



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:38 pm BST

PDB ID : 6KKH
Title : Crystal structure of the oxalate bound malyl-CoA lyase from *Roseiflexus castenholzii*
Authors : Tang, W.R.; Wang, Z.G.; Zhang, C.Y.; Wang, C.
Deposited on : 2019-07-25
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

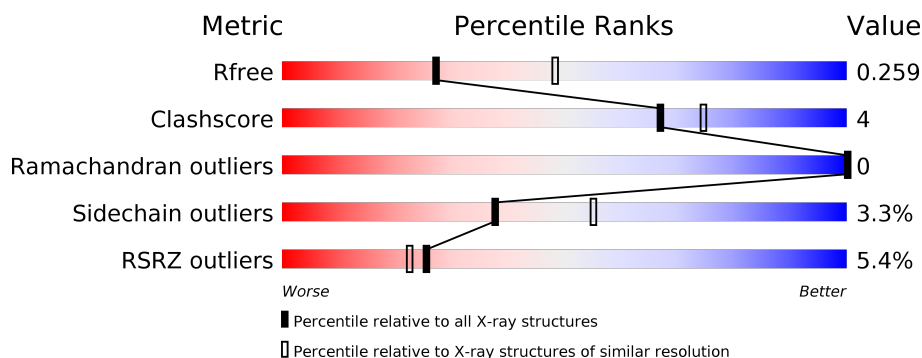
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div>3%</div> <div>82% 12% 5%</div> </div>
1	B	347	<div> <div>5%</div> <div>90% 8% ..</div> </div>
1	C	347	<div> <div>%</div> <div>93% 6% .</div> </div>
1	D	347	<div> <div>4%</div> <div>83% 12% 5%</div> </div>
1	E	347	<div> <div>%</div> <div>92% 8%</div> </div>
1	F	347	<div> <div>%</div> <div>92% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	347	
1	H	347	
1	I	347	
1	J	347	
1	K	347	
1	L	347	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	J	401	-	X	-	-

2 Entry composition

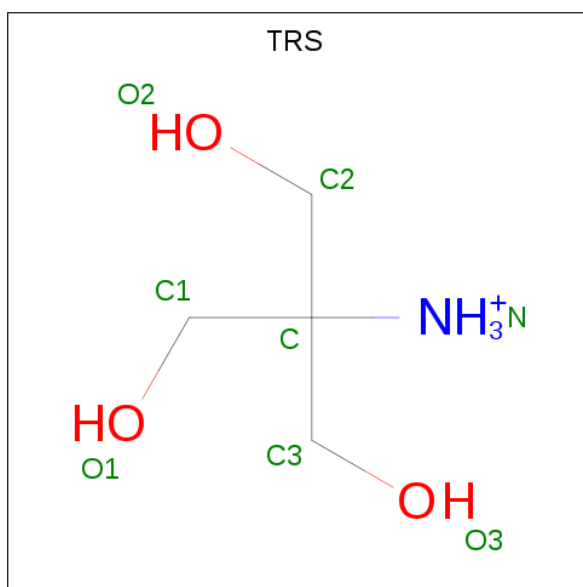
There are 5 unique types of molecules in this entry. The entry contains 31632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

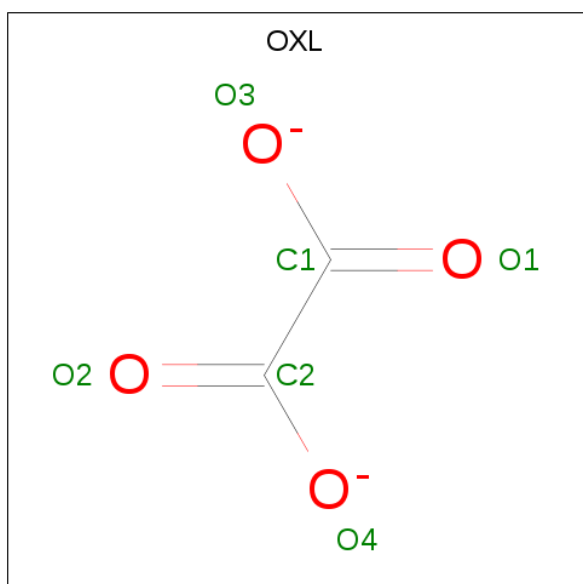
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2547	1640	444	449	14			
1	B	345	Total	C	N	O	S	0	0	0
			2679	1721	468	476	14			
1	C	343	Total	C	N	O	S	0	0	0
			2664	1714	464	471	15			
1	D	328	Total	C	N	O	S	0	0	0
			2555	1645	447	449	14			
1	E	347	Total	C	N	O	S	0	0	0
			2695	1732	470	478	15			
1	F	342	Total	C	N	O	S	0	0	0
			2655	1709	463	468	15			
1	G	325	Total	C	N	O	S	0	0	0
			2514	1615	442	444	13			
1	H	316	Total	C	N	O	S	0	0	0
			2435	1562	427	433	13			
1	I	345	Total	C	N	O	S	0	0	0
			2675	1718	466	476	15			
1	J	346	Total	C	N	O	S	0	0	0
			2692	1730	470	477	15			
1	K	327	Total	C	N	O	S	0	0	0
			2536	1629	445	448	14			
1	L	342	Total	C	N	O	S	0	0	0
			2655	1709	463	468	15			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	I	1	Total C O 6 2 4	0	0
3	L	1	Total C O 6 2 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	42	Total O 42 42	0	0
5	C	49	Total O 49 49	0	0
5	D	30	Total O 30 30	0	0
5	E	29	Total O 29 29	0	0
5	F	23	Total O 23 23	0	0
5	G	4	Total O 4 4	0	0
5	H	25	Total O 25 25	0	0
5	I	8	Total O 8 8	0	0
5	J	5	Total O 5 5	0	0
5	K	4	Total O 4 4	0	0

