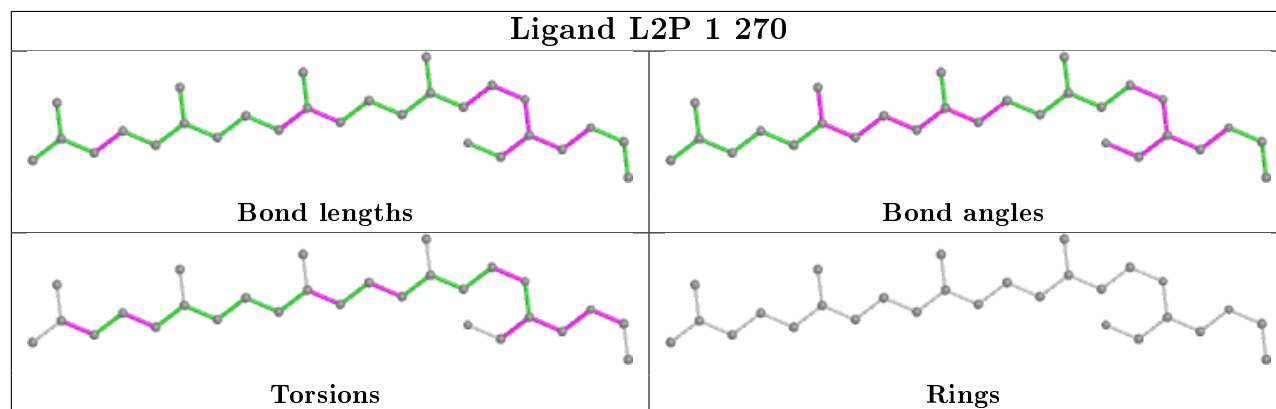
Ligand L3P 1 260

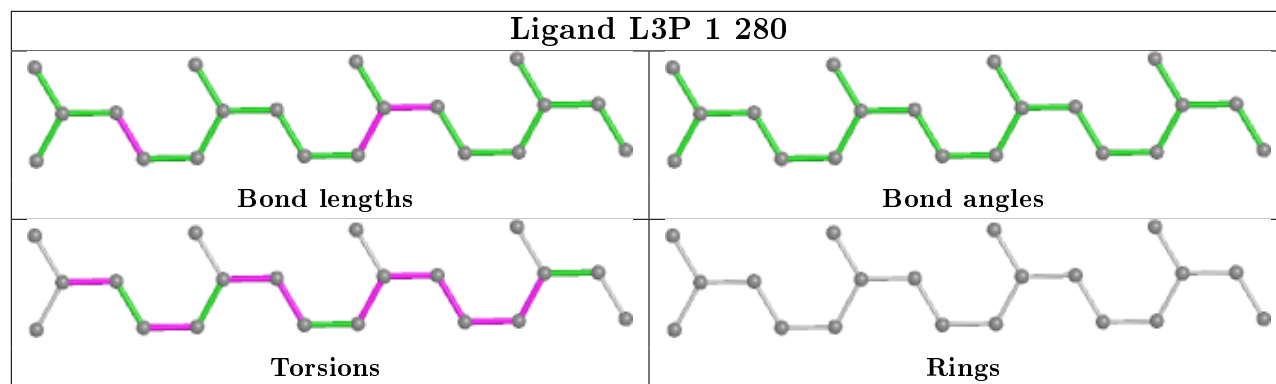


Ligand RET 1 250



Ligand L2P 1 270





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	1-1	215/248 (86%)	0.94	26 (12%) 4 6	20, 32, 61, 75	215 (100%)
1	2-1	215/248 (86%)	0.94	26 (12%) 4 6	20, 32, 61, 75	215 (100%)
All	All	430/496 (86%)	0.94	52 (12%) 4 6	20, 33, 61, 75	430 (100%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-1	233	ALA	15.5
1	2-1	233	ALA	15.5
1	1-1	78	ILE	10.4
1	2-1	78	ILE	10.4
1	1-1	64	TYR	10.1
1	2-1	64	TYR	10.1
1	1-1	232	GLU	9.1
1	2-1	232	GLU	9.1
1	1-1	77	PRO	8.6
1	2-1	77	PRO	8.6
1	1-1	8	PRO	7.0
1	2-1	8	PRO	7.0
1	1-1	199	VAL	6.8
1	2-1	199	VAL	6.8
1	1-1	65	GLY	6.4
1	2-1	65	GLY	6.4
1	1-1	10	TRP	5.1
1	2-1	10	TRP	5.1
1	1-1	33	GLY	4.9
