



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 4L80 / pdb_00004l80
Title : Crystal Structure of Chloroflexus aurantiacus malyl-CoA lyase in complex with magnesium, oxalate, and propionyl-CoA
Authors : Zarzycki, J.; Kerfeld, C.A.
Deposited on : 2013-06-15
Resolution : 2.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

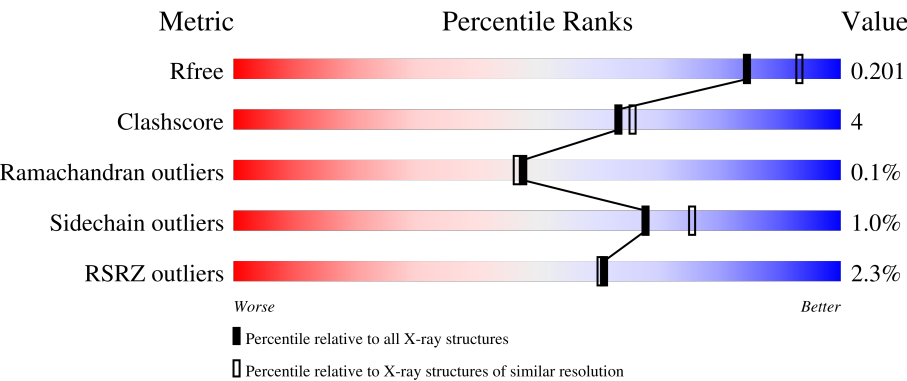
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



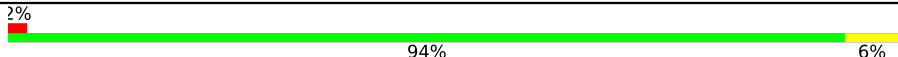
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	348	3% 88% 10% ..
1	B	348	% 90% 9%
1	C	348	3% 92% 7% .
1	D	348	2% 92% 6% .
1	E	348	2% 89% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	348	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	402	-	X	-	-
3	OXL	B	402	-	X	X	-
3	OXL	C	402	-	X	-	-
3	OXL	D	402	-	X	-	-
3	OXL	E	402	-	X	-	-
3	OXL	F	402	-	X	-	-

2 Entry composition [i](#)

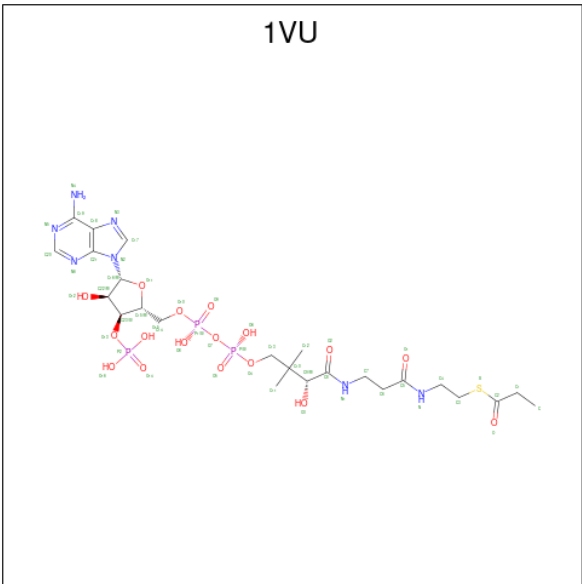
There are 6 unique types of molecules in this entry. The entry contains 18197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HpcH/HpaI aldolase.

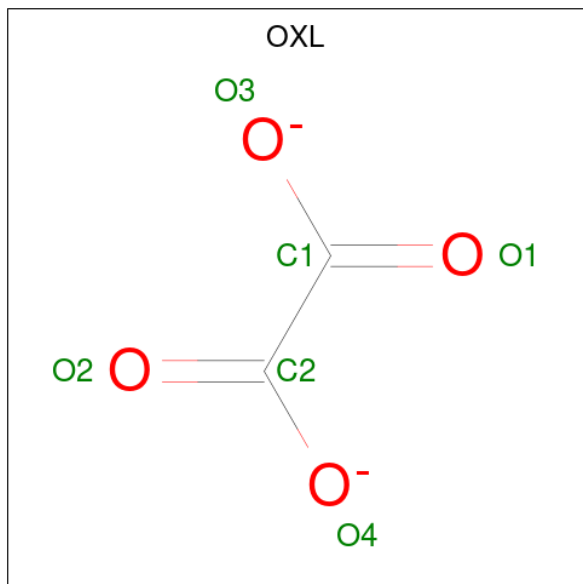
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2683	1722	470	478	13			
1	B	347	Total	C	N	O	S	0	1	0
			2701	1734	472	482	13			
1	C	347	Total	C	N	O	S	0	1	0
			2701	1734	472	482	13			
1	D	344	Total	C	N	O	S	0	1	0
			2679	1722	468	476	13			
1	E	344	Total	C	N	O	S	0	1	0
			2679	1722	468	476	13			
1	F	347	Total	C	N	O	S	0	0	0
			2695	1730	472	480	13			

- Molecule 2 is propionyl Coenzyme A (CCD ID: 1VU) (formula: C₂₄H₄₀N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0
2	B	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0
2	C	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0
2	D	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0
2	E	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0
2	F	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	0

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).

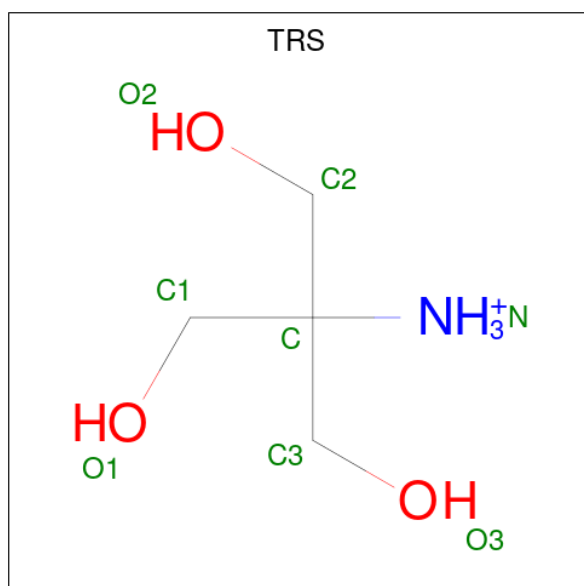


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O		
			6 2 4		0	0
3	B	1	Total	C O		
			6 2 4		0	0
3	C	1	Total	C O		
			6 2 4		0	0
3	D	1	Total	C O		
			6 2 4		0	0
3	E	1	Total	C O		
			6 2 4		0	0
3	F	1	Total	C O		
			6 2 4		0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	D	1	Total	C	N	O	0	0
			8	4	1	3		

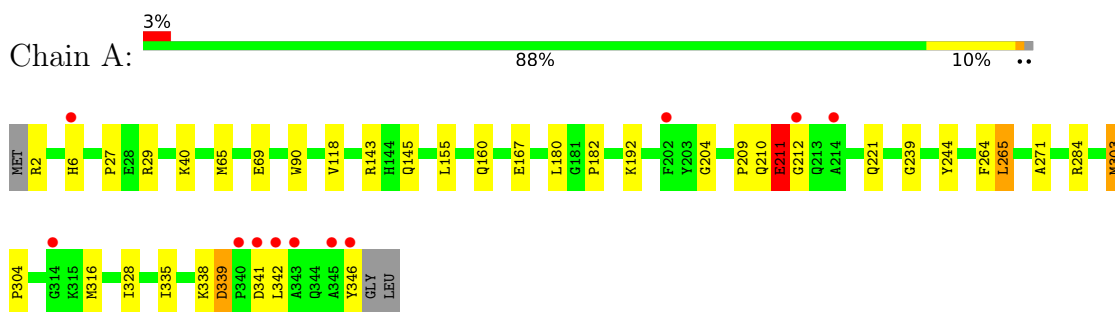
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total 278	O 278	0	0
6	B	260	Total 260	O 260	0	0
6	C	342	Total 342	O 342	0	0
6	D	286	Total 286	O 286	0	0
6	E	279	Total 279	O 279	0	0
6	F	244	Total 244	O 244	0	0

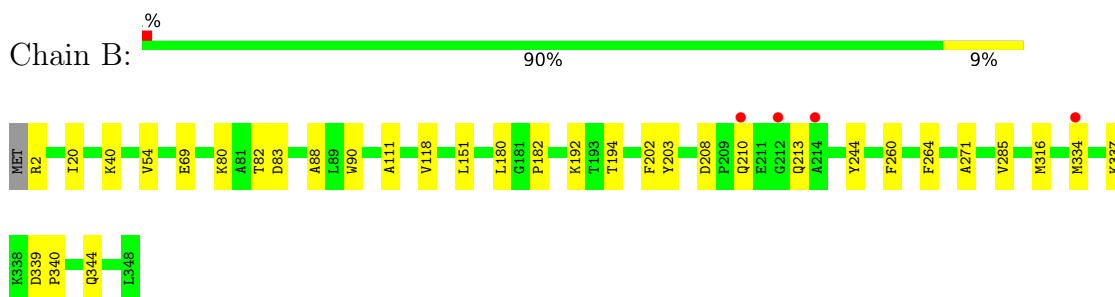
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

