Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 07:22 PM EDT

PDB ID	:	3ABW
Title	:	Crystal structure of pharaonis halorhodopsin in complex with azide ion
Authors	:	Kouyama, T.; Kanada, S.
Deposited on	:	2009-12-24
Resolution	:	1.90 Å(reported)

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

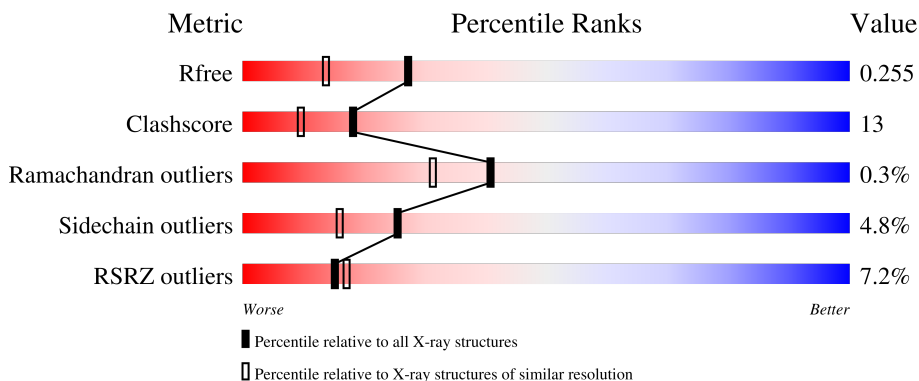|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.90 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		13
Ramachandran outliers		0.3%
Sidechain outliers		4.8%
RSRZ outliers		7.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	291	5% / 70% / 18% · 11%
1	B	291	5% / 64% / 24% · 11%
1	D	291	9% / 62% / 26% · 11%

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:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

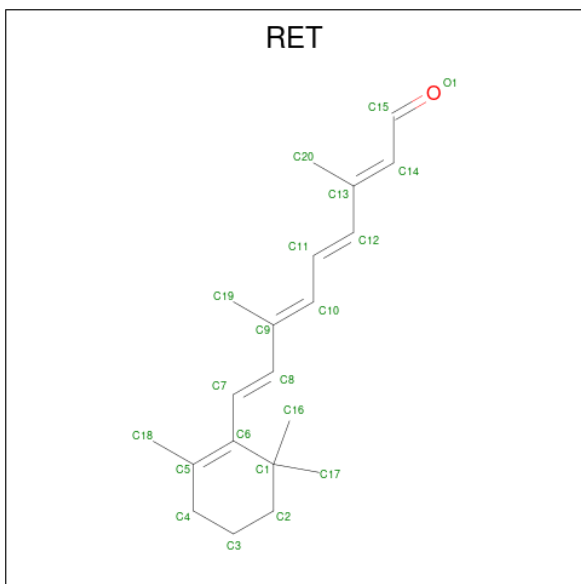| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	L3P	A	310	-	-	-	X
4	L3P	A	313	-	-	-	X
4	L3P	A	317	-	-	-	X
4	L3P	B	311	-	-	-	X
4	L3P	B	315	-	-	-	X
4	L3P	B	318	-	-	-	X
4	L3P	D	312	-	-	-	X
4	L3P	D	314	-	-	-	X
4	L3P	D	316	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6320 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 Halorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1967	1304	299	353	11			
1	B	259	Total	C	N	O	S	0	0	0
			1961	1301	298	351	11			
1	D	259	Total	C	N	O	S	0	0	0
			1961	1301	298	351	11			

- 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	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is BACTERIORUBERIN (three-letter code: 22B) (formula: $C_{50}H_{76}O_4$).

22B
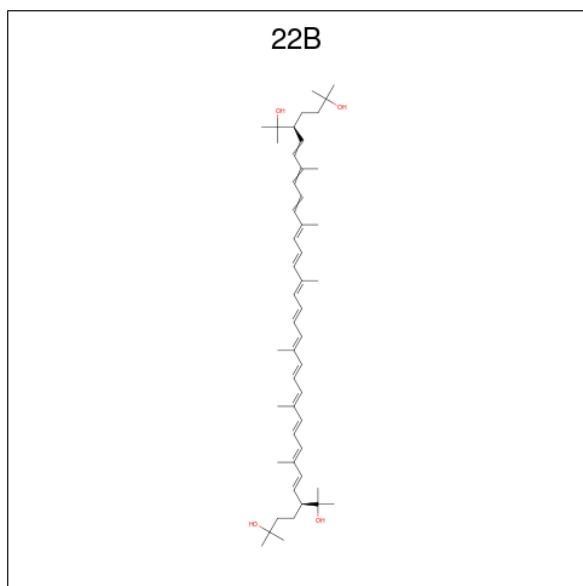
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 27	C 25	O 2	0	0
3	B	1	Total 27	C 25	O 2	0	0

- Molecule 4 is 2,3-DI-O-PHYTANLY-3-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCER OL-1'-PHOSPHATE (three-letter code: L3P) (formula: $C_{46}H_{94}O_{11}P_2$).

L3P
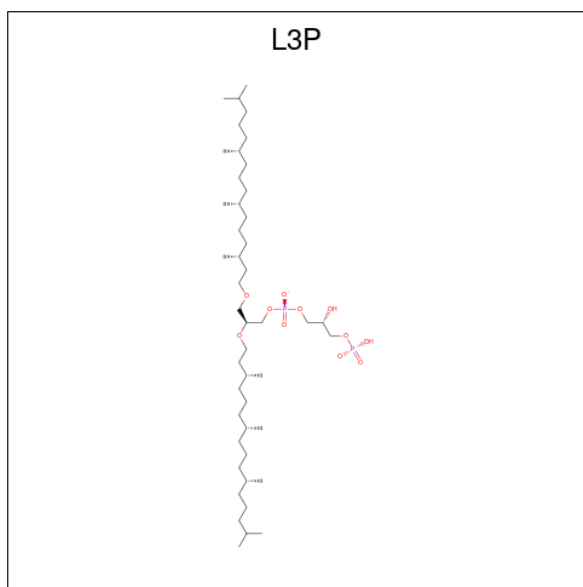
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C		0	0
			20 20			
4	A	1	Total C		0	0
			20 20			
4	A	1	Total C		0	0
			20 20			
4	B	1	Total C		0	0
			20 20			
4	B	1	Total C		0	0
			20 20			
4	B	1	Total C		0	0
			20 20			
4	D	1	Total C		0	0
			20 20			
4	D	1	Total C		0	0
			20 20			
4	D	1	Total C		0	0
			20 20			

- Molecule 5 is AZIDE ION (three-letter code: AZI) (formula: N_3).
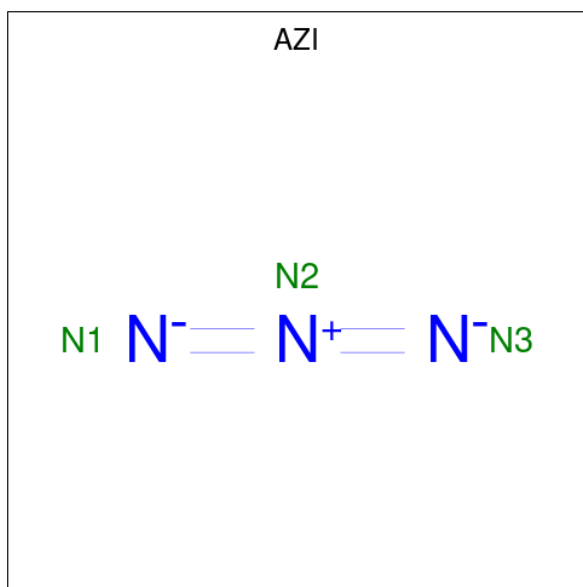
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total N		0	0
			3 3			
5	B	1	Total N		0	0
			3 3			
5	D	1	Total N		0	0
			3 3			

• Molecule 6 is water.

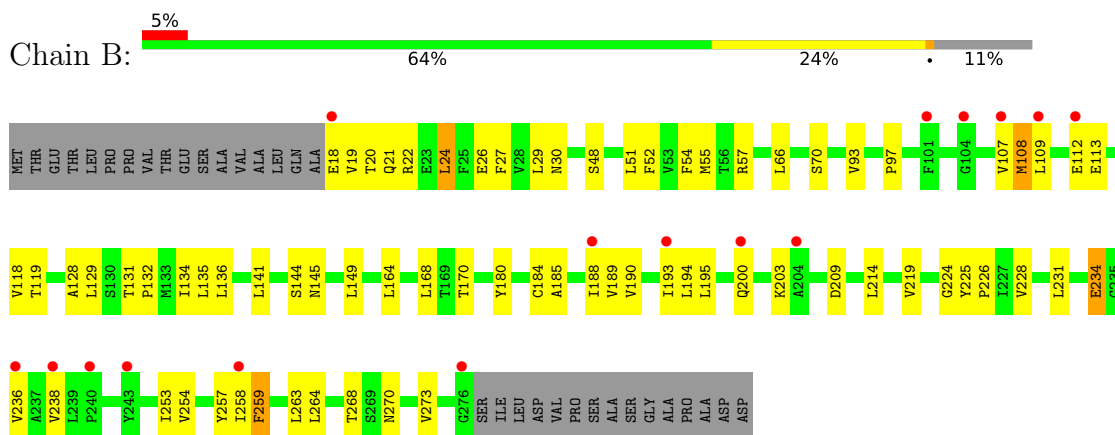| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total 49	O 49	0	0
6	B	48	Total 48	O 48	0	0
6	D	31	Total 31	O 31	0	0