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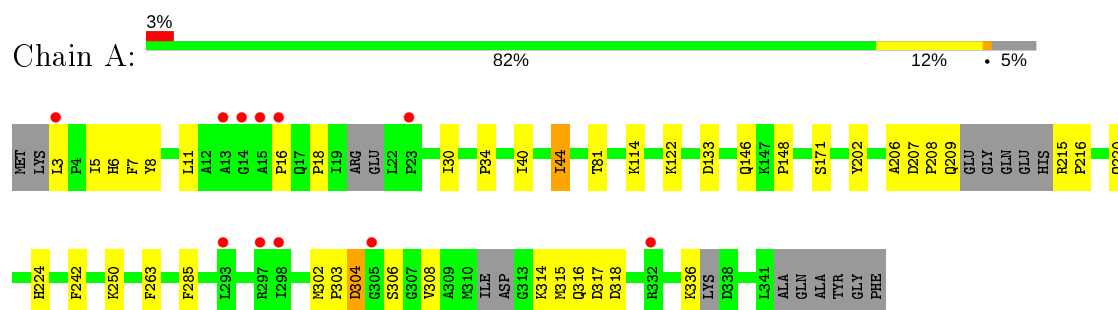
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	22	Total	O	0	0
			22	22		

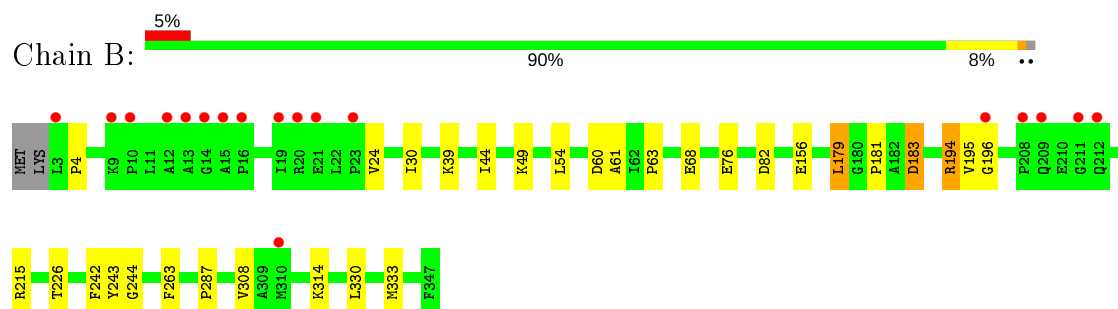
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