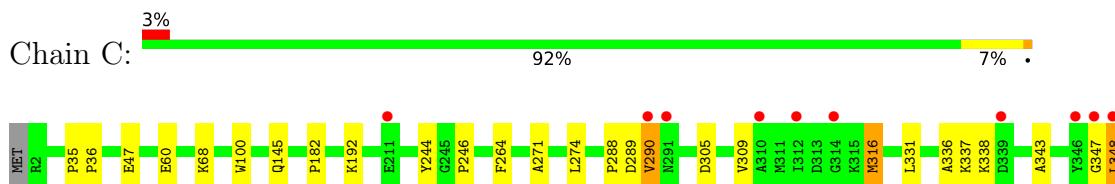
- Molecule 1: HpcH/HpaI aldolase



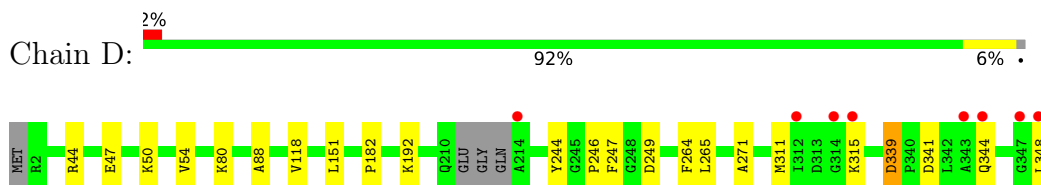
- Molecule 1: HpcH/HpaI aldolase



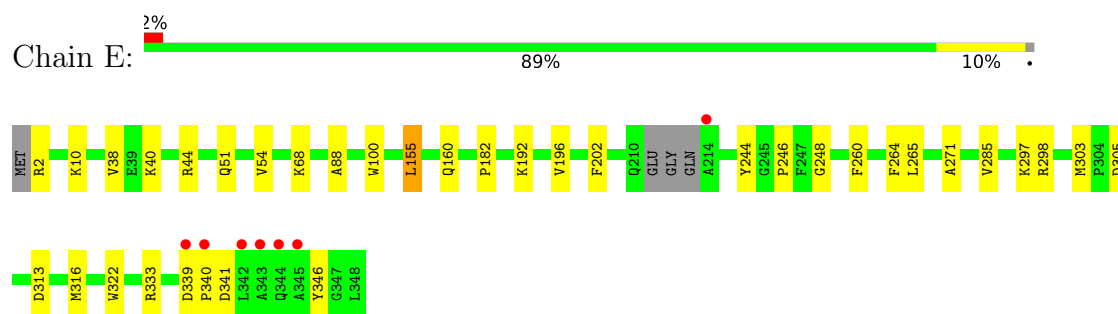
- Molecule 1: HpcH/HpaI aldolase



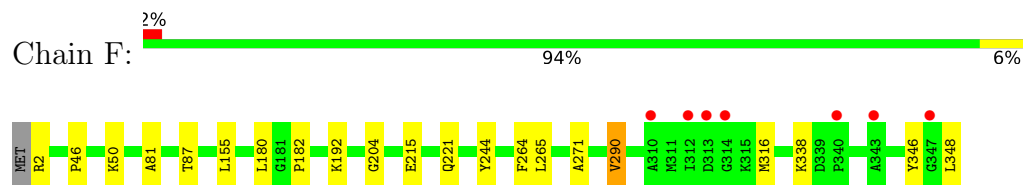
- Molecule 1: HpcH/HpaI aldolase



- Molecule 1: HpcH/HpaI aldolase



- Molecule 1: HpcH/HpaI aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	102.15Å 102.15Å 204.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 2.01 37.93 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.93-2.01) 98.5 (37.93-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1303	Depositor
R, R_{free}	0.172 , 0.201 0.173 , 0.201	Depositor DCC
R_{free} test set	1979 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18197	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: 1VU, TRS, MG, OXL

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	0.39	0/2750	0.77	5/3737 (0.1%)
1	B	0.36	0/2771	0.74	0/3765
1	C	0.32	0/2771	0.74	1/3765 (0.0%)
1	D	0.37	0/2748	0.76	2/3733 (0.1%)
1	E	0.35	1/2748 (0.0%)	0.75	0/3733
1	F	0.33	0/2762	0.73	0/3753
All	All	0.35	1/16550 (0.0%)	0.75	8/22486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	155	LEU	C-O	-5.42	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLY	N-CA-C	-7.58	102.65	114.10
1	A	303	MET	CA-C-N	7.04	127.02	119.28
1	A	303	MET	C-N-CA	7.04	127.02	119.28
1	A	339	ASP	CA-C-N	6.34	127.77	119.84
1	A	339	ASP	C-N-CA	6.34	127.77	119.84
1	C	290	VAL	N-CA-C	5.56	115.76	110.42
1	D	339	ASP	CA-C-N	5.12	125.16	119.32
1	D	339	ASP	C-N-CA	5.12	125.16	119.32

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	2683	0	2689	33	0
1	B	2701	0	2709	24	0
1	C	2701	0	2709	21	0
1	D	2679	0	2691	16	0
1	E	2679	0	2691	27	0
1	F	2695	0	2703	14	0
2	A	52	0	38	5	0
2	B	52	0	38	5	0
2	C	52	0	38	3	0
2	D	52	0	38	2	0
2	E	52	0	38	6	0
2	F	52	0	38	2	0
3	A	6	0	0	1	0
3	B	6	0	0	2	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	1	0
3	F	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	12	0	0
5	D	8	0	12	0	0
6	A	278	0	0	9	1
6	B	260	0	0	3	0
6	C	342	0	0	9	1
6	D	286	0	0	7	0
6	E	279	0	0	5	0
6	F	244	0	0	5	0
All	All	18197	0	16444	131	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 4.