1	2-1	33	GLY	4.9
1	1-1	63	GLY	3.8
1	2-1	63	GLY	3.8
1	1-1	12	TRP	3.6
1	2-1	12	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	1-1	9	GLU	3.5
1	2-1	9	GLU	3.5
1	1-1	35	SER	3.3
1	2-1	35	SER	3.3
1	1-1	79	TYR	3.3
1	2-1	79	TYR	3.3
1	1-1	128	THR	3.2
1	2-1	128	THR	3.2
1	1-1	201	LEU	3.1
1	2-1	201	LEU	3.1
1	1-1	80	TRP	2.8
1	2-1	80	TRP	2.8
1	1-1	200	PRO	2.7
1	2-1	200	PRO	2.7
1	1-1	202	ASN	2.4
1	2-1	202	ASN	2.4
1	1-1	50	PRO	2.3
1	1-1	131	TYR	2.3
1	2-1	50	PRO	2.3
1	2-1	131	TYR	2.3
1	1-1	196	ALA	2.2
1	2-1	196	ALA	2.2
1	1-1	206	LEU	2.1
1	2-1	206	LEU	2.1
1	1-1	166	GLU	2.1
1	2-1	166	GLU	2.1
1	1-1	231	GLY	2.0
1	2-1	231	GLY	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 carbohydrates in this entry.

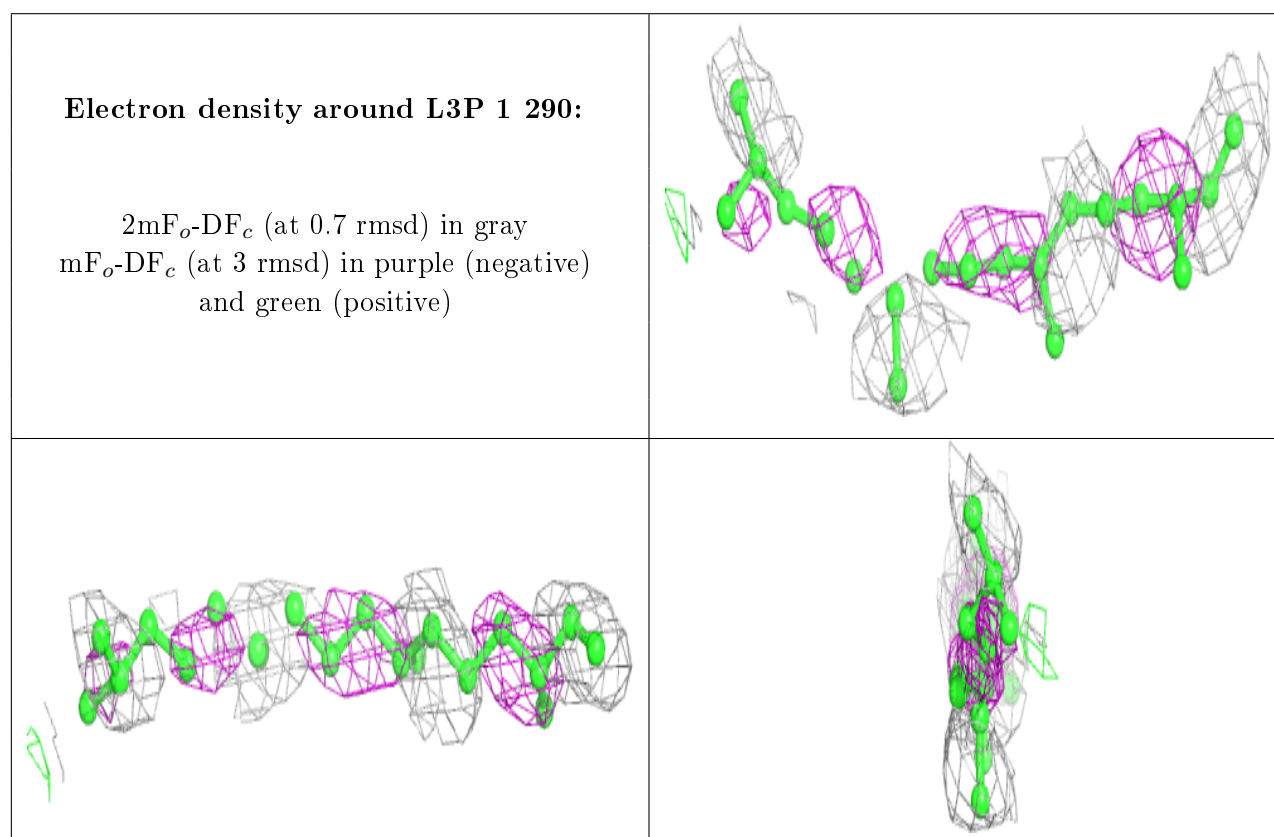
6.4 Ligands [i](#)