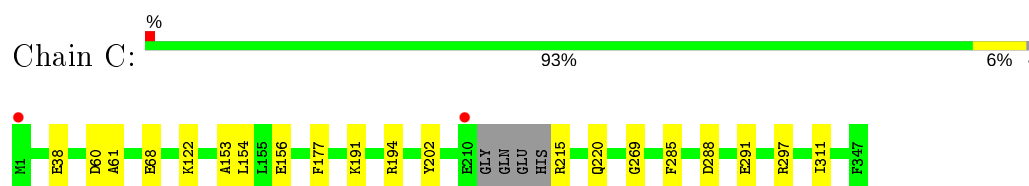
- Molecule 1: HpCh/HpaI aldolase



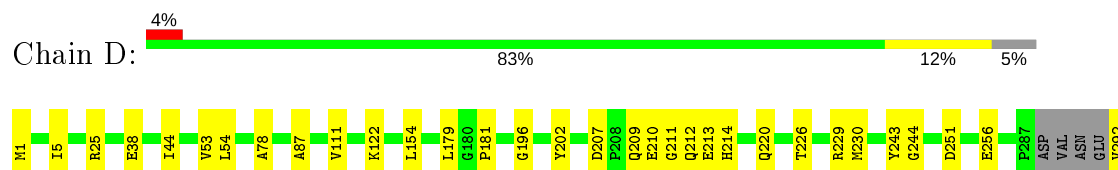
- Molecule 1: HpCh/HpaI aldolase



- Molecule 1: HpCh/HpaI aldolase

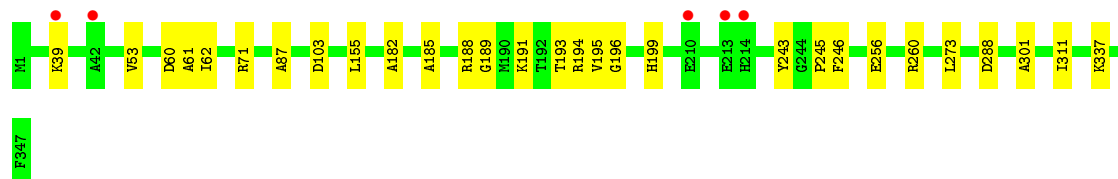
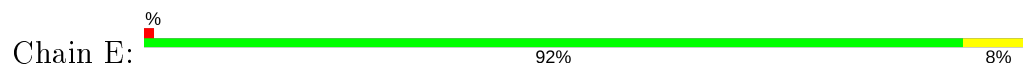


- Molecule 1: HpCh/HpaI aldolase

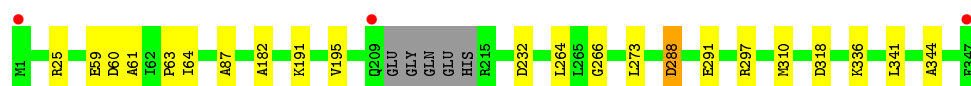




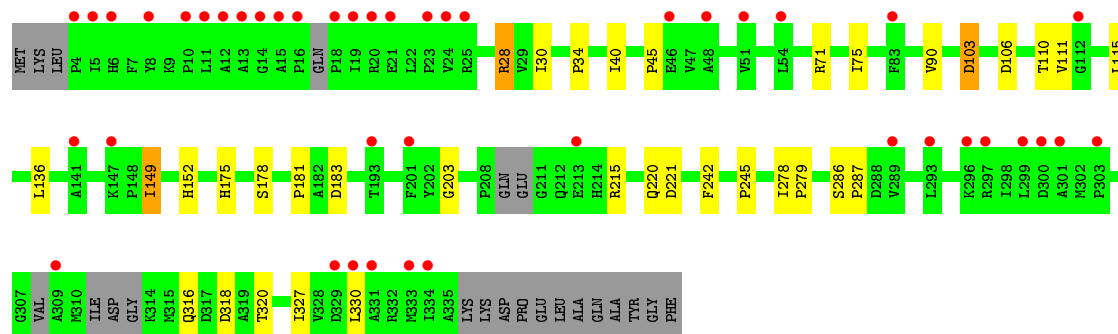
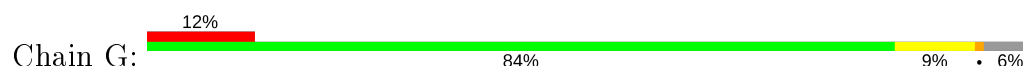
- Molecule 1: HpcH/HpaI aldolase



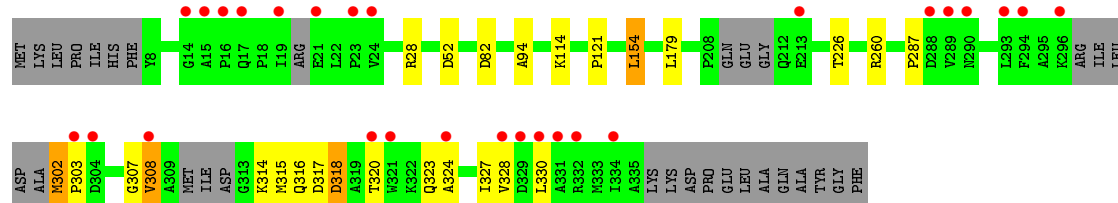
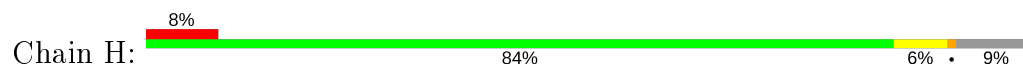
- Molecule 1: HpcH/HpaI aldolase