All (131) 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:210:GLN:O	1:A:211:GLU:HB3	1.54	1.05
1:A:209:PRO:O	6:A:626:HOH:O	1.82	0.97
1:E:316:MET:HE1	2:F:401:1VU:H31	1.30	0.95
2:C:401:1VU:O16	6:C:717:HOH:O	1.87	0.92
2:A:401:1VU:H31	1:C:316:MET:HE1	1.36	0.88
1:E:44:ARG:NH1	2:E:401:1VU:N6	2.25	0.84
1:A:2:ARG:N	6:A:729:HOH:O	2.08	0.83
2:D:401:1VU:H31	1:F:316:MET:HE1	1.42	0.83
2:D:401:1VU:O9	6:D:783:HOH:O	1.98	0.82
1:B:316:MET:SD	6:B:710:HOH:O	2.37	0.81
1:F:87:THR:OG1	6:F:695:HOH:O	1.98	0.81
1:C:47:GLU:OE1	6:C:699:HOH:O	1.98	0.81
1:E:297:LYS:NZ	1:E:346:TYR:O	2.13	0.81
1:E:339:ASP:OD2	6:E:665:HOH:O	2.04	0.75
1:A:27:PRO:HG2	1:A:338:LYS:HD3	1.68	0.75
1:C:305:ASP:OD2	6:C:817:HOH:O	2.05	0.75
1:C:145:GLN:NE2	6:C:802:HOH:O	1.96	0.74
1:D:47:GLU:OE2	6:D:750:HOH:O	2.04	0.74
1:D:339:ASP:OD2	6:D:566:HOH:O	2.06	0.72
1:D:80:LYS:NZ	6:D:758:HOH:O	2.22	0.72
1:B:316:MET:HE2	2:C:401:1VU:H20	1.70	0.72
1:A:210:GLN:O	1:A:211:GLU:CB	2.36	0.69
1:C:305:ASP:OD2	6:C:839:HOH:O	2.10	0.69
1:C:347:GLY:O	6:C:786:HOH:O	2.11	0.69
1:E:51:GLN:NE2	6:E:727:HOH:O	2.26	0.68
1:A:65:MET:SD	6:C:829:HOH:O	2.51	0.67
1:D:249:ASP:OD2	6:D:641:HOH:O	2.12	0.67
1:A:145:GLN:NE2	6:A:558:HOH:O	2.30	0.64
1:A:265:LEU:HD12	1:B:203:TYR:HB2	1.80	0.64
2:A:401:1VU:N	1:C:316:MET:HE1	2.10	0.63
2:B:401:1VU:H36	3:B:402:OXL:C1	2.29	0.62
1:E:44:ARG:HH12	2:E:401:1VU:H6	1.64	0.62
1:A:143:ARG:NH2	6:A:527:HOH:O	2.32	0.62
1:A:265:LEU:HD11	1:B:202:PHE:HB2	1.82	0.62
1:F:346:TYR:HB3	1:F:348:LEU:HD23	1.82	0.60
1:F:2:ARG:N	6:F:710:HOH:O	2.33	0.60
1:A:316:MET:HE2	2:B:401:1VU:H20	1.85	0.58
1:C:337:LYS:HD3	1:C:348:LEU:HD11	1.88	0.56
1:D:50:LYS:NZ	6:D:745:HOH:O	2.38	0.56
1:C:288:PRO:HG3	1:C:331:LEU:HD23	1.88	0.56
1:A:160:GLN:NE2	6:A:520:HOH:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:O	1:A:211:GLU:HG3	2.05	0.55
1:B:316:MET:HE1	1:C:274:LEU:HB3	1.89	0.54
2:A:401:1VU:H31	1:C:316:MET:CE	2.16	0.54
1:D:341:ASP:O	1:D:344:GLN:NE2	2.41	0.54
1:F:290:VAL:HG22	6:F:680:HOH:O	2.07	0.54
1:E:341:ASP:OD1	1:E:341:ASP:N	2.39	0.53
1:E:44:ARG:NH1	2:E:401:1VU:H6	2.23	0.53
1:B:80:LYS:HE3	1:B:111:ALA:HB1	1.91	0.52
1:B:82:THR:HG22	1:B:83:ASP:N	2.24	0.52
1:E:305:ASP:OD2	6:E:656:HOH:O	2.19	0.52
1:E:333:ARG:HG3	6:E:774:HOH:O	2.10	0.52
1:D:182:PRO:HD2	1:D:246:PRO:HD2	1.92	0.52
1:A:167:GLU:HG2	6:A:698:HOH:O	2.09	0.51
2:B:401:1VU:H36	3:B:402:OXL:C2	2.41	0.51
1:A:342:LEU:HD23	1:A:346:TYR:CE1	2.46	0.51
1:D:247:PHE:CE2	1:D:249:ASP:HB3	2.47	0.50
1:A:341:ASP:OD1	1:A:341:ASP:N	2.43	0.50
1:C:289:ASP:OD2	1:C:290:VAL:N	2.45	0.50
1:E:160:GLN:NE2	6:E:514:HOH:O	2.30	0.49
1:E:182:PRO:HD2	1:E:246:PRO:HD2	1.94	0.49
1:A:284:ARG:NH1	6:A:657:HOH:O	2.37	0.49
1:C:336:ALA:HB1	1:C:343:ALA:HA	1.95	0.49
1:A:40:LYS:HE2	2:A:401:1VU:O12	2.12	0.48
1:C:338:LYS:NZ	6:C:753:HOH:O	2.46	0.48
1:B:40:LYS:NZ	6:B:748:HOH:O	2.38	0.48
1:D:192:LYS:HG3	1:F:264:PHE:CZ	2.49	0.48
1:E:38:VAL:HG12	1:E:40:LYS:HG2	1.95	0.48
1:A:29:ARG:HD3	1:A:335:ILE:HD13	1.94	0.48
1:D:265:LEU:HD21	1:E:202:PHE:HB2	1.95	0.48
1:A:264:PHE:CZ	1:B:192:LYS:HG3	2.49	0.48
1:A:316:MET:SD	2:B:401:1VU:H30	2.54	0.47
1:E:303:MET:HB2	1:E:322:TRP:HD1	1.79	0.47
1:A:180:LEU:O	1:A:182:PRO:HD3	2.15	0.47
2:A:401:1VU:H36	3:A:402:OXL:C2	2.45	0.47
2:E:401:1VU:H21	2:E:401:1VU:O2	2.15	0.47
1:E:196:VAL:HB	1:E:248:GLY:HA3	1.97	0.47
1:A:244:TYR:O	1:A:271:ALA:HA	2.14	0.46
1:A:192:LYS:HG3	1:C:264:PHE:CZ	2.51	0.46
1:F:81:ALA:HB2	6:F:604:HOH:O	2.15	0.46
1:C:309:VAL:HG23	1:C:316:MET:HE3	1.98	0.46
1:B:2:ARG:O	1:E:2:ARG:NH2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:O	1:B:182:PRO:HD3	2.16	0.46
2:B:401:1VU:O2	2:B:401:1VU:H21	2.15	0.46
1:B:264:PHE:CZ	1:C:192:LYS:HG3	2.51	0.45
1:D:44:ARG:NH1	6:D:761:HOH:O	2.30	0.45
1:E:260:PHE:HB3	1:E:285:VAL:HG11	1.99	0.45
2:E:401:1VU:H36	3:E:402:OXL:C2	2.47	0.45
1:A:239:GLY:HA2	6:A:718:HOH:O	2.17	0.44
1:B:244:TYR:O	1:B:271:ALA:HA	2.17	0.44
1:C:244:TYR:O	1:C:271:ALA:HA	2.17	0.44
1:D:118:VAL:HG22	1:D:151:LEU:HB2	1.99	0.44
1:C:182:PRO:HD2	1:C:246:PRO:HD2	1.99	0.44
1:B:69:GLU:CD	1:B:69:GLU:H	2.25	0.44
1:E:10:LYS:HB3	1:E:10:LYS:HE2	1.74	0.44
1:B:54:VAL:HG22	1:B:88:ALA:HB3	2.00	0.43
1:D:244:TYR:O	1:D:271:ALA:HA	2.18	0.43
1:A:6:HIS:HB2	6:A:753:HOH:O	2.18	0.43
1:D:264:PHE:CZ	1:E:192:LYS:HG3	2.53	0.43
1:F:204:GLY:HA2	1:F:221:GLN:HG2	1.99	0.43
1:E:264:PHE:CZ	1:F:192:LYS:HG3	2.53	0.43
1:E:54:VAL:HG22	1:E:88:ALA:HB3	2.01	0.43
1:E:244:TYR:O	1:E:271:ALA:HA	2.19	0.43
1:F:46:PRO:O	1:F:50:LYS:HG2	2.19	0.43
1:A:339:ASP:HB3	1:A:342:LEU:HD13	2.01	0.43
1:B:337:LYS:HD2	1:B:337:LYS:N	2.33	0.43
1:B:260:PHE:HB3	1:B:285:VAL:HG11	2.00	0.42
1:B:118:VAL:HG22	1:B:151:LEU:HB2	2.01	0.42
1:E:298:ARG:NH2	1:E:313:ASP:OD2	2.52	0.42
1:E:316:MET:HE1	2:F:401:1VU:N	2.14	0.42
1:F:244:TYR:O	1:F:271:ALA:HA	2.19	0.42
1:A:303:MET:HA	1:A:304:PRO:HD2	1.85	0.42
2:C:401:1VU:H36	3:C:402:OXL:C1	2.49	0.42
1:B:208:ASP:O	1:B:210:GLN:NE2	2.53	0.42
1:A:328:ILE:HD12	1:B:194:THR:HG23	2.02	0.42
1:B:339:ASP:HA	1:B:340:PRO:HD2	1.80	0.42
1:B:90:TRP:CD1	1:B:118:VAL:HB	2.55	0.41
1:D:311:MET:HE3	2:E:401:1VU:H16	2.02	0.41
1:F:2:ARG:N	6:F:719:HOH:O	2.52	0.41
1:D:54:VAL:HG22	1:D:88:ALA:HB3	2.02	0.41
1:A:90:TRP:CD1	1:A:118:VAL:HB	2.56	0.41
1:E:339:ASP:HA	1:E:340:PRO:HD2	1.91	0.41
1:C:35:PRO:HA	1:C:36:PRO:HD3	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:NH2	1:F:2:ARG:O	2.53	0.41
1:B:340:PRO:O	1:B:344:GLN:HG2	2.21	0.41
1:E:68:LYS:HG3	1:E:100:TRP:CE2	2.56	0.41
1:F:180:LEU:O	1:F:182:PRO:HD3	2.21	0.40
1:A:204:GLY:HA2	1:A:221:GLN:HG2	2.03	0.40
1:A:65:MET:HG3	6:C:839:HOH:O	2.21	0.40
1:C:68:LYS:HG3	1:C:100:TRP:CE2	2.57	0.40
1:B:334:MET:HG3	6:B:646:HOH: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:539:HOH:O	6:C:521:HOH:O[4_555]	1.85	0.35

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	343/348 (99%)	332 (97%)	10 (3%)	1 (0%)	36	35
1	B	346/348 (99%)	333 (96%)	13 (4%)	0	100	100
1	C	346/348 (99%)	334 (96%)	12 (4%)	0	100	100
1	D	341/348 (98%)	328 (96%)	13 (4%)	0	100	100
1	E	341/348 (98%)	329 (96%)	12 (4%)	0	100	100
1	F	345/348 (99%)	334 (97%)	10 (3%)	1 (0%)	36	35
All	All	2062/2088 (99%)	1990 (96%)	70 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	GLU
1	F	338	LYS