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.
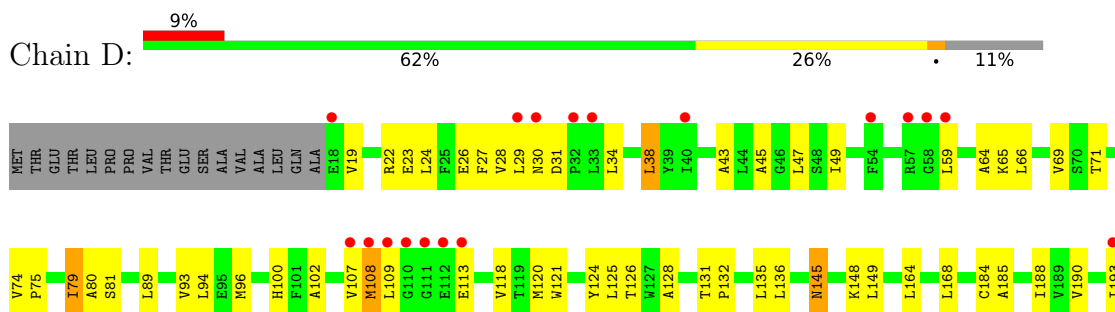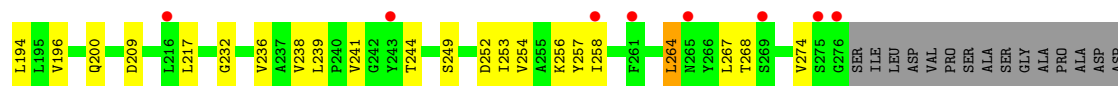
• Molecule 1: Halorhodopsin

Chain A:

• Molecule 1: Halorhodopsin

Chain B:

• Molecule 1: Halorhodopsin

Chain D:

L194 L195 V196 Q200 D209 L216 L217 G232 V236 A237 V238 L239 P240 V241 G242 Y243 T244 S249 D252 I253 V254 A255 K256 Y257 I258 F261 L264 N265 Y266 L267 T268 S269 V274 S275 G276 SER ILE LEU ASP VAL PRO SER ALA SER GLY ALA PRO ALA ASP ASP
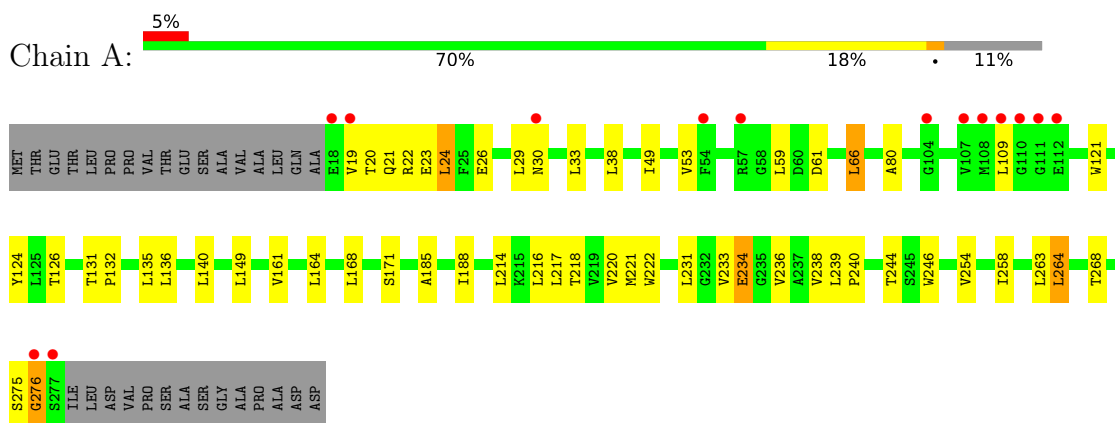
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.09Å 98.79Å 100.14Å 90.00° 127.85° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 36.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.9 (15.00-1.90) 87.8 (36.46-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.263 0.235 , 0.255	Depositor DCC
R_{free} test set	4064 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 74.7	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6320	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: L3P, RET, 22B, AZI

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	0.37	0/2013	0.57	0/2756
1	B	0.34	0/2007	0.54	0/2748
1	D	0.33	0/2007	0.54	0/2748
All	All	0.35	0/6027	0.55	0/8252

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	1967	0	2018	41	0
1	B	1961	0	2013	65	0
1	D	1961	0	2013	63	0
2	A	20	0	27	0	0
2	B	20	0	27	2	0
2	D	20	0	27	1	0
3	A	27	0	37	0	0
3	B	27	0	37	0	0
4	A	60	0	117	3	0
4	B	60	0	117	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	60	0	117	6	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	D	3	0	0	0	0
6	A	49	0	0	1	1
6	B	48	0	0	1	0
6	D	31	0	0	0	0
All	All	6320	0	6550	171	1

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 13.