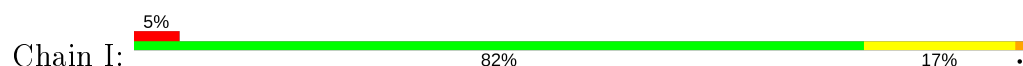
- Molecule 1: HpcH/HpaI aldolase

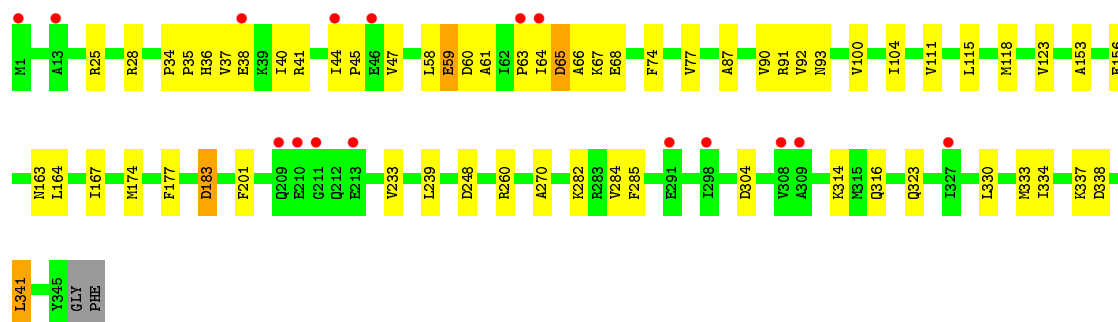


- Molecule 1: HpcH/HpaI aldolase

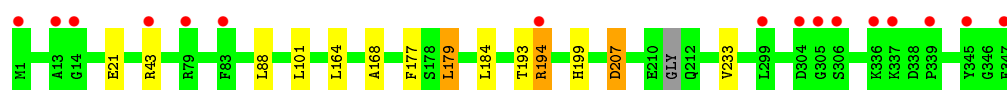


- Molecule 1: HpcH/HpaI aldolase

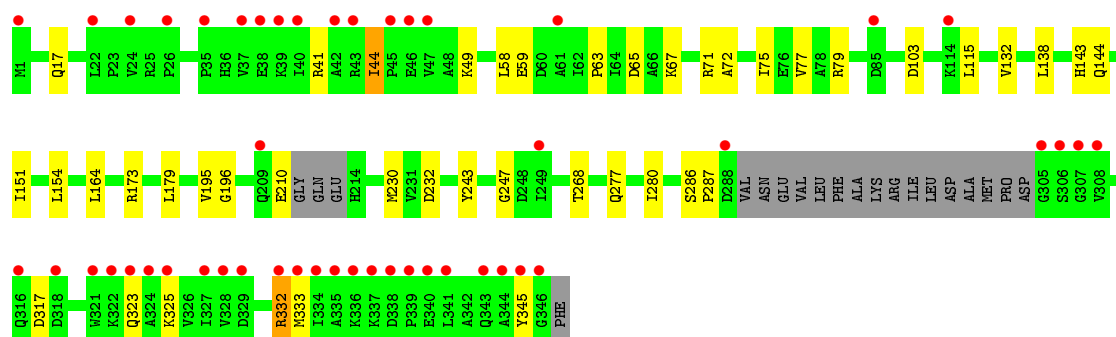
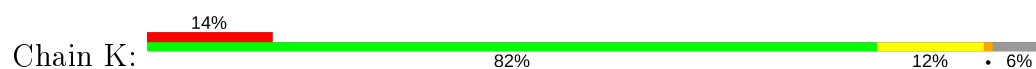




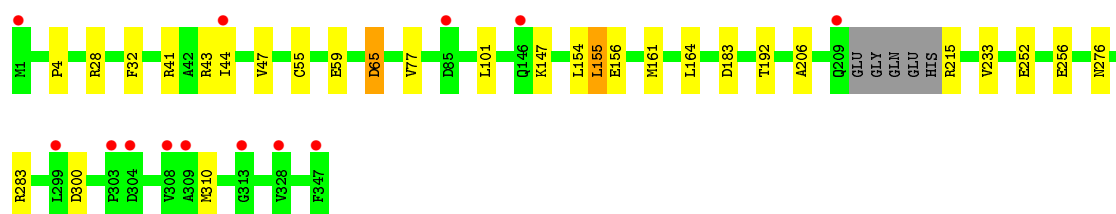
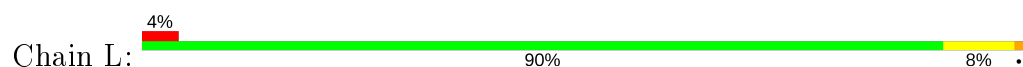
- Molecule 1: HpcH/HpaI aldolase



- Molecule 1: HpcH/HpaI aldolase



- Molecule 1: HpcH/HpaI aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.90Å 156.65Å 155.09Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	49.48 – 2.64 49.44 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.48-2.64) 98.8 (49.44-2.64)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.199 , 0.260 0.203 , 0.259	Depositor DCC
R_{free} test set	6782 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31632	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: OXL, TRS, MG