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	275/277 (99%)	271 (98%)	4 (2%)	57	64
1	B	277/277 (100%)	275 (99%)	2 (1%)	76	82
1	C	277/277 (100%)	274 (99%)	3 (1%)	65	73
1	D	275/277 (99%)	273 (99%)	2 (1%)	76	82
1	E	275/277 (99%)	273 (99%)	2 (1%)	76	82
1	F	276/277 (100%)	272 (99%)	4 (1%)	59	66
All	All	1655/1662 (100%)	1638 (99%)	17 (1%)	68	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	155	LEU
1	A	211	GLU
1	A	265	LEU
1	B	20	ILE
1	B	213	GLN
1	C	60	GLU
1	C	316	MET
1	C	348	LEU
1	D	315	LYS
1	D	348	LEU
1	E	155	LEU
1	E	265	LEU
1	F	155	LEU
1	F	215	GLU
1	F	265	LEU
1	F	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	220	GLN
1	C	7	ASN
1	C	135	GLN
1	C	317	GLN
1	D	7	ASN
1	E	135	GLN
1	E	160	GLN
1	F	220	GLN
1	F	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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	OXL	E	402	4	5,5,5	2.54	1 (20%)	6,6,6	1.95	2 (33%)
2	1VU	B	401	-	52,54,54	1.52	10 (19%)	73,80,80	1.97	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1VU	D	401	-	52,54,54	1.64	10 (19%)	73,80,80	1.74	13 (17%)
2	1VU	F	401	-	52,54,54	1.79	11 (21%)	73,80,80	1.71	15 (20%)
3	OXL	B	402	4	5,5,5	2.55	1 (20%)	6,6,6	1.95	2 (33%)
3	OXL	D	402	4	5,5,5	2.55	1 (20%)	6,6,6	1.94	2 (33%)
2	1VU	A	401	-	52,54,54	1.67	11 (21%)	73,80,80	1.90	16 (21%)
2	1VU	C	401	-	52,54,54	1.66	10 (19%)	73,80,80	1.75	13 (17%)
5	TRS	D	404	-	7,7,7	0.74	0	9,9,9	0.51	0
3	OXL	A	402	4	5,5,5	2.54	1 (20%)	6,6,6	1.95	2 (33%)
3	OXL	C	402	4	5,5,5	2.55	1 (20%)	6,6,6	1.94	2 (33%)
3	OXL	F	402	4	5,5,5	2.55	1 (20%)	6,6,6	1.95	2 (33%)
5	TRS	A	404	-	7,7,7	0.76	0	9,9,9	0.41	0
2	1VU	E	401	-	52,54,54	1.40	8 (15%)	73,80,80	1.99	18 (24%)

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	OXL	E	402	4	-	4/4/4/4	-
2	1VU	B	401	-	-	5/53/69/69	0/3/3/3
2	1VU	D	401	-	-	6/53/69/69	0/3/3/3
2	1VU	F	401	-	-	7/53/69/69	0/3/3/3
3	OXL	B	402	4	-	4/4/4/4	-
3	OXL	D	402	4	-	4/4/4/4	-
2	1VU	A	401	-	-	6/53/69/69	0/3/3/3
2	1VU	C	401	-	-	3/53/69/69	0/3/3/3
5	TRS	D	404	-	-	0/9/9/9	-
3	OXL	A	402	4	-	4/4/4/4	-
3	OXL	C	402	4	-	4/4/4/4	-
3	OXL	F	402	4	-	4/4/4/4	-
5	TRS	A	404	-	-	0/9/9/9	-
2	1VU	E	401	-	-	3/53/69/69	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	1VU	P-O7	-5.62	1.53	1.59
3	C	402	OXL	C2-C1	-4.77	1.46	1.54
3	D	402	OXL	C2-C1	-4.76	1.46	1.54
3	F	402	OXL	C2-C1	-4.76	1.46	1.54
2	A	401	1VU	P-O7	-4.76	1.54	1.59
3	B	402	OXL	C2-C1	-4.76	1.46	1.54
3	A	402	OXL	C2-C1	-4.74	1.46	1.54
3	E	402	OXL	C2-C1	-4.74	1.46	1.54
2	E	401	1VU	C2-S	-4.30	1.66	1.76
2	B	401	1VU	C17-N2	-4.10	1.30	1.37
2	D	401	1VU	C17-N2	-4.08	1.30	1.37
2	F	401	1VU	C18-N3	-4.00	1.31	1.39
2	D	401	1VU	C21-N2	-3.94	1.29	1.37
2	C	401	1VU	C18-N3	-3.93	1.31	1.39
2	A	401	1VU	C2-S	-3.85	1.67	1.76
2	A	401	1VU	C18-N3	-3.85	1.32	1.39
2	D	401	1VU	C2-S	-3.85	1.67	1.76
2	C	401	1VU	C17-N2	-3.72	1.31	1.37
2	D	401	1VU	C18-N3	-3.68	1.32	1.39
2	B	401	1VU	C21-N2	-3.67	1.30	1.37
2	F	401	1VU	C21-N2	-3.58	1.30	1.37
2	F	401	1VU	C2-S	-3.57	1.67	1.76
2	F	401	1VU	C17-N2	-3.55	1.31	1.37
2	C	401	1VU	C21-N2	-3.55	1.30	1.37
2	A	401	1VU	P1-O7	-3.38	1.55	1.59
2	E	401	1VU	C18-N3	-3.37	1.32	1.39
2	A	401	1VU	C17-N2	-3.31	1.31	1.37
2	C	401	1VU	O1-C5	-3.26	1.16	1.23
2	B	401	1VU	C18-N3	-3.25	1.33	1.39
2	A	401	1VU	O1-C5	-3.20	1.16	1.23
2	B	401	1VU	P1-O8	-3.16	1.40	1.55
2	C	401	1VU	P2-O14	-3.15	1.40	1.50
2	D	401	1VU	O1-C5	-3.13	1.17	1.23
2	A	401	1VU	C21-N2	-3.04	1.31	1.37
2	F	401	1VU	P1-O7	-2.91	1.56	1.59
2	C	401	1VU	O2-C8	-2.87	1.17	1.23
2	C	401	1VU	C2-S	-2.81	1.69	1.76
2	F	401	1VU	O1-C5	-2.73	1.17	1.23
2	C	401	1VU	P1-O8	-2.71	1.42	1.55
2	F	401	1VU	O2-C8	-2.70	1.18	1.23
2	E	401	1VU	P1-O9	2.67	1.60	1.50
2	C	401	1VU	P1-O7	-2.64	1.56	1.59
2	C	401	1VU	P-O5	-2.63	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	1VU	P2-O14	-2.61	1.42	1.50
2	E	401	1VU	C21-N2	-2.59	1.32	1.37
2	A	401	1VU	P1-O8	-2.59	1.43	1.55
2	B	401	1VU	O2-C8	-2.55	1.18	1.23
2	B	401	1VU	C2-S	-2.54	1.70	1.76
2	D	401	1VU	P1-O7	-2.54	1.56	1.59
2	D	401	1VU	P1-O8	-2.54	1.43	1.55
2	E	401	1VU	O1-C5	-2.48	1.18	1.23
2	D	401	1VU	O2-C8	-2.40	1.18	1.23
2	B	401	1VU	P2-O14	-2.37	1.43	1.50
2	E	401	1VU	C17-N2	-2.35	1.33	1.37
2	F	401	1VU	P1-O8	-2.34	1.44	1.55
2	A	401	1VU	P-O5	-2.34	1.42	1.50
2	D	401	1VU	P-O5	-2.30	1.42	1.50
2	F	401	1VU	C3-S	-2.25	1.72	1.81
2	E	401	1VU	P1-O8	-2.24	1.45	1.55
2	B	401	1VU	P-O5	-2.22	1.43	1.50
2	E	401	1VU	O2-C8	-2.16	1.19	1.23
2	B	401	1VU	O1-C5	-2.14	1.19	1.23
2	A	401	1VU	P2-O14	-2.10	1.43	1.50
2	B	401	1VU	P1-O9	2.08	1.58	1.50
2	D	401	1VU	C21-N6	-2.06	1.30	1.34
2	A	401	1VU	O2-C8	-2.03	1.19	1.23