All (171) 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:238:VAL:HG23	1:A:239:LEU:HD13	1.49	0.93
1:D:185:ALA:O	1:D:188:ILE:HG12	1.74	0.87
1:B:254:VAL:HG13	1:B:258:ILE:HD11	1.57	0.85
1:B:254:VAL:HA	1:B:258:ILE:HG12	1.63	0.81
1:D:43:ALA:O	1:D:47:LEU:HD13	1.83	0.78
1:B:20:THR:HG22	1:B:22:ARG:H	1.48	0.76
1:D:238:VAL:HG23	1:D:239:LEU:HD13	1.67	0.75
1:D:100:HIS:HD2	1:D:102:ALA:H	1.34	0.75
1:B:190:VAL:O	1:B:193:ILE:HG13	1.87	0.74
1:B:200:GLN:HA	1:B:203:LYS:HE2	1.68	0.74
1:D:254:VAL:HA	1:D:258:ILE:HG22	1.70	0.73
1:D:190:VAL:O	1:D:193:ILE:HG13	1.87	0.73
1:D:145:ASN:C	1:D:145:ASN:HD22	1.93	0.72
1:B:193:ILE:HD12	1:B:194:LEU:N	2.06	0.71
1:D:108:MET:HA	1:D:113:GLU:HA	1.70	0.70
1:B:270:ASN:O	1:B:273:VAL:HG12	1.92	0.70
1:B:164:LEU:HD21	4:B:315:L3P:H243	1.74	0.70
1:B:185:ALA:O	1:B:188:ILE:HG12	1.92	0.69
1:B:164:LEU:O	1:B:168:LEU:HD13	1.93	0.68
1:A:185:ALA:O	1:A:188:ILE:HG13	1.94	0.68
1:B:119:THR:HG23	1:B:234:GLU:OE1	1.95	0.67
1:A:238:VAL:HG23	1:A:239:LEU:CD1	2.24	0.66
1:D:193:ILE:HD12	1:D:194:LEU:N	2.11	0.65
1:A:214:LEU:CD1	1:A:263:LEU:HD13	2.26	0.65
1:D:65:LYS:O	1:D:69:VAL:HG23	1.97	0.65
1:B:29:LEU:O	1:B:30:ASN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ALA:HB1	4:A:317:L3P:H292	1.78	0.64
1:B:19:VAL:HG21	1:B:93:VAL:HG11	1.79	0.64
1:A:264:LEU:O	1:A:268:THR:HG22	1.98	0.64
1:D:232:GLY:HA3	1:D:244:THR:HG21	1.80	0.64
1:A:20:THR:HG22	1:A:22:ARG:H	1.62	0.63
1:B:108:MET:HA	1:B:113:GLU:HA	1.81	0.63
1:D:100:HIS:CD2	1:D:102:ALA:H	2.16	0.63
1:D:19:VAL:HG21	1:D:93:VAL:HG11	1.80	0.63
1:B:141:LEU:HD22	1:B:263:LEU:CD1	2.31	0.61
1:D:164:LEU:O	1:D:168:LEU:HD23	2.00	0.61
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.82	0.60
1:A:254:VAL:O	1:A:258:ILE:HG13	2.02	0.60
1:B:254:VAL:HG13	1:B:258:ILE:CD1	2.31	0.59
1:A:217:LEU:HD21	1:A:258:ILE:HD11	1.83	0.59
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.33	0.59
1:D:22:ARG:O	1:D:26:GLU:HG2	2.04	0.57
1:D:254:VAL:O	1:D:258:ILE:HG22	2.04	0.57
1:A:29:LEU:O	1:A:30:ASN:HB2	2.03	0.57
1:B:48:SER:HB3	1:B:52:PHE:CE2	2.39	0.57
1:B:224:GLY:O	1:B:228:VAL:HG23	2.04	0.57
1:D:131:THR:OG1	1:D:132:PRO:HD3	2.05	0.56
1:D:121:TRP:HA	1:D:124:TYR:CD2	2.41	0.56
1:B:144:SER:OG	1:B:149:LEU:HD22	2.06	0.55
1:A:164:LEU:HD21	4:A:313:L3P:H241	1.89	0.55
1:B:20:THR:HG22	1:B:22:ARG:N	2.21	0.55
1:B:108:MET:HA	1:B:112:GLU:O	2.06	0.55
1:A:20:THR:O	1:A:24:LEU:HD22	2.07	0.54
1:D:145:ASN:ND2	1:D:148:LYS:H	2.05	0.54
1:D:45:ALA:O	1:D:49:ILE:HG13	2.08	0.54
1:B:21:GLN:HE21	4:B:311:L3P:H143	1.73	0.54
1:A:275:SER:O	1:A:276:GLY:C	2.44	0.54
1:B:270:ASN:HB3	1:B:273:VAL:HG12	1.90	0.53
1:A:20:THR:CG2	1:A:22:ARG:HG2	2.38	0.53
1:D:254:VAL:HA	1:D:258:ILE:CG2	2.38	0.53
1:B:70:SER:OG	1:B:136:LEU:HD12	2.08	0.53
1:D:108:MET:HB2	1:D:113:GLU:HG3	1.90	0.53
1:A:20:THR:HG21	1:A:22:ARG:NH1	2.22	0.53
1:D:217:LEU:HD11	1:D:254:VAL:CG1	2.39	0.53
1:D:145:ASN:HD21	1:D:148:LYS:HG3	1.74	0.53
1:A:20:THR:HG21	1:A:22:ARG:HG2	1.92	0.52
1:D:267:LEU:HD11	1:D:274:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HD21	1:D:120:MET:HE3	1.92	0.51
1:D:252:ASP:O	1:D:256:LYS:HB2	2.10	0.51
1:B:109:LEU:HD22	1:B:109:LEU:N	2.25	0.51
1:B:136:LEU:HD13	1:B:136:LEU:C	2.30	0.51
1:D:28:VAL:HG13	1:D:34:LEU:CD1	2.41	0.51
1:D:71:THR:HG21	1:D:264:LEU:HD13	1.92	0.51
1:D:145:ASN:HD21	1:D:148:LYS:H	1.59	0.50
1:B:231:LEU:HA	1:B:236:VAL:HG12	1.94	0.50
1:D:126:THR:HG22	4:D:314:L3P:H291	1.93	0.50
1:B:108:MET:HG2	1:B:113:GLU:HA	1.93	0.50
1:A:254:VAL:HA	1:A:258:ILE:HG12	1.93	0.50
1:D:125:LEU:HD13	4:D:316:L3P:H262	1.94	0.50
1:D:196:VAL:O	1:D:200:GLN:HG2	2.11	0.49
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.48	0.49
4:D:316:L3P:H152	4:D:316:L3P:H191	1.95	0.48
1:A:20:THR:HG22	1:A:21:GLN:N	2.26	0.48
1:B:168:LEU:HD22	4:D:314:L3P:H242	1.94	0.48
1:D:80:ALA:HB1	4:D:314:L3P:H303	1.95	0.48
1:B:141:LEU:HD22	1:B:263:LEU:HD11	1.96	0.48
1:D:28:VAL:HG13	1:D:34:LEU:HD12	1.94	0.48
1:A:254:VAL:HA	1:A:258:ILE:CG1	2.44	0.48
1:A:234:GLU:HG3	6:A:511:HOH:O	2.13	0.48
1:B:20:THR:HG22	1:B:21:GLN:N	2.28	0.48
1:D:254:VAL:CA	1:D:258:ILE:HG22	2.42	0.48
1:B:70:SER:CB	1:B:136:LEU:HD12	2.44	0.48
1:A:22:ARG:HG3	1:A:23:GLU:N	2.29	0.47
1:B:26:GLU:O	1:B:29:LEU:O	2.32	0.47
1:A:218:THR:HG23	1:A:222:TRP:NE1	2.30	0.47
1:B:268:THR:HG23	6:B:516:HOH:O	2.14	0.47
1:B:97:PRO:HB3	1:B:170:THR:O	2.16	0.46
1:B:19:VAL:CG2	1:B:93:VAL:HG11	2.46	0.46
1:B:193:ILE:HD12	1:B:193:ILE:C	2.35	0.46
1:D:29:LEU:C	1:D:31:ASP:H	2.19	0.46
1:D:184:CYS:O	1:D:188:ILE:HG23	2.16	0.46
1:A:233:VAL:HG23	1:A:234:GLU:OE1	2.16	0.46
1:A:33:LEU:HD22	1:A:246:TRP:CD1	2.50	0.46
1:B:93:VAL:HG13	1:B:93:VAL:O	2.15	0.46
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.98	0.46
1:A:19:VAL:HG12	1:A:109:LEU:HD23	1.97	0.46
1:B:54:PHE:O	1:B:57:ARG:HG2	2.16	0.46
1:B:258:ILE:HG13	1:B:259:PHE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HB3	1:B:273:VAL:CG1	2.45	0.46
1:B:141:LEU:HD22	1:B:263:LEU:HD13	1.97	0.46
1:D:38:LEU:HD21	1:D:120:MET:CE	2.45	0.46
1:B:195:LEU:HD21	1:B:219:VAL:HG21	1.98	0.45
1:D:94:LEU:HD11	1:D:168:LEU:HD13	1.97	0.45
1:D:23:GLU:HB3	1:D:109:LEU:HB3	1.98	0.45
1:A:49:ILE:O	1:A:53:VAL:HG23	2.16	0.45
1:B:107:VAL:O	1:B:108:MET:HB2	2.16	0.45
1:D:89:LEU:HD21	4:D:314:L3P:H23	1.99	0.45
1:D:193:ILE:HD12	1:D:193:ILE:C	2.36	0.45
1:D:29:LEU:O	1:D:30:ASN:HB2	2.17	0.45
1:D:232:GLY:CA	1:D:244:THR:HG21	2.47	0.44
1:B:188:ILE:HG13	1:B:189:VAL:N	2.33	0.44
1:D:145:ASN:C	1:D:145:ASN:ND2	2.65	0.44
1:B:134:ILE:HG23	1:B:259:PHE:CZ	2.52	0.44
1:A:26:GLU:O	1:A:29:LEU:O	2.36	0.44
1:A:131:THR:N	1:A:132:PRO:CD	2.81	0.43
1:B:184:CYS:O	1:B:188:ILE:HG23	2.18	0.43
1:D:59:LEU:HD21	1:D:268:THR:HG22	2.00	0.43
1:A:66:LEU:HD13	1:A:140:LEU:HD11	2.00	0.43
1:B:214:LEU:CD1	1:B:263:LEU:HD13	2.48	0.43
1:D:249:SER:O	1:D:253:ILE:HG13	2.18	0.43
1:B:20:THR:CG2	1:B:21:GLN:N	2.82	0.43
1:B:180:TYR:CD2	2:B:292:RET:H32	2.53	0.43
1:A:240:PRO:O	1:A:244:THR:HG23	2.18	0.43
1:B:236:VAL:HG22	1:B:236:VAL:O	2.18	0.43
1:D:107:VAL:O	1:D:108:MET:HB3	2.19	0.43
1:A:220:VAL:HG12	1:A:221:MET:CE	2.49	0.43
1:B:149:LEU:HB3	4:B:318:L3P:H271	2.01	0.43
1:B:51:LEU:O	1:B:55:MET:HG3	2.20	0.42
1:B:253:ILE:HA	1:B:257:TYR:CD2	2.54	0.42
1:A:19:VAL:O	1:A:19:VAL:HG23	2.19	0.42
1:D:74:VAL:HB	1:D:75:PRO:CD	2.49	0.42
2:D:292:RET:H7	2:D:292:RET:H181	1.84	0.42
1:D:75:PRO:O	1:D:79:ILE:HG13	2.20	0.42
1:D:128:ALA:O	1:D:132:PRO:HG2	2.20	0.42
2:B:292:RET:H7	2:B:292:RET:H181	1.81	0.41
1:A:20:THR:CG2	1:A:21:GLN:N	2.83	0.41
1:A:161:VAL:HG12	4:B:311:L3P:H291	2.02	0.41
1:D:168:LEU:HD22	1:D:168:LEU:N	2.36	0.41
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:CE1	1:B:118:VAL:HG21	2.55	0.41
1:B:128:ALA:O	1:B:132:PRO:HG2	2.20	0.41
1:B:225:TYR:N	1:B:226:PRO:HD2	2.36	0.41
1:D:81:SER:CB	1:D:126:THR:HG21	2.51	0.41
1:A:33:LEU:HD22	1:A:246:TRP:HD1	1.85	0.41
1:B:108:MET:HG2	1:B:113:GLU:CA	2.51	0.41
1:A:61:ASP:OD2	1:A:275:SER:HA	2.20	0.41
1:B:29:LEU:O	1:B:30:ASN:CB	2.62	0.41
1:B:129:LEU:C	1:B:132:PRO:HD2	2.42	0.41
1:B:131:THR:N	1:B:132:PRO:CD	2.84	0.41
1:B:145:ASN:O	1:B:149:LEU:HD23	2.20	0.41
1:D:27:PHE:CZ	1:D:118:VAL:HG21	2.55	0.41
1:D:241:VAL:HA	1:D:244:THR:OG1	2.21	0.40
1:D:64:ALA:O	1:D:267:LEU:HD21	2.21	0.40
1:A:121:TRP:HA	1:A:124:TYR:CD2	2.55	0.40
1:A:126:THR:HG22	4:A:317:L3P:H302	2.03	0.40
1:A:171:SER:HB2	1:B:22:ARG:HA	2.04	0.40
1:A:231:LEU:O	1:A:238:VAL:HG22	2.20	0.40
1:D:108:MET:HB2	1:D:113:GLU:CG	2.51	0.40
1:D:27:PHE:CE1	1:D:118:VAL:HG21	2.56	0.40
1:D:96:MET:HG3	1:D:102:ALA:HB3	2.04	0.40
1:D:236:VAL:HG22	1:D:236:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:600:HOH:O	6:A:600:HOH:O[2_656]	1.79	0.41

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	258/291 (89%)	253 (98%)	4 (2%)	1 (0%)	34	24
1	B	257/291 (88%)	248 (96%)	9 (4%)	0	100	100
1	D	257/291 (88%)	250 (97%)	6 (2%)	1 (0%)	34	24
All	All	772/873 (88%)	751 (97%)	19 (2%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	GLY
1	D	108	MET