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.

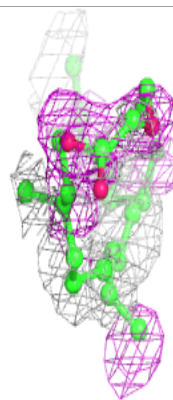
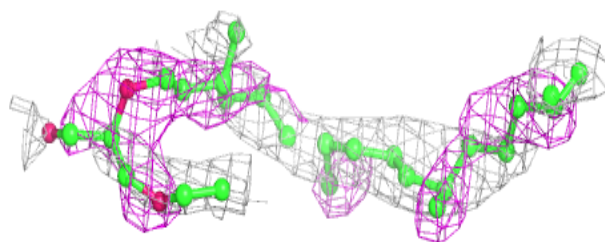
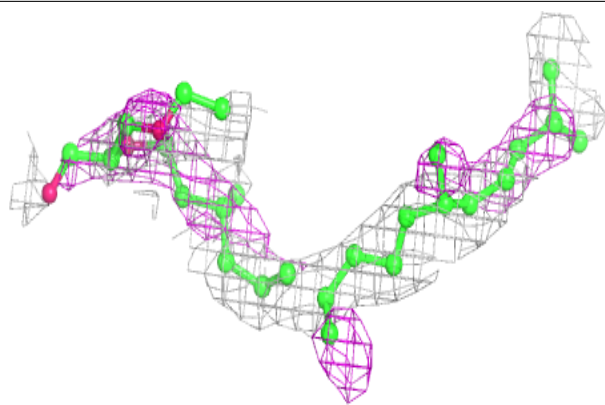
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	L3P	1-1	290	20/59	0.29	0.68	94,97,100,100	0
4	L3P	2-1	290	20/59	0.29	0.68	94,97,100,100	0
5	L2P	2-1	270	28/46	0.48	0.56	84,92,110,110	0
5	L2P	1-1	270	28/46	0.48	0.56	84,92,110,110	0
4	L3P	2-1	260	40/59	0.54	0.54	60,78,89,90	4
4	L3P	1-1	260	40/59	0.54	0.54	60,78,89,90	4
4	L3P	1-1	280	20/59	0.55	0.60	83,85,88,88	0
2	SO4	2-1	700	5/5	0.55	0.47	136,136,137,137	5
2	SO4	1-1	700	5/5	0.55	0.47	157,157,158,158	5
4	L3P	2-1	280	20/59	0.55	0.60	83,85,88,88	0
3	RET	2-1	250	20/21	0.94	0.19	30,37,39,40	20
3	RET	1-1	250	20/21	0.94	0.19	23,29,31,31	20

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.

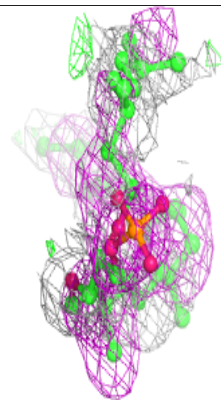
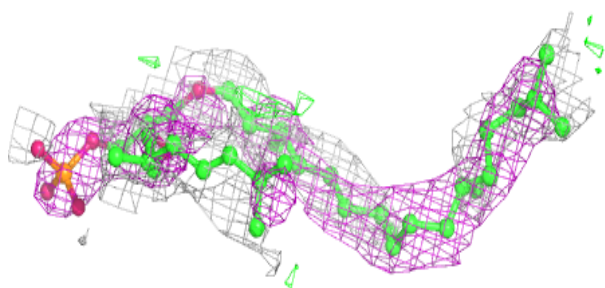
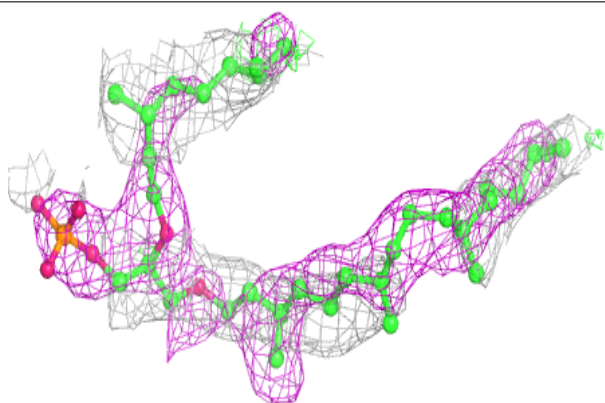