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	1VU	C18-C21-N6	-6.60	117.63	126.72
2	F	401	1VU	C18-C21-N6	-6.06	118.37	126.72
2	C	401	1VU	C1-C2-S	6.00	121.13	113.56
2	B	401	1VU	C18-C21-N6	-5.94	118.54	126.72
2	A	401	1VU	C18-C21-N6	-5.91	118.58	126.72
2	B	401	1VU	C1-C2-S	5.87	120.97	113.56
2	B	401	1VU	N5-C20-N6	-5.64	120.04	128.58
2	A	401	1VU	C1-C2-S	5.41	120.39	113.56
2	C	401	1VU	C18-C21-N6	-5.35	119.35	126.72
2	C	401	1VU	O-C2-C1	-5.25	115.85	123.72
2	F	401	1VU	C1-C2-S	5.24	120.17	113.56
2	A	401	1VU	N5-C20-N6	-5.10	120.87	128.58
2	B	401	1VU	O-C2-C1	-5.04	116.18	123.72
2	E	401	1VU	N5-C20-N6	-4.96	121.07	128.58
2	D	401	1VU	C18-C21-N6	-4.96	119.88	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	1VU	C1-C2-S	4.75	119.56	113.56
2	E	401	1VU	N6-C21-N2	4.45	134.73	127.17
2	B	401	1VU	N2-C17-N3	-4.26	107.89	113.94
2	D	401	1VU	N5-C20-N6	-4.25	122.14	128.58
2	E	401	1VU	C20-N6-C21	4.16	121.99	111.83
2	D	401	1VU	C21-C18-N3	-4.07	105.93	110.58
2	B	401	1VU	C20-N6-C21	4.04	121.69	111.83
2	A	401	1VU	O-C2-C1	-3.97	117.77	123.72
2	E	401	1VU	N2-C17-N3	-3.91	108.39	113.94
2	D	401	1VU	N2-C17-N3	-3.89	108.42	113.94
2	A	401	1VU	N2-C17-N3	-3.89	108.42	113.94
2	A	401	1VU	C20-N6-C21	3.86	121.25	111.83
2	E	401	1VU	C1-C2-S	3.79	118.34	113.56
2	B	401	1VU	C21-C18-N3	-3.78	106.26	110.58
2	F	401	1VU	C21-C18-N3	-3.73	106.32	110.58
2	B	401	1VU	N6-C21-N2	3.73	133.51	127.17
2	A	401	1VU	N6-C21-N2	3.73	133.50	127.17
2	F	401	1VU	O-C2-C1	-3.69	118.19	123.72
2	B	401	1VU	C21-N2-C17	3.68	109.60	105.74
2	B	401	1VU	C4-N-C5	3.65	129.62	122.82
2	C	401	1VU	N6-C21-N2	3.64	133.35	127.17
2	F	401	1VU	N6-C21-N2	3.52	133.16	127.17
2	A	401	1VU	C21-C18-N3	-3.51	106.57	110.58
2	D	401	1VU	O-C2-C1	-3.41	118.61	123.72
2	D	401	1VU	C20-N6-C21	3.28	119.84	111.83
2	D	401	1VU	C18-N3-C17	3.26	108.57	103.45
2	C	401	1VU	O7-P1-O9	-3.26	100.91	110.70
2	F	401	1VU	C20-N6-C21	3.25	119.77	111.83
2	F	401	1VU	N5-C20-N6	-3.24	123.68	128.58
2	D	401	1VU	C21-N2-C17	3.22	109.12	105.74
3	F	402	OXL	O4-C2-C1	3.20	119.04	112.83
3	A	402	OXL	O3-C1-C2	3.20	119.03	112.83
3	E	402	OXL	O4-C2-C1	3.19	119.03	112.83
3	B	402	OXL	O4-C2-C1	3.19	119.01	112.83
3	C	402	OXL	O4-C2-C1	3.18	119.00	112.83
3	D	402	OXL	O4-C2-C1	3.18	119.00	112.83
3	B	402	OXL	O3-C1-C2	3.18	119.00	112.83
3	C	402	OXL	O3-C1-C2	3.17	118.98	112.83
3	D	402	OXL	O3-C1-C2	3.17	118.98	112.83
3	F	402	OXL	O3-C1-C2	3.17	118.98	112.83
3	E	402	OXL	O3-C1-C2	3.17	118.98	112.83
3	A	402	OXL	O4-C2-C1	3.16	118.96	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	1VU	C18-N3-C17	3.16	108.41	103.45
2	C	401	1VU	N2-C17-N3	-3.13	109.50	113.94
2	F	401	1VU	N2-C17-N3	-3.09	109.55	113.94
2	B	401	1VU	C18-N3-C17	3.08	108.30	103.45
2	E	401	1VU	C18-N3-C17	3.07	108.28	103.45
2	C	401	1VU	C21-C18-N3	-3.07	107.07	110.58
2	E	401	1VU	O15-P2-O13	3.02	117.61	105.85
2	E	401	1VU	C21-C18-N3	-3.00	107.15	110.58
2	C	401	1VU	N5-C20-N6	-2.99	124.05	128.58
2	D	401	1VU	O6-P-O7	2.99	115.35	107.27
2	E	401	1VU	P2-O13-C23	-2.95	115.54	123.43
2	D	401	1VU	N6-C21-N2	2.93	132.16	127.17
2	D	401	1VU	C7-N1-C8	2.91	127.77	122.55
2	E	401	1VU	O6-P-O7	2.87	115.04	107.27
2	F	401	1VU	C18-N3-C17	2.82	107.89	103.45
2	A	401	1VU	P2-O13-C23	2.81	130.94	123.43
2	A	401	1VU	C21-N2-C17	2.81	108.69	105.74
2	E	401	1VU	C23-C22-C16	2.74	105.92	99.89
2	E	401	1VU	C21-N2-C17	2.66	108.53	105.74
2	C	401	1VU	C18-N3-C17	2.65	107.61	103.45
2	C	401	1VU	C21-N2-C17	2.65	108.52	105.74
2	F	401	1VU	C3-S-C2	2.57	109.44	101.84
2	E	401	1VU	C3-S-C2	2.52	109.28	101.84
2	C	401	1VU	C20-N6-C21	2.51	117.97	111.83
2	C	401	1VU	C19-C18-C21	2.46	120.54	117.18
2	E	401	1VU	O-C2-S	-2.46	119.55	122.68
2	F	401	1VU	C12-C10-C9	2.46	112.96	108.77
2	C	401	1VU	O7-P-O5	2.46	118.09	110.70
2	F	401	1VU	C18-C21-N2	2.43	108.46	105.81
2	E	401	1VU	O4-P-O5	2.36	118.28	108.94
2	A	401	1VU	C12-C10-C9	2.33	112.75	108.77
2	A	401	1VU	C7-N1-C8	2.27	126.63	122.55
2	D	401	1VU	C12-C10-C9	2.27	112.64	108.77
2	A	401	1VU	C11-C10-C9	-2.25	104.93	108.77
2	E	401	1VU	C7-C6-C5	-2.20	108.73	112.39
2	A	401	1VU	O15-P2-O13	2.15	114.22	105.85
2	A	401	1VU	C11-C10-C13	2.08	111.66	108.22
2	F	401	1VU	O7-P1-O9	-2.08	104.45	110.70
2	E	401	1VU	C7-N1-C8	2.06	126.25	122.55
2	F	401	1VU	C19-C18-C21	2.04	119.96	117.18
2	B	401	1VU	C6-C5-N	-2.02	112.66	116.34
2	F	401	1VU	C3-C4-N	-2.02	108.19	112.41

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	1VU	C14-O10-P1-O7
2	A	401	1VU	C-C1-C2-S
2	A	401	1VU	C-C1-C2-O
2	B	401	1VU	C13-O4-P-O5
2	B	401	1VU	C-C1-C2-S
2	B	401	1VU	C-C1-C2-O
2	C	401	1VU	C14-O10-P1-O9
2	C	401	1VU	C-C1-C2-S
2	C	401	1VU	C-C1-C2-O
2	D	401	1VU	C14-O10-P1-O8
2	D	401	1VU	C14-O10-P1-O7
2	D	401	1VU	C-C1-C2-S
2	D	401	1VU	C-C1-C2-O
2	E	401	1VU	C-C1-C2-S
2	E	401	1VU	C-C1-C2-O
2	F	401	1VU	C14-O10-P1-O7
2	F	401	1VU	C-C1-C2-S
2	F	401	1VU	C-C1-C2-O
3	B	402	OXL	O1-C1-C2-O2
3	B	402	OXL	O3-C1-C2-O4
3	B	402	OXL	O1-C1-C2-O4
3	B	402	OXL	O3-C1-C2-O2
3	D	402	OXL	O1-C1-C2-O2
3	E	402	OXL	O1-C1-C2-O2
3	D	402	OXL	O3-C1-C2-O4
3	E	402	OXL	O3-C1-C2-O4
3	D	402	OXL	O1-C1-C2-O4
3	D	402	OXL	O3-C1-C2-O2
2	E	401	1VU	C23-O13-P2-O14
3	E	402	OXL	O1-C1-C2-O4
3	E	402	OXL	O3-C1-C2-O2
2	A	401	1VU	C22-C16-N2-C17
3	A	402	OXL	O3-C1-C2-O4
3	C	402	OXL	O3-C1-C2-O4
3	F	402	OXL	O3-C1-C2-O4
2	B	401	1VU	C12-C10-C13-O4
3	F	402	OXL	O1-C1-C2-O2
2	A	401	1VU	C14-O10-P1-O9
2	F	401	1VU	C14-O10-P1-O9
3	A	402	OXL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	402	OXL	O1-C1-C2-O2
2	F	401	1VU	O1-C5-N-C4
3	F	402	OXL	O1-C1-C2-O4
3	F	402	OXL	O3-C1-C2-O2
2	A	401	1VU	O11-C16-N2-C17
3	A	402	OXL	O1-C1-C2-O4
3	A	402	OXL	O3-C1-C2-O2
3	C	402	OXL	O1-C1-C2-O4
3	C	402	OXL	O3-C1-C2-O2
2	D	401	1VU	O10-C14-C15-O11
2	F	401	1VU	C6-C5-N-C4
2	B	401	1VU	C11-C10-C13-O4
2	D	401	1VU	P-O7-P1-O8
2	F	401	1VU	P-O7-P1-O8