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	209/233 (90%)	198 (95%)	11 (5%)	22	13
1	B	208/233 (89%)	199 (96%)	9 (4%)	29	19
1	D	208/233 (89%)	198 (95%)	10 (5%)	25	16
All	All	625/699 (89%)	595 (95%)	30 (5%)	25	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	LEU
1	A	59	LEU
1	A	66	LEU
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	216	LEU
1	A	234	GLU
1	A	264	LEU

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Mol	Chain	Res	Type
1	B	18	GLU
1	B	24	LEU
1	B	66	LEU
1	B	108	MET
1	B	135	LEU
1	B	209	ASP
1	B	234	GLU
1	B	259	PHE
1	B	264	LEU
1	D	24	LEU
1	D	38	LEU
1	D	66	LEU
1	D	79	ILE
1	D	135	LEU
1	D	136	LEU
1	D	145	ASN
1	D	149	LEU
1	D	209	ASP
1	D	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	265	ASN
1	B	41	ASN
1	B	265	ASN
1	D	100	HIS
1	D	145	ASN

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 ⓘ

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	22B	B	300	-	25,26,53	3.29	10 (40%)	30,35,72	2.16	9 (30%)
4	L3P	B	311	-	19,19,58	1.93	8 (42%)	22,22,73	1.14	2 (9%)
4	L3P	D	312	-	19,19,58	1.94	8 (42%)	22,22,73	1.22	2 (9%)
4	L3P	B	318	-	19,19,58	1.96	8 (42%)	22,22,73	1.31	2 (9%)
4	L3P	D	314	-	19,19,58	1.92	8 (42%)	22,22,73	1.20	2 (9%)
2	RET	B	292	1	20,20,21	2.17	6 (30%)	27,27,28	1.71	9 (33%)
5	AZI	D	401	-	0,2,2	-	-	0,1,1	-	-
4	L3P	A	310	-	19,19,58	1.98	8 (42%)	22,22,73	1.37	3 (13%)
4	L3P	A	317	-	19,19,58	1.97	8 (42%)	22,22,73	1.35	2 (9%)
4	L3P	D	316	-	19,19,58	2.00	8 (42%)	22,22,73	1.32	2 (9%)
5	AZI	A	401	-	0,2,2	-	-	0,1,1	-	-
2	RET	D	292	1	20,20,21	2.14	6 (30%)	27,27,28	1.65	7 (25%)
5	AZI	B	401	-	0,2,2	-	-	0,1,1	-	-
2	RET	A	292	1	20,20,21	2.11	6 (30%)	27,27,28	1.64	8 (29%)
4	L3P	B	315	-	19,19,58	1.92	8 (42%)	22,22,73	1.14	2 (9%)
3	22B	A	300	-	25,26,53	3.30	10 (40%)	30,35,72	2.10	9 (30%)
4	L3P	A	313	-	19,19,58	1.93	8 (42%)	22,22,73	1.11	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	22B	B	300	-	-	8/31/31/65	-
4	L3P	B	311	-	-	5/20/20/67	-
4	L3P	D	312	-	-	6/20/20/67	-
4	L3P	B	318	-	-	6/20/20/67	-
4	L3P	D	314	-	-	7/20/20/67	-
2	RET	B	292	1	-	0/13/30/31	0/1/1/1
4	L3P	A	310	-	-	9/20/20/67	-
4	L3P	A	317	-	-	6/20/20/67	-
4	L3P	D	316	-	-	8/20/20/67	-
2	RET	D	292	1	-	0/13/30/31	0/1/1/1
2	RET	A	292	1	-	0/13/30/31	0/1/1/1
4	L3P	B	315	-	-	6/20/20/67	-
3	22B	A	300	-	-	8/31/31/65	-
4	L3P	A	313	-	-	4/20/20/67	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	22B	C2-C3	12.32	1.63	1.49
3	B	300	22B	C2-C3	12.26	1.63	1.49
2	B	292	RET	C1-C6	6.06	1.62	1.53
2	D	292	RET	C1-C6	5.99	1.62	1.53
2	A	292	RET	C1-C6	5.97	1.62	1.53
3	B	300	22B	C21-C2	4.67	1.59	1.53
3	A	300	22B	C21-C2	4.66	1.59	1.53
2	A	292	RET	C5-C6	4.24	1.41	1.34
2	D	292	RET	C5-C6	4.18	1.41	1.34
3	B	300	22B	O27-C23	3.99	1.54	1.44
2	B	292	RET	C5-C6	3.96	1.41	1.34
3	A	300	22B	C16-C1	3.93	1.59	1.52
3	A	300	22B	O27-C23	3.92	1.54	1.44
3	B	300	22B	C16-C1	3.91	1.59	1.52
3	B	300	22B	C19-C9	3.71	1.58	1.50
3	A	300	22B	C19-C9	3.69	1.58	1.50
2	B	292	RET	C14-C13	3.23	1.36	1.33
3	A	300	22B	C17-C1	3.22	1.57	1.52
2	D	292	RET	C14-C13	3.19	1.36	1.33
3	B	300	22B	C17-C1	3.11	1.57	1.52
4	A	310	L3P	C15-C13	2.99	1.68	1.52
3	B	300	22B	C20-C13	2.96	1.57	1.50
2	B	292	RET	C7-C6	2.94	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	314	L3P	C15-C13	2.93	1.68	1.52
4	A	317	L3P	C15-C13	2.92	1.67	1.52
4	B	315	L3P	C15-C13	2.92	1.67	1.52
4	D	312	L3P	C15-C13	2.92	1.67	1.52
3	B	300	22B	C22-C21	2.89	1.61	1.53
4	D	316	L3P	C15-C13	2.89	1.67	1.52
4	B	311	L3P	C15-C13	2.88	1.67	1.52
4	A	313	L3P	C15-C13	2.88	1.67	1.52
4	B	318	L3P	C15-C13	2.88	1.67	1.52
3	A	300	22B	C20-C13	2.87	1.56	1.50
3	A	300	22B	C22-C21	2.87	1.61	1.53
2	D	292	RET	C7-C6	2.82	1.55	1.45
4	B	311	L3P	C26-C27	2.79	1.64	1.52
2	A	292	RET	C7-C6	2.76	1.54	1.45
4	A	317	L3P	C17-C18	2.73	1.66	1.52
4	D	316	L3P	C17-C18	2.72	1.66	1.52
4	A	310	L3P	C26-C27	2.71	1.63	1.52
4	A	317	L3P	C25-C23	2.70	1.66	1.52
4	D	316	L3P	C25-C23	2.70	1.66	1.52
4	A	310	L3P	C25-C23	2.68	1.66	1.52
3	B	300	22B	C18-C5	2.67	1.56	1.50
4	D	316	L3P	C26-C27	2.67	1.63	1.52
4	D	314	L3P	C26-C27	2.67	1.63	1.52
4	B	318	L3P	C17-C18	2.67	1.66	1.52
4	A	310	L3P	C19-C18	2.66	1.61	1.52
4	D	316	L3P	C19-C18	2.66	1.61	1.52
3	A	300	22B	C18-C5	2.66	1.56	1.50
4	B	318	L3P	C19-C18	2.64	1.61	1.52
4	A	317	L3P	C26-C27	2.64	1.63	1.52
4	D	312	L3P	C25-C23	2.64	1.66	1.52
4	D	312	L3P	C26-C27	2.63	1.63	1.52
4	B	318	L3P	C25-C23	2.63	1.66	1.52
4	D	314	L3P	C25-C23	2.62	1.66	1.52
4	A	310	L3P	C14-C13	2.61	1.61	1.52
4	B	311	L3P	C25-C23	2.61	1.66	1.52
4	A	313	L3P	C14-C13	2.60	1.61	1.52
4	B	318	L3P	C26-C27	2.60	1.63	1.52
4	B	315	L3P	C25-C23	2.59	1.66	1.52
4	B	315	L3P	C19-C18	2.59	1.61	1.52
4	D	316	L3P	C14-C13	2.59	1.61	1.52
4	D	312	L3P	C14-C13	2.58	1.61	1.52
4	A	313	L3P	C25-C23	2.58	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	312	L3P	C19-C18	2.57	1.61	1.52
2	B	292	RET	C2-C3	-2.56	1.46	1.52
4	B	318	L3P	C14-C13	2.55	1.60	1.52
4	A	317	L3P	C14-C13	2.55	1.60	1.52
4	B	315	L3P	C14-C13	2.55	1.60	1.52
4	B	315	L3P	C26-C27	2.54	1.63	1.52
4	B	311	L3P	C19-C18	2.53	1.60	1.52
4	A	313	L3P	C26-C27	2.53	1.63	1.52
4	A	317	L3P	C19-C18	2.53	1.60	1.52
4	D	314	L3P	C14-C13	2.52	1.60	1.52
4	A	313	L3P	C19-C18	2.51	1.60	1.52
4	D	312	L3P	C17-C18	2.51	1.65	1.52
4	A	310	L3P	C17-C18	2.50	1.65	1.52
4	B	311	L3P	C14-C13	2.48	1.60	1.52
4	D	314	L3P	C19-C18	2.47	1.60	1.52
4	B	315	L3P	C17-C18	2.45	1.65	1.52
2	A	292	RET	C2-C3	-2.45	1.46	1.52
4	B	311	L3P	C17-C18	2.45	1.65	1.52
4	D	316	L3P	C26-C25	2.45	1.62	1.52
4	D	314	L3P	C17-C18	2.45	1.65	1.52
4	A	313	L3P	C26-C25	2.45	1.62	1.52
4	A	313	L3P	C17-C18	2.44	1.65	1.52
4	A	317	L3P	C26-C25	2.43	1.62	1.52
4	D	312	L3P	C26-C25	2.39	1.62	1.52
4	B	318	L3P	C26-C25	2.38	1.62	1.52
4	A	310	L3P	C26-C25	2.38	1.62	1.52
4	D	314	L3P	C26-C25	2.37	1.62	1.52
4	B	311	L3P	C26-C25	2.37	1.62	1.52
4	B	315	L3P	C26-C25	2.37	1.62	1.52
2	D	292	RET	C2-C3	-2.37	1.46	1.52
3	A	300	22B	C4-C3	2.18	1.37	1.32
4	D	316	L3P	C16-C15	2.18	1.61	1.52
4	B	318	L3P	C16-C15	2.14	1.61	1.52
4	A	317	L3P	C16-C15	2.13	1.61	1.52
2	D	292	RET	C2-C1	2.13	1.59	1.54
4	B	315	L3P	C16-C15	2.12	1.61	1.52
4	A	313	L3P	C16-C15	2.12	1.61	1.52
4	D	314	L3P	C16-C15	2.09	1.61	1.52
4	B	311	L3P	C16-C15	2.07	1.61	1.52
4	D	312	L3P	C16-C15	2.07	1.61	1.52
4	A	310	L3P	C16-C15	2.06	1.61	1.52
3	B	300	22B	C4-C3	2.05	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	292	RET	C14-C13	2.04	1.35	1.33
2	A	292	RET	C2-C1	2.04	1.58	1.54
2	B	292	RET	C18-C5	2.04	1.54	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	300	22B	C2-C3-C4	6.00	134.91	125.15
3	A	300	22B	C2-C3-C4	5.71	134.43	125.15
3	A	300	22B	C20-C13-C12	4.22	124.73	118.08
3	B	300	22B	C21-C22-C23	4.00	124.08	116.39
3	B	300	22B	C20-C13-C12	3.83	124.10	118.08
3	A	300	22B	C21-C22-C23	3.75	123.61	116.39
4	A	310	L3P	C26-C25-C23	3.71	127.92	115.92
4	A	317	L3P	C26-C25-C23	3.69	127.83	115.92
4	D	312	L3P	C26-C25-C23	3.58	127.50	115.92
4	D	316	L3P	C26-C25-C23	3.51	127.27	115.92
4	D	314	L3P	C26-C25-C23	3.51	127.26	115.92
4	B	318	L3P	C26-C25-C23	3.46	127.12	115.92
3	B	300	22B	C16-C1-C2	3.45	116.69	111.72
3	B	300	22B	C17-C1-C16	-3.30	105.84	110.56
2	A	292	RET	C20-C13-C12	3.30	123.27	118.08
3	A	300	22B	C17-C1-C16	-3.29	105.85	110.56
4	B	311	L3P	C26-C25-C23	3.24	126.38	115.92
2	D	292	RET	C1-C6-C7	3.23	124.92	115.78
3	B	300	22B	C4-C5-C6	-3.23	113.98	118.94
2	B	292	RET	C1-C6-C7	3.16	124.71	115.78
3	B	300	22B	C18-C5-C4	3.09	122.95	118.08
4	A	317	L3P	C16-C17-C18	3.08	125.86	115.92
3	A	300	22B	C16-C1-C2	3.06	116.14	111.72
3	A	300	22B	C4-C5-C6	-3.03	114.29	118.94
3	A	300	22B	C18-C5-C4	3.00	122.81	118.08
4	D	316	L3P	C16-C17-C18	2.98	125.55	115.92
2	D	292	RET	C1-C6-C5	-2.97	118.43	122.61
4	B	318	L3P	C16-C17-C18	2.96	125.49	115.92
2	B	292	RET	C20-C13-C12	2.92	122.67	118.08
4	B	315	L3P	C26-C25-C23	2.88	125.24	115.92
4	A	310	L3P	C21-C20-C18	2.84	125.11	115.92
2	A	292	RET	C1-C6-C7	2.70	123.41	115.78
2	D	292	RET	C2-C1-C6	2.65	114.56	110.48
2	A	292	RET	C1-C6-C5	-2.65	118.88	122.61
4	A	310	L3P	C16-C17-C18	2.60	124.33	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	292	RET	C17-C1-C6	2.60	114.51	110.30
2	B	292	RET	C2-C1-C6	2.59	114.47	110.48
2	B	292	RET	C1-C6-C5	-2.56	119.00	122.61
4	A	313	L3P	C26-C25-C23	2.53	124.10	115.92
2	A	292	RET	C12-C13-C14	-2.50	110.88	118.80
2	A	292	RET	C2-C1-C6	2.47	114.29	110.48
3	A	300	22B	C12-C13-C14	-2.46	111.00	118.80
2	A	292	RET	C8-C9-C10	-2.46	115.17	118.94
2	D	292	RET	C20-C13-C12	2.43	121.91	118.08
2	B	292	RET	C8-C9-C10	-2.42	115.22	118.94
2	B	292	RET	C2-C3-C4	2.35	116.63	111.38
2	D	292	RET	C8-C9-C10	-2.31	115.39	118.94
2	B	292	RET	C19-C9-C8	2.29	121.68	118.08
3	B	300	22B	C24-C23-C22	2.22	118.26	111.42
2	D	292	RET	C19-C9-C8	2.21	121.56	118.08
2	A	292	RET	C19-C9-C8	2.20	121.55	118.08
3	A	300	22B	C24-C23-C22	2.20	118.20	111.42
4	D	314	L3P	C16-C17-C18	2.19	123.00	115.92
4	D	312	L3P	C16-C17-C18	2.18	122.98	115.92
2	A	292	RET	C17-C1-C6	2.18	113.83	110.30
2	B	292	RET	C7-C6-C5	-2.14	116.29	121.46
3	B	300	22B	C12-C13-C14	-2.13	112.04	118.80
2	D	292	RET	C17-C1-C6	2.12	113.73	110.30
4	B	311	L3P	C16-C17-C18	2.12	122.76	115.92
4	B	315	L3P	C16-C17-C18	2.05	122.55	115.92