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	0.45	0/2610	0.59	0/3546
1	B	0.38	0/2749	0.55	0/3738
1	C	0.42	0/2732	0.56	0/3712
1	D	0.35	0/2621	0.54	0/3560
1	E	0.36	0/2765	0.53	0/3757
1	F	0.32	0/2723	0.50	0/3700
1	G	0.32	0/2577	0.51	0/3500
1	H	0.35	0/2494	0.53	0/3388
1	I	0.37	0/2744	0.54	0/3731
1	J	0.32	0/2761	0.49	0/3751
1	K	0.33	0/2601	0.51	0/3533
1	L	0.35	0/2723	0.52	0/3700
All	All	0.36	0/32100	0.53	0/43616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2547	0	2552	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2679	0	2672	21	0
1	C	2664	0	2672	10	0
1	D	2555	0	2559	33	0
1	E	2695	0	2695	16	0
1	F	2655	0	2666	16	0
1	G	2514	0	2499	17	0
1	H	2435	0	2425	26	0
1	I	2675	0	2674	55	0
1	J	2692	0	2693	7	0
1	K	2536	0	2537	24	0
1	L	2655	0	2666	13	0
2	A	8	0	12	2	0
2	B	8	0	12	0	0
2	G	8	0	12	1	0
2	J	8	0	12	0	0
3	C	6	0	0	1	0
3	F	6	0	0	1	0
3	I	6	0	0	0	0
3	L	6	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
5	A	31	0	0	0	0
5	B	42	0	0	0	0
5	C	49	0	0	0	0
5	D	30	0	0	2	0
5	E	29	0	0	0	0
5	F	23	0	0	1	0
5	G	4	0	0	0	0
5	H	25	0	0	0	0
5	I	8	0	0	0	0
5	J	5	0	0	0	0
5	K	4	0	0	0	0
5	L	22	0	0	0	0
All	All	31632	0	31358	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (247) 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:D:210:GLU:HG3	1:D:211:GLY:N	1.36	1.17
1:D:210:GLU:CG	1:D:211:GLY:H	1.57	1.10
1:D:210:GLU:CG	1:D:211:GLY:N	2.17	1.00
1:D:209:GLN:O	1:D:210:GLU:HG2	1.61	1.00
1:A:8:TYR:O	1:A:18:PRO:HG2	1.63	0.99
1:L:155:LEU:HD11	1:L:161:MET:SD	2.09	0.93
1:H:315:MET:C	1:H:316:GLN:OE1	2.09	0.90
1:D:210:GLU:HG3	1:D:211:GLY:H	0.73	0.88
1:I:44:ILE:HG21	1:I:77:VAL:CG1	2.04	0.88
1:H:316:GLN:N	1:H:316:GLN:OE1	2.08	0.87
1:I:44:ILE:HG22	1:I:45:PRO:HD3	1.57	0.86
1:A:306:SER:OG	1:F:64:ILE:HG13	1.75	0.85
1:K:173:ARG:HH11	1:K:173:ARG:HG2	1.42	0.84
1:I:63:PRO:HG2	1:I:66:ALA:HB3	1.60	0.81
1:I:63:PRO:HG2	1:I:66:ALA:CB	2.10	0.80
1:H:260:ARG:HD3	1:I:201:PHE:HB3	1.63	0.78
1:A:306:SER:HB3	1:F:63:PRO:HA	1.67	0.76
1:B:181:PRO:HB2	1:B:196:GLY:HA2	1.68	0.75
1:A:81:THR:O	1:A:114:LYS:NZ	2.20	0.74
1:E:193:THR:O	1:E:194:ARG:HD3	1.87	0.74
1:H:260:ARG:CD	1:I:201:PHE:HB3	2.18	0.73
1:K:173:ARG:HH11	1:K:173:ARG:CG	2.03	0.71
1:I:37:VAL:HG12	1:I:40:ILE:H	1.56	0.70
1:I:44:ILE:HG21	1:I:77:VAL:HG11	1.75	0.69
1:I:44:ILE:HG21	1:I:77:VAL:HG13	1.73	0.69
1:L:155:LEU:CD1	1:L:161:MET:SD	2.81	0.68
1:I:59:GLU:HB3	1:I:93:ASN:HA	1.74	0.68
1:I:65:ASP:OD1	1:I:65:ASP:N	2.27	0.67
1:I:163:ASN:O	1:I:167:ILE:HG13	1.94	0.67