Electron density around L2P 1 270:

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

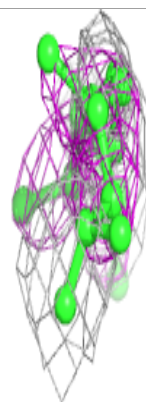
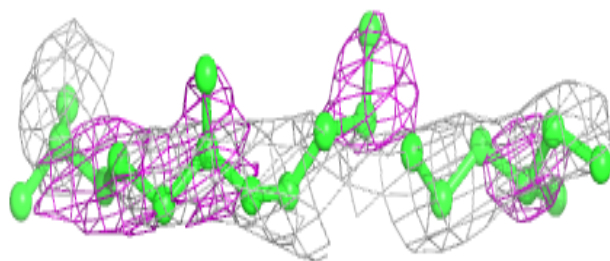
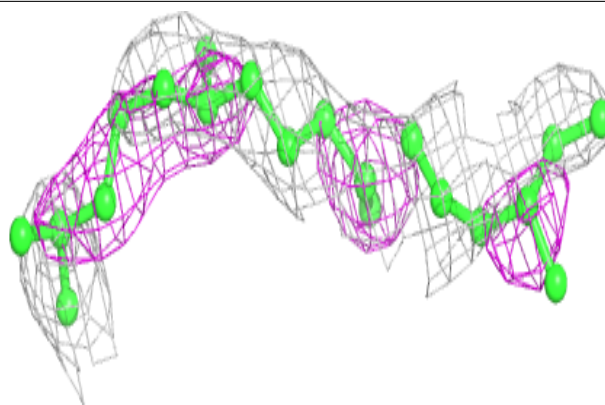
**Electron density around L3P 1 260:**

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

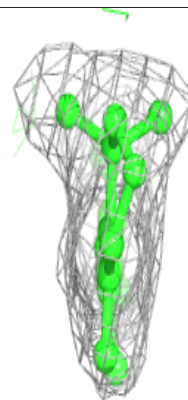
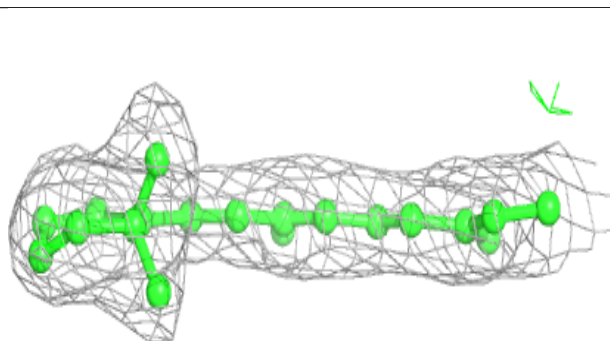
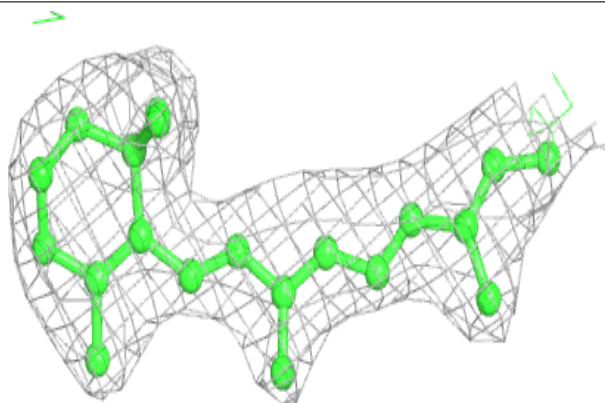


Electron density around L3P 1 280:

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

**Electron density around RET 1 250:**

$2mF_o-DF_c$ (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.