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	22B	C1-C2-C3-C4
3	A	300	22B	C2-C3-C4-C5
3	A	300	22B	C7-C8-C9-C10
3	A	300	22B	C7-C8-C9-C19
3	A	300	22B	C21-C22-C23-C24
3	A	300	22B	C21-C22-C23-O27
3	B	300	22B	C1-C2-C3-C4
3	B	300	22B	C2-C3-C4-C5
3	B	300	22B	C7-C8-C9-C10
3	B	300	22B	C7-C8-C9-C19
3	B	300	22B	C21-C22-C23-C24
3	B	300	22B	C21-C22-C23-O27

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Mol	Chain	Res	Type	Atoms
4	A	310	L3P	C15-C16-C17-C18
4	A	313	L3P	C15-C16-C17-C18
4	A	317	L3P	C15-C16-C17-C18
4	B	311	L3P	C15-C16-C17-C18
4	B	315	L3P	C15-C16-C17-C18
4	B	318	L3P	C15-C16-C17-C18
4	D	312	L3P	C15-C16-C17-C18
4	D	314	L3P	C15-C16-C17-C18
4	D	316	L3P	C15-C16-C17-C18
4	A	310	L3P	C19-C18-C20-C21
4	D	316	L3P	C18-C20-C21-C22
4	A	313	L3P	C25-C26-C27-C28
4	B	318	L3P	C25-C26-C27-C28
4	A	310	L3P	C18-C20-C21-C22
3	A	300	22B	C21-C22-C23-C25
3	B	300	22B	C21-C22-C23-C25
4	B	315	L3P	C26-C27-C28-C29
4	B	318	L3P	C26-C27-C28-C29
4	D	312	L3P	C25-C26-C27-C28
4	A	310	L3P	C26-C27-C28-C29
4	A	317	L3P	C26-C27-C28-C29
4	A	317	L3P	C26-C27-C28-C30
4	B	315	L3P	C26-C27-C28-C30
4	B	318	L3P	C26-C27-C28-C30
4	D	312	L3P	C26-C27-C28-C29
4	A	310	L3P	C26-C27-C28-C30
4	D	312	L3P	C26-C27-C28-C30
4	D	316	L3P	C26-C27-C28-C30
4	B	318	L3P	C13-C15-C16-C17
4	A	310	L3P	C22-C23-C25-C26
4	D	316	L3P	C17-C18-C20-C21
4	D	316	L3P	C26-C27-C28-C29
4	A	313	L3P	C26-C27-C28-C30
4	A	313	L3P	C26-C27-C28-C29
4	A	310	L3P	C24-C23-C25-C26
4	D	316	L3P	C19-C18-C20-C21
4	A	317	L3P	C13-C15-C16-C17
3	A	300	22B	C21-C2-C3-C4
3	B	300	22B	C21-C2-C3-C4
4	B	315	L3P	C25-C26-C27-C28
4	A	310	L3P	C25-C26-C27-C28
4	B	315	L3P	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	317	L3P	C17-C18-C20-C21
4	D	314	L3P	C17-C18-C20-C21
4	D	314	L3P	C22-C23-C25-C26
4	A	317	L3P	C19-C18-C20-C21
4	B	311	L3P	C16-C17-C18-C19
4	D	314	L3P	C24-C23-C25-C26
4	D	316	L3P	C13-C15-C16-C17
4	D	314	L3P	C19-C18-C20-C21
4	A	310	L3P	C13-C15-C16-C17
4	B	311	L3P	C16-C17-C18-C20
4	D	314	L3P	C16-C17-C18-C20
4	B	318	L3P	C19-C18-C20-C21
4	D	312	L3P	C16-C17-C18-C20
4	D	314	L3P	C16-C17-C18-C19
4	B	311	L3P	C19-C18-C20-C21
4	D	312	L3P	C16-C17-C18-C19
4	B	311	L3P	C13-C15-C16-C17
4	D	316	L3P	C25-C26-C27-C28
4	B	315	L3P	C22-C23-C25-C26