1:K:277:GLN:HA	1:K:280:ILE:HD12	1.76	0.67
1:A:209:GLN:HG3	1:A:209:GLN:O	1.94	0.67
1:B:194:ARG:NE	1:B:194:ARG:HA	2.11	0.66
1:L:65:ASP:OD1	1:L:65:ASP:N	2.29	0.65
1:B:263:PHE:CZ	1:C:191:LYS:HG2	2.31	0.65
1:H:302:MET:HE1	1:H:317:ASP:HA	1.77	0.64
1:H:302:MET:HE2	1:H:317:ASP:C	2.17	0.64
1:H:307:GLY:O	1:I:61:ALA:HA	1.98	0.64
1:A:5:ILE:HD12	1:A:6:HIS:NE2	2.13	0.63
1:D:210:GLU:CG	1:D:212:GLN:H	2.12	0.62
1:D:230:MET:SD	5:D:429:HOH:O	2.56	0.62
1:D:209:GLN:O	1:D:210:GLU:CG	2.44	0.61
1:B:24:VAL:HG12	1:B:333:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ARG:HD3	1:F:232:ASP:OD1	2.01	0.61
1:B:215:ARG:HH22	1:D:251:ASP:CG	2.04	0.61
1:G:136:LEU:HD22	1:G:149:ILE:HD11	1.81	0.60
1:H:324:ALA:O	1:H:327:ILE:HG22	2.02	0.59
1:E:189:GLY:O	1:F:266:GLY:HA2	2.03	0.59
1:K:287:PRO:HD2	1:K:345:TYR:OH	2.01	0.59
1:B:194:ARG:CA	1:B:194:ARG:HE	2.17	0.58
1:I:34:PRO:HB2	1:I:36:HIS:CE1	2.39	0.58
1:K:75:ILE:HD13	1:K:79:ARG:NH2	2.18	0.57
1:A:3:LEU:O	1:A:7:PHE:HB2	2.05	0.57
1:H:260:ARG:HD2	1:I:201:PHE:O	2.04	0.57
1:D:78:ALA:HB3	1:D:111:VAL:HG11	1.87	0.56
1:L:164:LEU:HG	1:L:233:VAL:HG11	1.88	0.56
1:I:123:VAL:HG12	1:I:167:ILE:HD13	1.88	0.56
1:I:63:PRO:CG	1:I:66:ALA:HB3	2.33	0.55
1:F:182:ALA:HB3	3:F:401:OXL:O2	2.07	0.55
1:A:302:MET:CE	1:A:316:GLN:HB3	2.37	0.55
1:H:302:MET:CE	1:H:317:ASP:C	2.74	0.55
1:C:156:GLU:OE2	3:C:401:OXL:O1	2.25	0.55
1:I:37:VAL:HG11	1:I:40:ILE:HD12	1.89	0.54
1:I:44:ILE:CG2	1:I:45:PRO:HD3	2.35	0.54
1:K:58:LEU:O	1:K:67:LYS:NZ	2.32	0.54
1:B:44:ILE:HG23	1:B:54:LEU:HD21	1.89	0.54
1:A:302:MET:HE3	1:A:317:ASP:N	2.22	0.54
1:J:179:LEU:HD21	1:J:184:LEU:HD23	1.89	0.53
1:D:44:ILE:HG23	1:D:54:LEU:HD21	1.90	0.53
1:H:320:THR:HA	1:H:323:GLN:HE21	1.73	0.53
1:H:302:MET:HE2	1:H:317:ASP:O	2.09	0.53
1:I:25:ARG:CZ	1:I:87:ALA:HB2	2.39	0.53
1:H:318:ASP:OD1	1:H:318:ASP:N	2.43	0.52
1:A:206:ALA:HB3	1:A:216:PRO:HD2	1.92	0.52
1:G:90:VAL:HG12	1:G:115:LEU:HD11	1.92	0.52
1:H:28:ARG:HD3	1:H:52:ASP:OD2	2.08	0.52
1:J:207:ASP:OD2	1:J:207:ASP:N	2.43	0.52
1:B:63:PRO:HA	1:D:310:MET:HE3	1.92	0.52
1:I:63:PRO:HG2	1:I:66:ALA:HB2	1.91	0.52
1:D:230:MET:HB2	5:D:429:HOH:O	2.10	0.51
1:H:287:PRO:HD3	1:H:330:LEU:HD22	1.92	0.51
1:G:28:ARG:NH1	1:G:286:SER:OG	2.43	0.51
1:K:173:ARG:CG	1:K:173:ARG:NH1	2.70	0.51
1:A:34:PRO:HG2	1:A:40:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:VAL:O	1:I:111:VAL:HG22	2.11	0.51
1:D:229:ARG:HG3	1:D:229:ARG:HH11	1.76	0.50
1:A:206:ALA:O	1:A:215:ARG:HD2	2.11	0.50
1:B:181:PRO:CB	1:B:196:GLY:HA2	2.39	0.50
1:E:196:GLY:O	1:E:243:TYR:OH	2.28	0.50