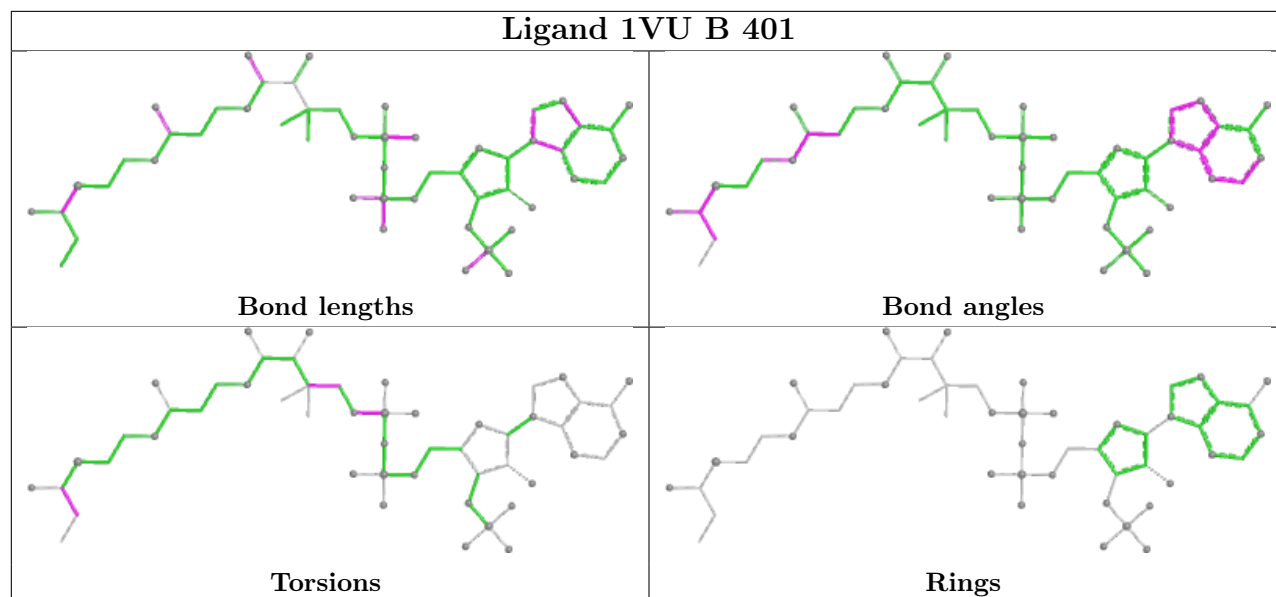
There are no ring outliers.

10 monomers are involved in 23 short contacts:

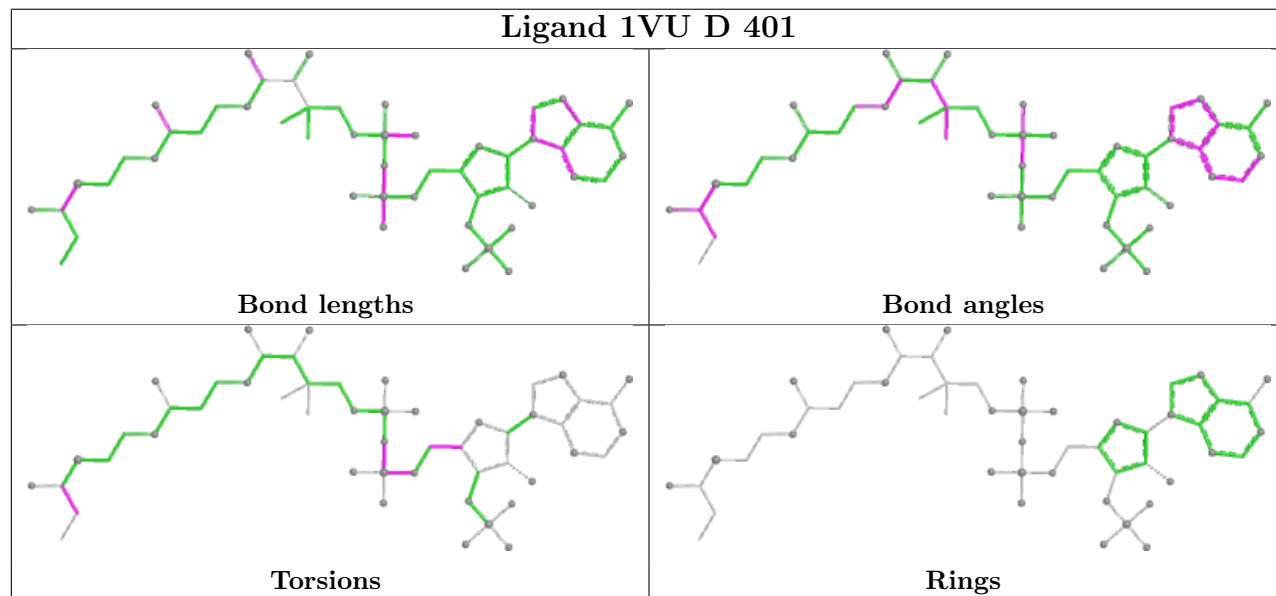
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	OXL	1	0
2	B	401	1VU	5	0
2	D	401	1VU	2	0
2	F	401	1VU	2	0
3	B	402	OXL	2	0
2	A	401	1VU	5	0
2	C	401	1VU	3	0
3	A	402	OXL	1	0
3	C	402	OXL	1	0
2	E	401	1VU	6	0