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	311	L3P	2	0
4	B	318	L3P	1	0
4	D	314	L3P	4	0
2	B	292	RET	2	0
4	A	317	L3P	2	0
4	D	316	L3P	2	0
2	D	292	RET	1	0
4	B	315	L3P	1	0
4	A	313	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 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 22B B 300

Bond lengths | Bond angles
Torsions | Rings

Ligand L3P B 311

Bond lengths | Bond angles
Torsions | Rings

Ligand L3P D 312

Bond lengths | Bond angles
Torsions | Rings

Ligand L3P B 318

Bond lengths | Bond angles
Torsions | Rings

Ligand L3P D 314

Bond lengths

Bond angles

Torsions

Rings

Ligand RET B 292

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 310

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 317

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P D 316

Bond lengths

Bond angles

Torsions

Rings

Ligand RET D 292

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 292

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P B 315

Bond lengths

Bond angles

Torsions

Rings

Ligand 22B A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 313

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	260/291 (89%)	0.13	14 (5%)	25	29	16, 23, 47, 69	0
1	B	259/291 (89%)	0.23	16 (6%)	20	23	18, 29, 43, 58	0
1	D	259/291 (89%)	0.49	26 (10%)	7	8	20, 32, 56, 80	0
All	All	778/873 (89%)	0.28	56 (7%)	15	17	16, 28, 49, 80	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	GLY	11.4
1	D	276	GLY	8.8
1	D	109	LEU	8.0
1	D	110	GLY	7.2
1	D	112	GLU	7.2
1	A	111	GLY	5.9
1	A	277	SER	5.5
1	D	111	GLY	5.5
1	A	109	LEU	5.0
1	A	110	GLY	4.9
1	B	104	GLY	4.8
1	D	30	ASN	4.8
1	D	108	MET	4.5
1	D	18	GLU	4.4
1	D	243	TYR	4.3
1	D	113	GLU	4.3
1	A	276	GLY	4.1
1	A	30	ASN	4.0
1	A	107	VAL	3.7
1	D	269	SER	3.6
1	D	29	LEU	3.5
1	B	112	GLU	3.3
1	D	193	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	275	SER	3.0
1	A	104	GLY	3.0
1	B	101	PHE	3.0
1	A	19	VAL	3.0
1	A	112	GLU	2.9
1	D	32	PRO	2.9
1	B	18	GLU	2.9
1	A	54	PHE	2.9
1	B	243	TYR	2.8
1	A	57	ARG	2.8
1	D	258	ILE	2.7
1	A	18	GLU	2.6
1	A	108	MET	2.6
1	B	204	ALA	2.5
1	D	54	PHE	2.5
1	B	109	LEU	2.4
1	D	33	LEU	2.3
1	D	216	LEU	2.3
1	D	57	ARG	2.3
1	B	258	ILE	2.2
1	D	261	PHE	2.2
1	D	58	GLY	2.2
1	B	240	PRO	2.2
1	D	59	LEU	2.2
1	D	265	ASN	2.2
1	D	40	ILE	2.1
1	B	236	VAL	2.1
1	D	107	VAL	2.1
1	B	107	VAL	2.1
1	B	188	ILE	2.0
1	B	200	GLN	2.0
1	B	238	VAL	2.0
1	B	193	ILE	2.0