1:F:60:ASP:O	1:F:61:ALA:HB3	2.12	0.50
1:E:193:THR:C	1:E:194:ARG:HD3	2.31	0.50
1:B:215:ARG:NH2	1:D:251:ASP:OD1	2.44	0.50
1:C:269:GLY:HA2	1:C:285:PHE:CG	2.47	0.50
1:H:327:ILE:HG23	1:H:328:VAL:N	2.26	0.50
1:E:185:ALA:O	1:E:188:ARG:O	2.30	0.50
1:H:327:ILE:CG2	1:H:328:VAL:N	2.75	0.49
1:H:302:MET:HE1	1:H:317:ASP:CA	2.43	0.49
1:I:92:VAL:HG11	1:I:118:MET:CE	2.43	0.49
1:K:71:ARG:NH1	1:K:103:ASP:OD1	2.45	0.49
1:A:302:MET:HE3	1:A:316:GLN:HB3	1.94	0.49
1:I:35:PRO:O	1:I:41:ARG:HD2	2.12	0.49
1:I:44:ILE:HD12	1:I:47:VAL:HG21	1.95	0.49
1:K:41:ARG:HB2	1:K:77:VAL:HG22	1.95	0.49
1:A:11:LEU:HD22	1:A:133:ASP:OD1	2.13	0.49
1:H:121:PRO:HA	1:H:154:LEU:HB2	1.95	0.49
1:D:196:GLY:O	1:D:243:TYR:OH	2.31	0.48
1:E:245:PRO:HB2	1:E:273:LEU:HD11	1.95	0.48
1:I:314:LYS:HE2	1:I:316:GLN:HE22	1.78	0.48
1:D:202:TYR:CE2	1:D:220:GLN:HB2	2.48	0.48
1:F:25:ARG:CZ	1:F:87:ALA:HB2	2.44	0.48
1:A:133:ASP:OD2	1:A:171:SER:OG	2.25	0.48
1:I:60:ASP:HB2	1:I:91:ARG:NH2	2.27	0.48
1:E:53:VAL:HG22	1:E:87:ALA:HB3	1.96	0.48
1:B:194:ARG:NE	1:B:194:ARG:CA	2.72	0.48
1:B:30:ILE:HD11	1:B:242:PHE:CD2	2.49	0.48
1:C:194:ARG:NH1	1:D:207:ASP:OD2	2.38	0.48
1:F:195:VAL:HG12	1:F:195:VAL:O	2.14	0.48
1:C:202:TYR:CE2	1:C:220:GLN:HB2	2.49	0.47
1:K:332:ARG:CG	1:K:332:ARG:HH11	2.26	0.47
1:K:332:ARG:HG2	1:K:332:ARG:HH11	1.78	0.47
1:E:191:LYS:HB2	1:F:264:LEU:HD23	1.96	0.47
1:I:28:ARG:HH22	1:I:282:LYS:HD2	1.78	0.47
1:I:44:ILE:HD12	1:I:47:VAL:CG2	2.44	0.47
1:I:153:ALA:HB3	1:I:177:PHE:CD1	2.49	0.47
1:C:297:ARG:NH2	1:C:311:ILE:HG23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:ILE:HB	1:G:279:PRO:HD3	1.96	0.47
1:I:164:LEU:HG	1:I:233:VAL:HG11	1.96	0.47
1:I:34:PRO:HD2	1:I:40:ILE:HD13	1.97	0.47
1:B:194:ARG:HA	1:B:194:ARG:HE	1.77	0.47
1:D:212:GLN:OE1	1:D:214:HIS:N	2.36	0.47
1:J:164:LEU:HG	1:J:233:VAL:HG11	1.97	0.47
1:J:101:LEU:HD11	1:K:138:LEU:HB3	1.97	0.47
1:D:310:MET:SD	1:D:310:MET:C	2.94	0.46
1:G:181:PRO:HD3	1:G:245:PRO:HD2	1.96	0.46
1:D:210:GLU:HG2	1:D:212:GLN:H	1.78	0.46
1:K:196:GLY:O	1:K:243:TYR:OH	2.33	0.46
1:B:156:GLU:HB3	1:B:183:ASP:HB3	1.98	0.46
1:A:314:LYS:O	1:A:316:GLN:NE2	2.49	0.46
1:E:301:ALA:CB	1:E:311:ILE:HD11	2.45	0.46
1:D:292:VAL:HG13	1:D:292:VAL:O	2.15	0.46
1:K:179:LEU:HB2	1:K:230:MET:HE1	1.98	0.46
1:A:224:HIS:CD2	2:A:401:TRS:H22	2.51	0.46
1:D:210:GLU:HG3	1:D:211:GLY:CA	2.36	0.46
1:G:71:ARG:HD3	1:G:103:ASP:HA	1.97	0.46
1:I:338:ASP:HB3	1:I:341:LEU:HD11	1.97	0.46
1:D:310:MET:HE2	1:D:313:GLY:HA2	1.97	0.46
1:H:260:ARG:HD3	1:I:201:PHE:CB	2.40	0.46