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

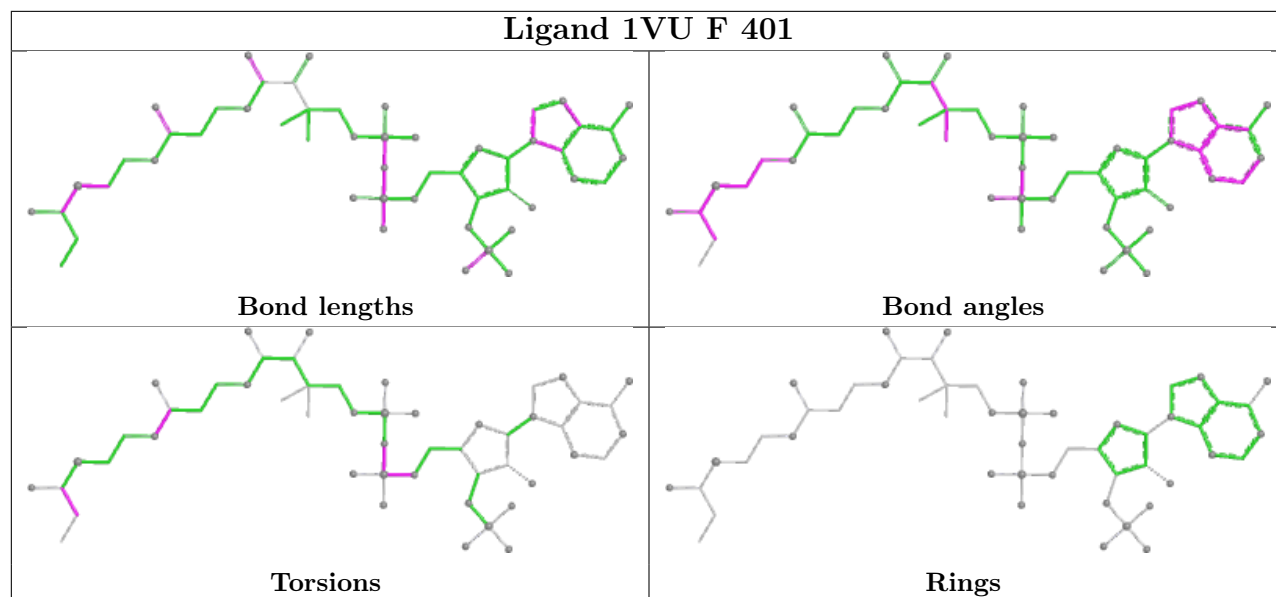
Ligand 1VU B 401



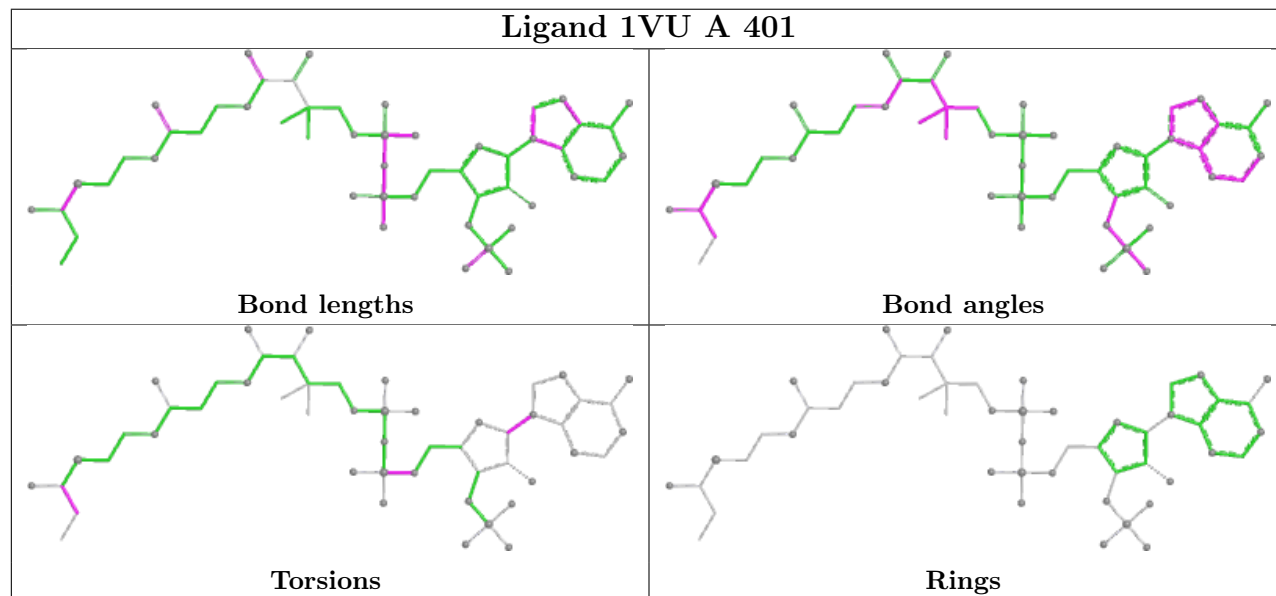
Ligand 1VU D 401

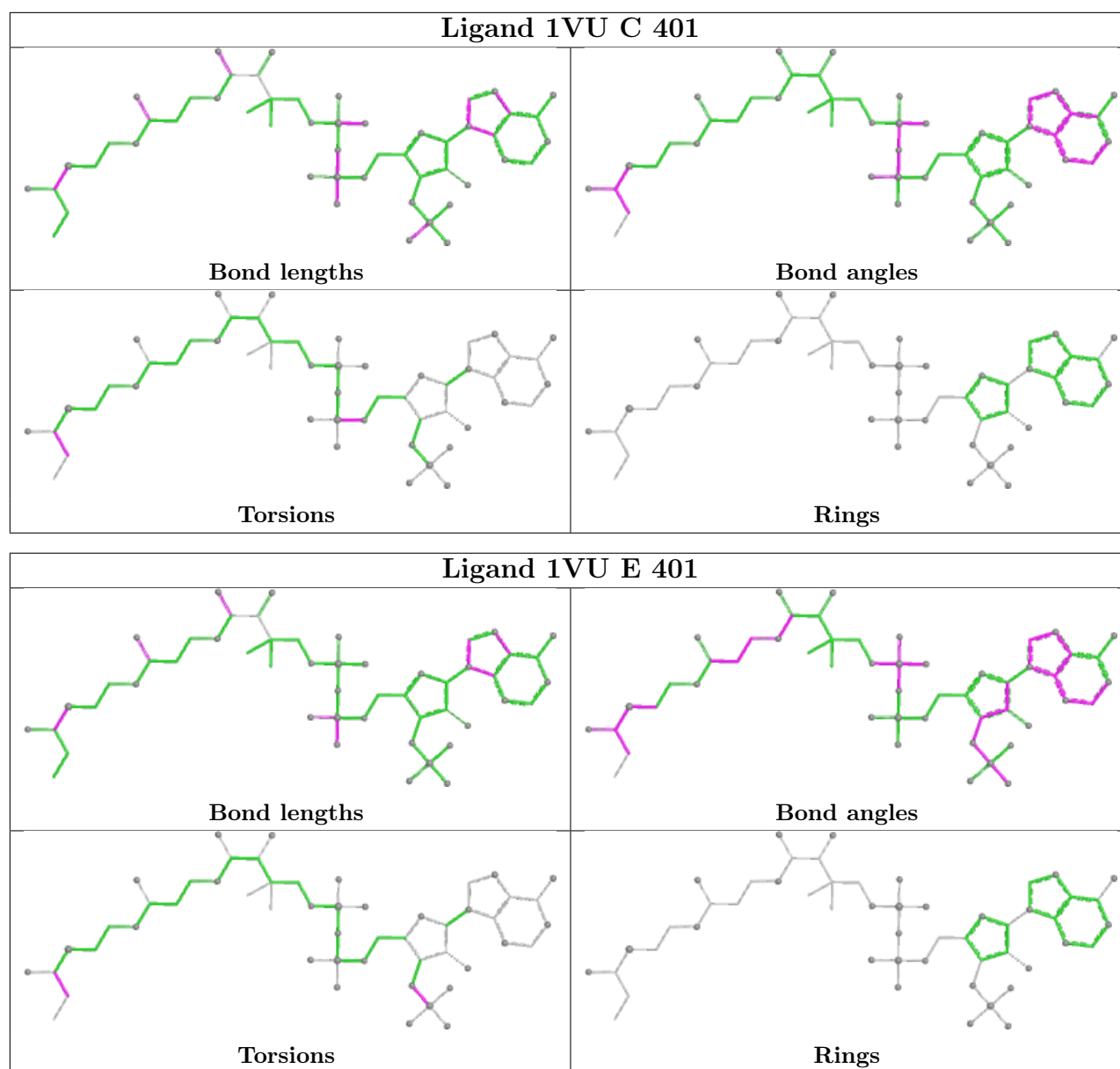


Ligand 1VU F 401



Ligand 1VU A 401





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	345/348 (99%)	-0.16	11 (3%)	50	49	13, 22, 52, 84	0
1	B	347/348 (99%)	-0.14	4 (1%)	76	76	13, 26, 46, 87	1 (0%)
1	C	347/348 (99%)	-0.29	10 (2%)	53	52	11, 20, 51, 71	1 (0%)
1	D	344/348 (98%)	-0.11	8 (2%)	61	60	12, 25, 50, 68	1 (0%)
1	E	344/348 (98%)	-0.16	7 (2%)	65	64	12, 24, 47, 73	1 (0%)
1	F	347/348 (99%)	-0.01	7 (2%)	65	64	15, 27, 51, 66	0
All	All	2074/2088 (99%)	-0.15	47 (2%)	61	60	11, 24, 50, 87	4 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	4.8
1	C	348	LEU	4.2
1	B	214	ALA	4.1
1	A	343	ALA	3.6
1	A	212	GLY	3.6
1	E	343	ALA	3.5
1	E	345	ALA	3.4
1	E	214	ALA	3.4
1	D	314	GLY	3.3
1	F	343	ALA	3.2
1	A	346	TYR	3.1
1	A	214	ALA	3.1
1	C	347	GLY	3.0
1	A	340	PRO	3.0
1	A	342	LEU	3.0
1	A	341	ASP	2.8
1	E	339	ASP	2.8
1	D	214	ALA	2.7
1	F	347	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	2.6
1	C	211	GLU	2.5
1	F	314	GLY	2.5
1	C	312	ILE	2.5
1	F	312	ILE	2.5
1	D	315	LYS	2.4
1	F	340	PRO	2.4
1	B	334	MET	2.3
1	F	310	ALA	2.3
1	C	291	ASN	2.3
1	D	347	GLY	2.3
1	B	210	GLN	2.3
1	E	342	LEU	2.3
1	E	344	GLN	2.3
1	D	348	LEU	2.3
1	E	340	PRO	2.2
1	C	339	ASP	2.2
1	F	313	ASP	2.2
1	A	314	GLY	2.2
1	C	314	GLY	2.2
1	C	310	ALA	2.2
1	D	343	ALA	2.1
1	C	346	TYR	2.1
1	A	202	PHE	2.1
1	D	312	ILE	2.1
1	A	6	HIS	2.1
1	C	290	VAL	2.1
1	D	344	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