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 (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	D	316	20/59	0.27	0.66	95,96,96,96	0
4	L3P	B	318	20/59	0.39	0.66	90,94,95,95	0
4	L3P	A	310	20/59	0.45	0.59	79,85,90,90	0
3	22B	A	300	27/54	0.48	0.30	70,74,79,79	0
4	L3P	B	315	20/59	0.49	0.71	114,115,117,117	0
4	L3P	A	313	20/59	0.51	0.56	94,95,96,96	0
4	L3P	A	317	20/59	0.53	0.62	86,87,94,94	0
4	L3P	D	312	20/59	0.56	0.63	108,110,111,111	0
4	L3P	D	314	20/59	0.60	0.58	83,86,92,93	0
4	L3P	B	311	20/59	0.64	0.71	113,114,116,116	0
3	22B	B	300	27/54	0.76	0.19	43,46,50,52	0
2	RET	D	292	20/21	0.89	0.14	24,26,30,30	0
2	RET	B	292	20/21	0.93	0.12	21,23,26,26	0
5	AZI	D	401	3/3	0.93	0.14	37,37,40,43	0
5	AZI	A	401	3/3	0.94	0.08	24,24,28,30	0
2	RET	A	292	20/21	0.94	0.12	15,19,23,23	0
5	AZI	B	401	3/3	0.95	0.09	27,27,32,33	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.
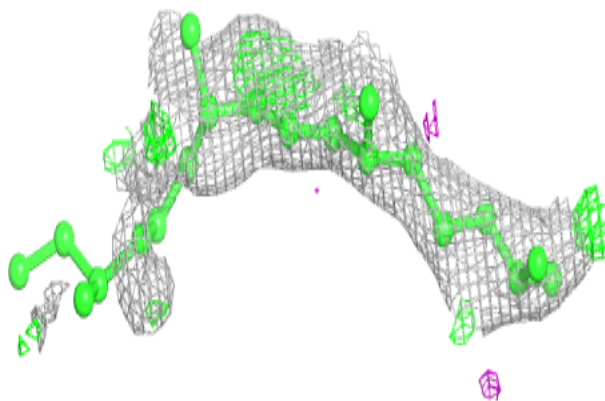
Electron density around L3P D 316:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
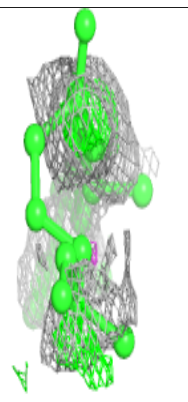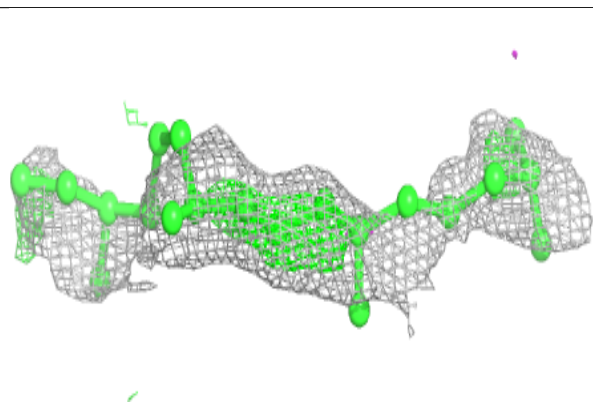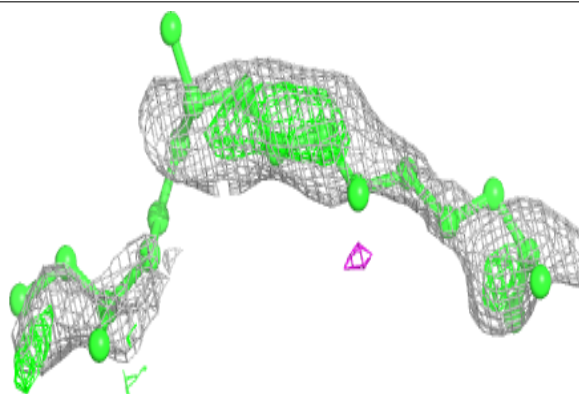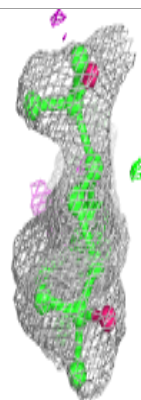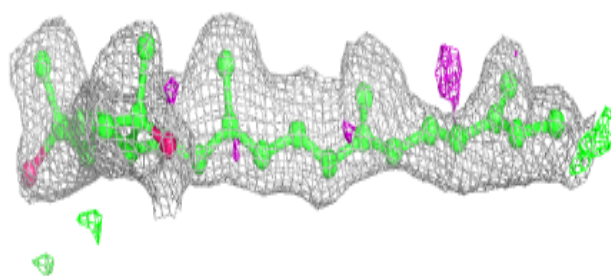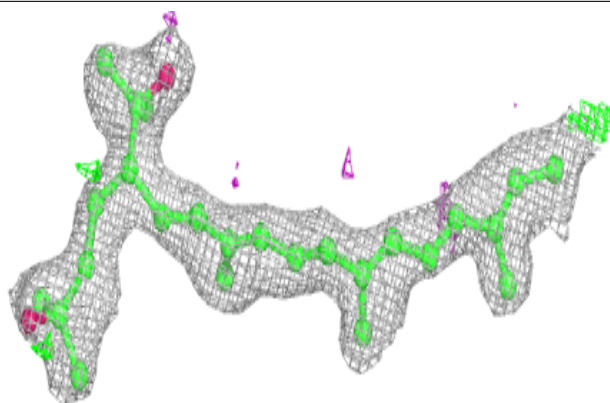$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
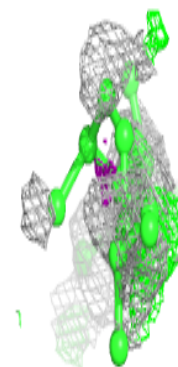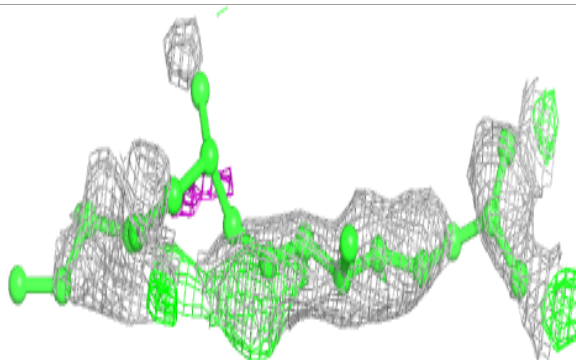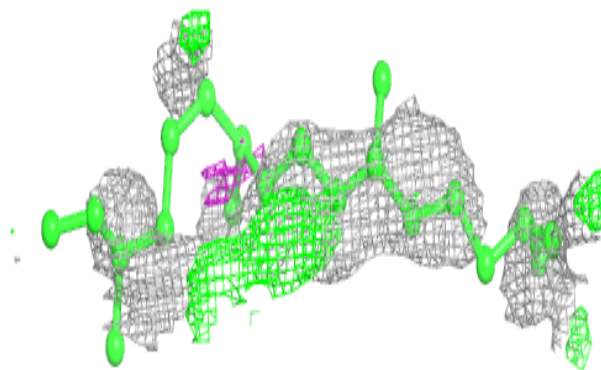
Electron density around L3P B 318:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
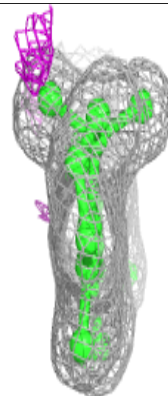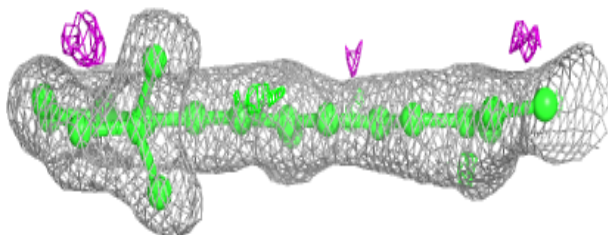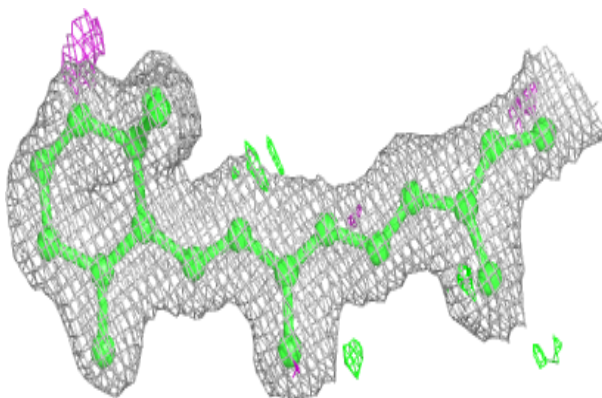$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
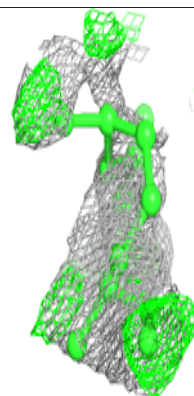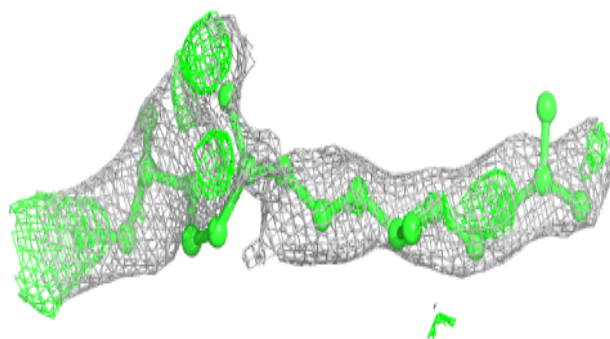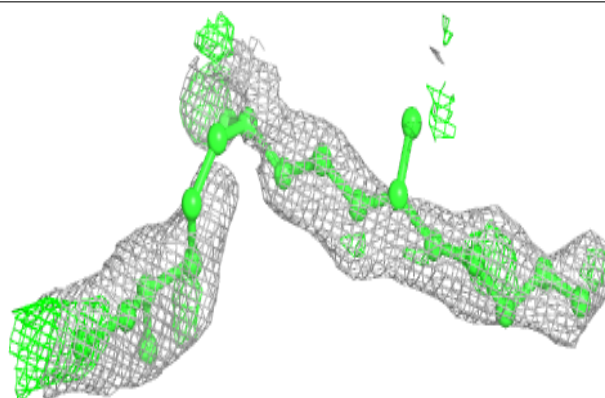
Electron density around L3P A 310:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
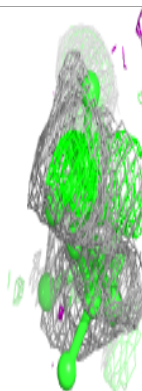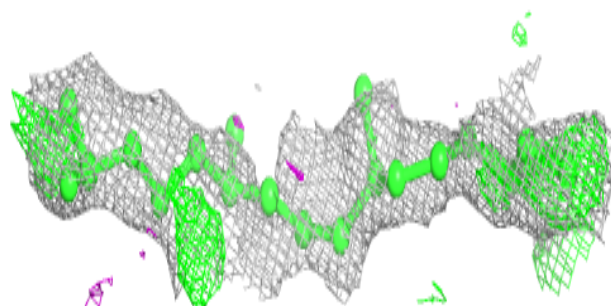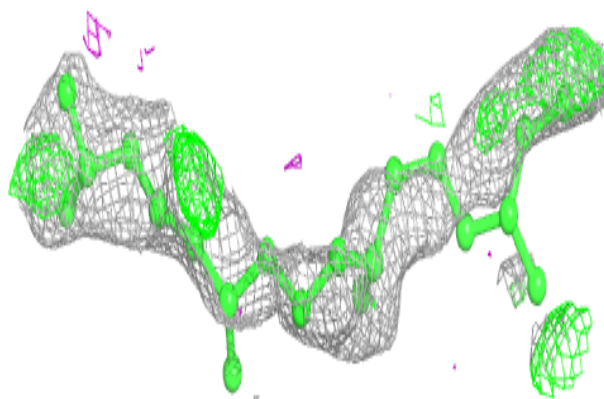
Electron density around 22B A 300:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
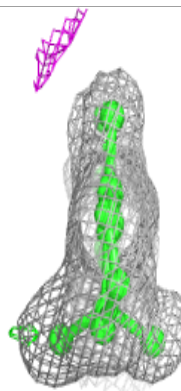$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
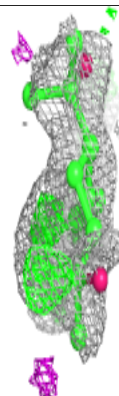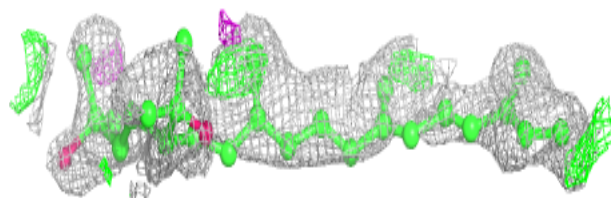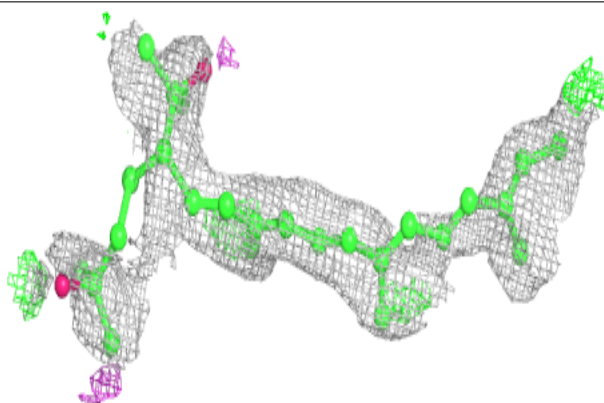
Electron density around L3P B 315:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
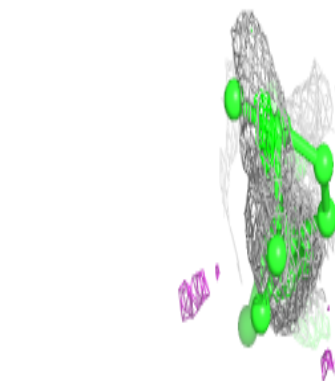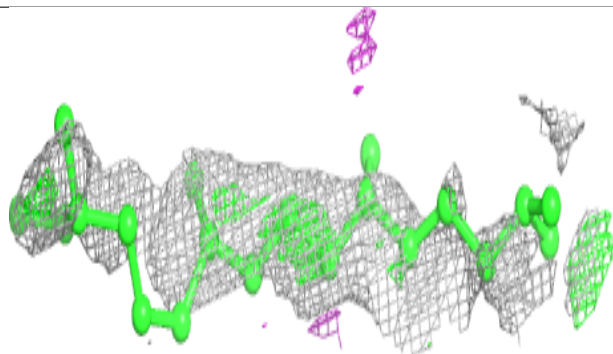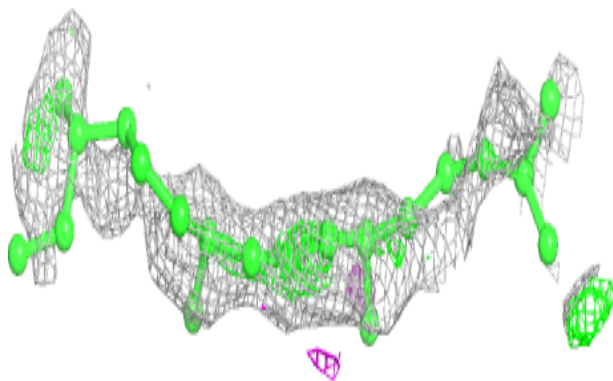
Electron density around L3P A 313:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
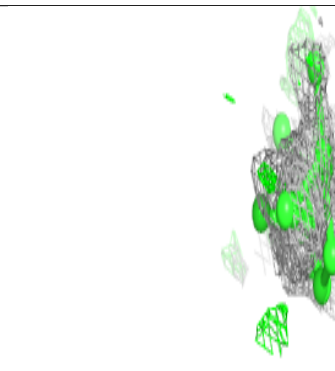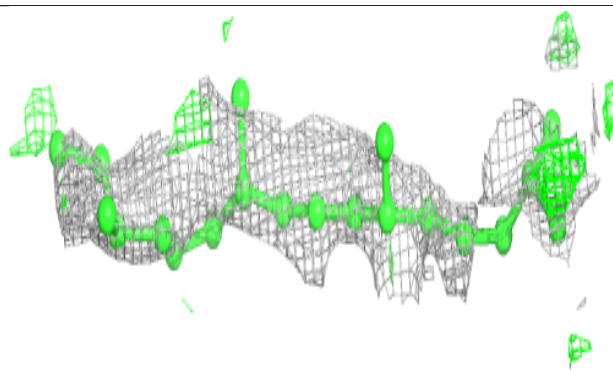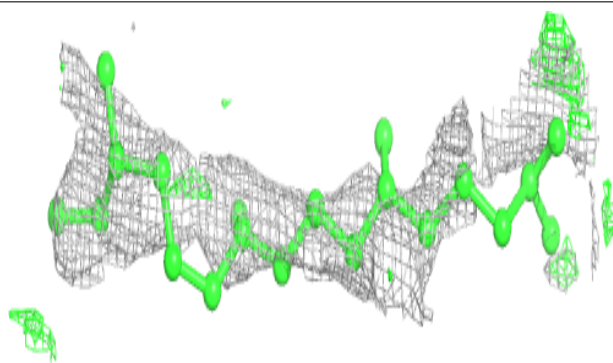
Electron density around L3P A 317:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
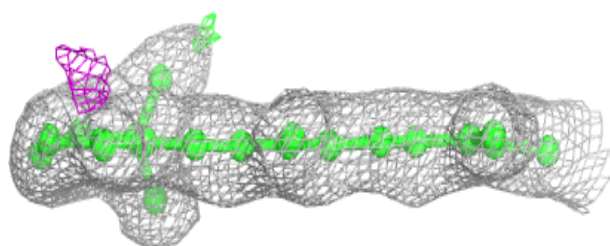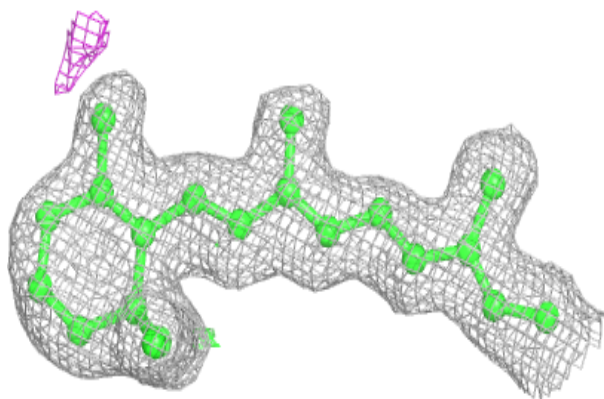mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
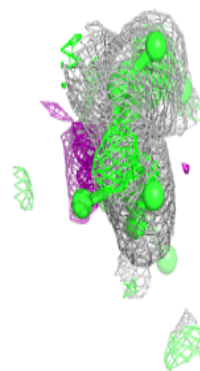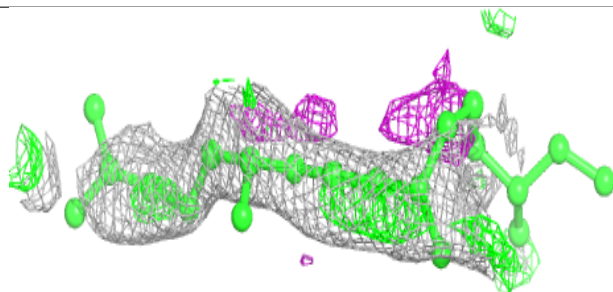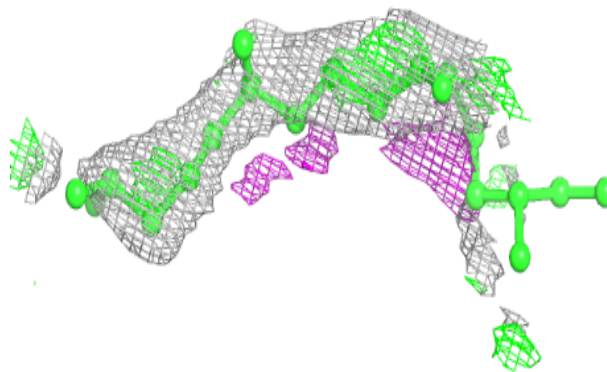
Electron density around L3P D 312:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
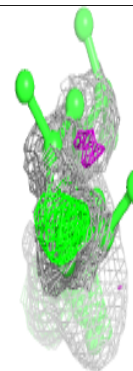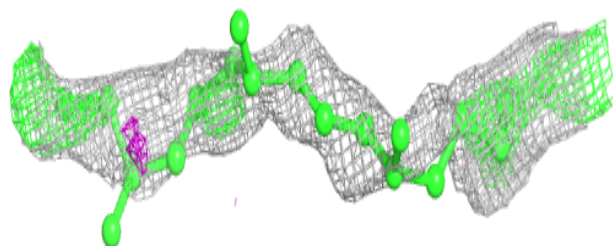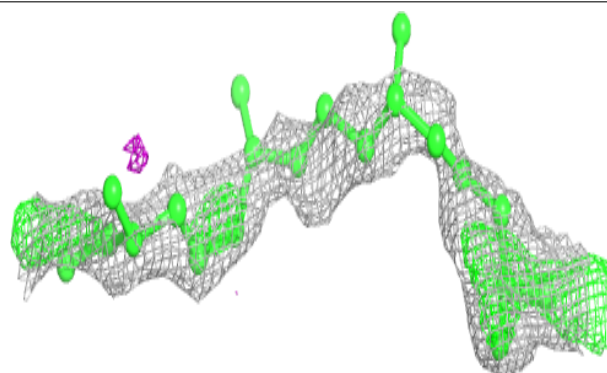
Electron density around L3P D 314:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
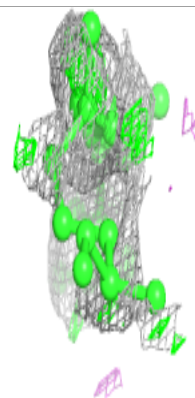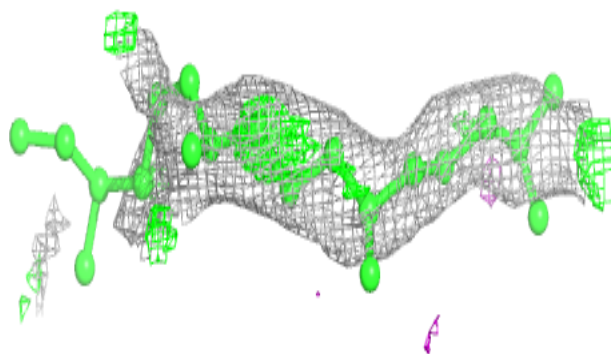
Electron density around L3P B 311:

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 22B B 300:

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 D 292:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

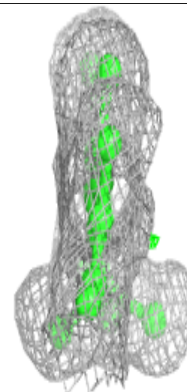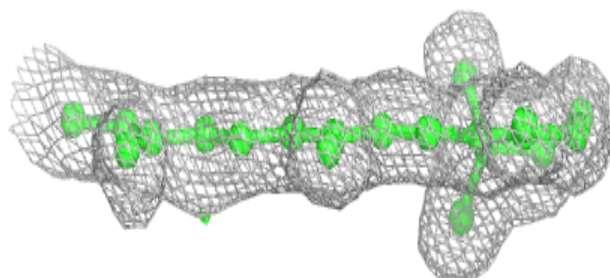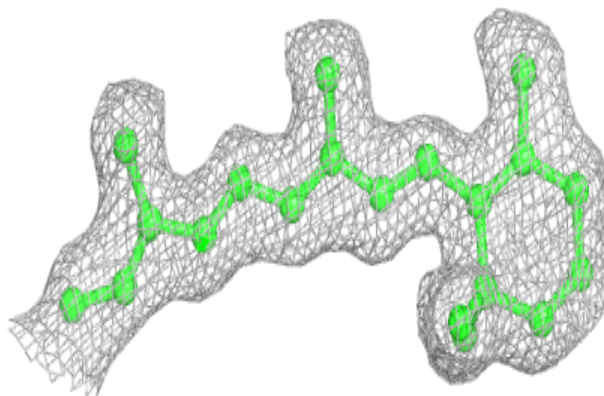**Electron density around RET B 292:**

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 292:

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.