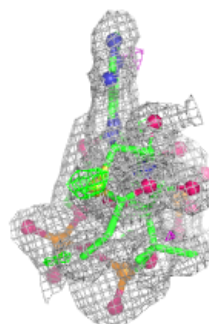
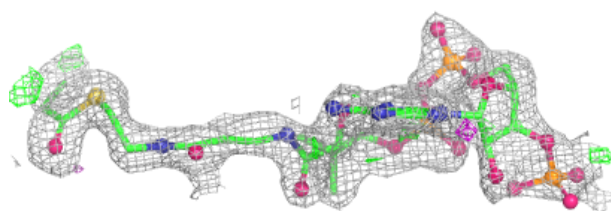
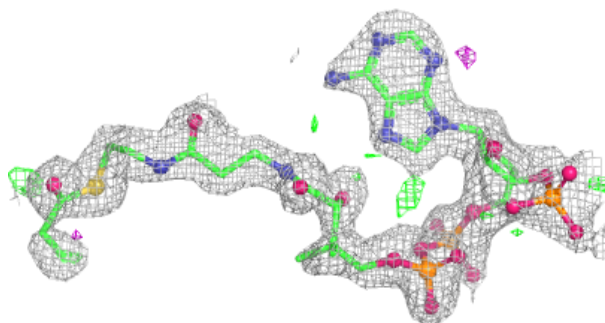
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1VU	E	401	52/52	0.84	0.12	19,40,61,72	52
2	1VU	B	401	52/52	0.89	0.10	26,37,53,55	52
2	1VU	F	401	52/52	0.89	0.10	23,38,55,63	52
2	1VU	A	401	52/52	0.90	0.10	21,36,48,55	52
2	1VU	D	401	52/52	0.90	0.10	26,39,60,65	0
2	1VU	C	401	52/52	0.93	0.08	16,26,45,49	0
3	OXL	A	402	6/6	0.93	0.08	19,22,24,30	0
3	OXL	B	402	6/6	0.93	0.10	22,23,28,36	0
3	OXL	F	402	6/6	0.94	0.08	18,20,27,28	0
3	OXL	E	402	6/6	0.95	0.07	19,22,26,27	6
3	OXL	D	402	6/6	0.95	0.08	22,22,27,31	0
4	MG	F	403	1/1	0.95	0.05	24,24,24,24	0
3	OXL	C	402	6/6	0.96	0.07	16,18,24,28	0
4	MG	E	403	1/1	0.97	0.03	24,24,24,24	0
5	TRS	D	404	8/8	0.97	0.05	16,19,21,22	0
4	MG	D	403	1/1	0.98	0.03	24,24,24,24	0
4	MG	A	403	1/1	0.98	0.03	21,21,21,21	0
4	MG	B	403	1/1	0.98	0.04	26,26,26,26	0
5	TRS	A	404	8/8	0.98	0.04	14,16,17,17	0
4	MG	C	403	1/1	0.98	0.02	15,15,15,15	0

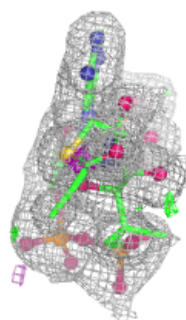
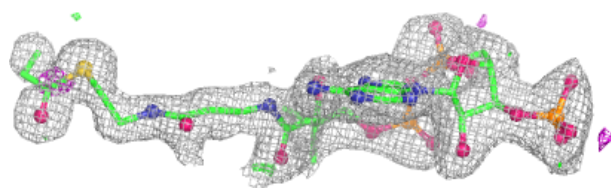
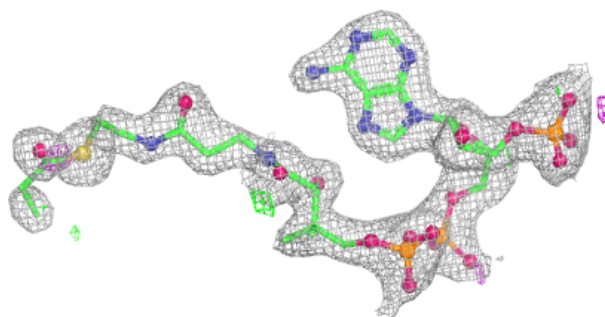
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1VU E 401:

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

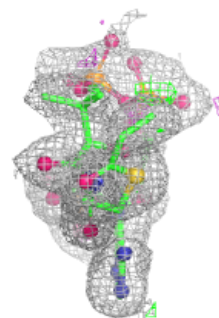
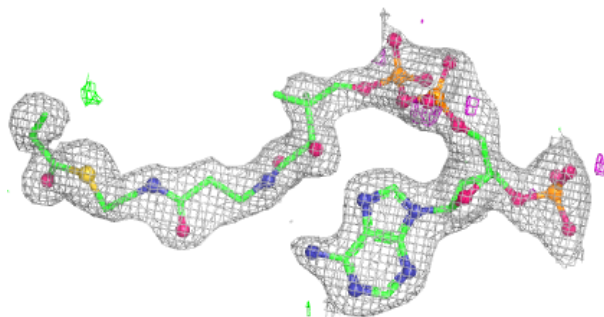
**Electron density around 1VU B 401:**

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

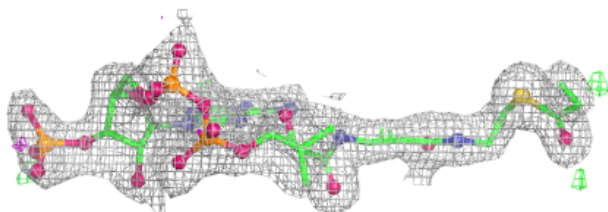
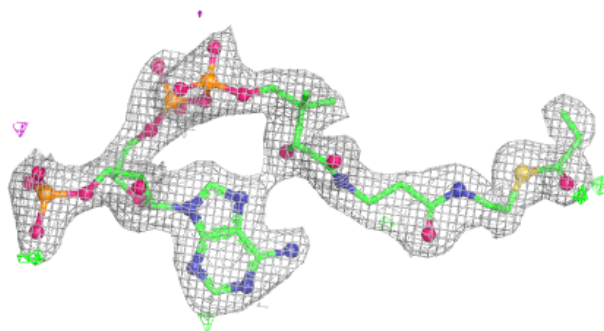


Electron density around 1VU F 401:

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

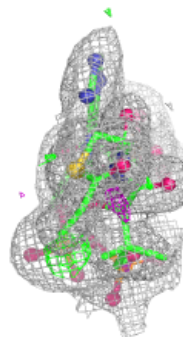
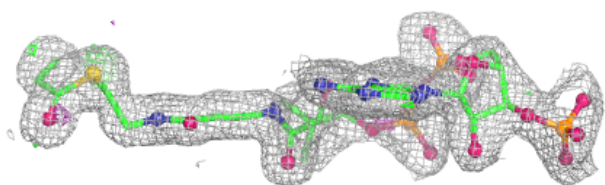
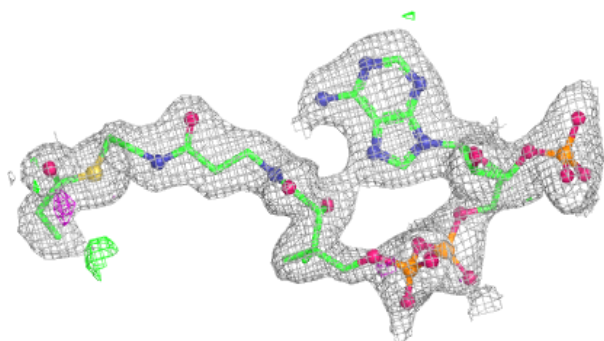
**Electron density around 1VU A 401:**

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

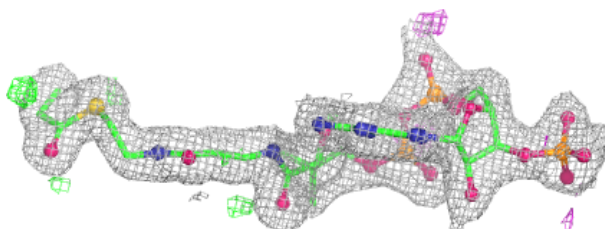
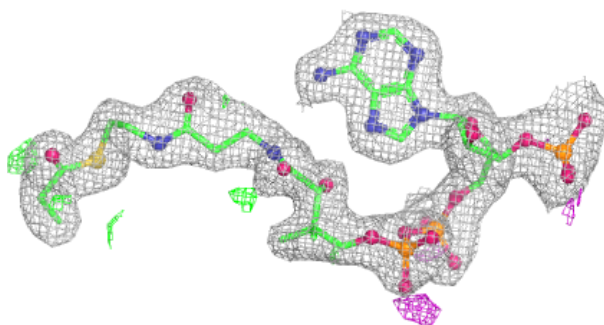


Electron density around 1VU D 401:

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

**Electron density around 1VU C 401:**

$2mF_o-DF_c$ (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.