1:J:193:THR:HG23	1:J:199:HIS:CD2	2.51	0.46
1:B:60:ASP:O	1:B:61:ALA:HB3	2.16	0.45
1:L:256:GLU:OE2	1:L:283:ARG:NH1	2.48	0.45
1:I:330:LEU:O	1:I:334:ILE:HG12	2.16	0.45
1:B:179:LEU:O	1:B:244:GLY:HA3	2.16	0.45
1:D:210:GLU:HG3	1:D:212:GLN:H	1.80	0.45
1:B:194:ARG:HH21	1:B:195:VAL:H	1.63	0.45
1:A:308:VAL:CG2	1:F:61:ALA:O	2.65	0.45
1:D:202:TYR:CD2	1:D:220:GLN:HB2	2.52	0.45
1:K:164:LEU:HD21	1:K:230:MET:HA	1.99	0.45
1:B:287:PRO:HG3	1:B:330:LEU:HD23	1.97	0.45
1:K:41:ARG:HB2	1:K:77:VAL:CG2	2.46	0.45
1:I:90:VAL:HG12	1:I:115:LEU:HD11	1.99	0.45
1:I:100:VAL:O	1:I:104:ILE:HG13	2.17	0.45
1:A:208:PRO:HD2	1:A:208:PRO:O	2.17	0.45
1:B:196:GLY:O	1:B:243:TYR:OH	2.34	0.45
1:D:179:LEU:O	1:D:244:GLY:HA3	2.17	0.45
1:I:67:LYS:HD2	1:I:93:ASN:HD21	1.81	0.44
1:K:195:VAL:HB	1:K:247:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:ALA:O	1:I:177:PHE:HA	2.18	0.44
1:I:156:GLU:HB3	1:I:183:ASP:HB3	2.00	0.44
1:H:287:PRO:CD	1:H:330:LEU:HD22	2.48	0.44
1:E:71:ARG:HD3	1:E:103:ASP:HA	2.00	0.44
1:G:34:PRO:O	1:G:40:ILE:HD11	2.18	0.44
1:J:168:ALA:HB2	1:J:177:PHE:HZ	1.82	0.44
1:L:32:PHE:HA	1:L:55:CYS:O	2.18	0.44
1:A:304:ASP:OD1	1:A:304:ASP:N	2.48	0.44
1:D:179:LEU:O	1:D:181:PRO:HD3	2.18	0.43
1:I:34:PRO:HB2	1:I:36:HIS:HE1	1.83	0.43
1:L:156:GLU:OE1	1:L:183:ASP:OD2	2.36	0.43
1:L:41:ARG:HG3	1:L:77:VAL:CG2	2.48	0.43
1:I:92:VAL:HG11	1:I:118:MET:HE3	2.00	0.43
1:G:316:GLN:HE22	1:G:320:THR:HB	1.83	0.43
1:C:154:LEU:HG	1:C:156:GLU:HG3	1.99	0.43
1:F:341:LEU:HA	1:F:344:ALA:HB3	1.99	0.43
1:A:16:PRO:HB2	1:A:148:PRO:HD3	2.00	0.43
1:I:44:ILE:N	1:I:45:PRO:CD	2.81	0.43
1:A:30:ILE:HD11	1:A:242:PHE:CD2	2.54	0.43
1:A:224:HIS:CG	2:A:401:TRS:H22	2.53	0.43
1:G:110:THR:HG23	1:G:111:VAL:HG22	2.01	0.43
1:I:174:MET:HB3	1:I:239:LEU:HD21	2.01	0.43
1:K:75:ILE:HD13	1:K:79:ARG:HH21	1.83	0.43
1:D:315:MET:HG2	1:D:316:GLN:N	2.32	0.43
1:H:94:ALA:HA	1:H:121:PRO:HG2	2.01	0.43
1:I:58:LEU:HD12	1:I:92:VAL:HA	2.00	0.43
1:G:287:PRO:HG3	1:G:330:LEU:HD12	2.01	0.42
1:A:44:ILE:HD13	1:A:44:ILE:HA	1.83	0.42
1:D:210:GLU:HG3	1:D:212:GLN:N	2.34	0.42
1:I:334:ILE:HG22	1:I:341:LEU:HD13	2.01	0.42
1:K:132:VAL:HG12	1:K:151:ILE:HD11	2.02	0.42
1:C:60:ASP:O	1:C:61:ALA:HB3	2.19	0.42
1:A:263:PHE:CZ	1:F:191:LYS:HG2	2.55	0.42
1:D:25:ARG:CZ	1:D:87:ALA:HB2	2.49	0.42
1:A:202:TYR:CE2	1:A:220:GLN:HB2	2.54	0.42
1:G:152:HIS:HE2	1:G:178:SER:CB	2.32	0.42
1:G:30:ILE:HD11	1:G:242:PHE:CD2	2.54	0.42
1:G:221:ASP:O	2:G:401:TRS:O1	2.28	0.42
1:L:44:ILE:HA	1:L:47:VAL:HG22	2.01	0.42
1:A:114:LYS:CE	1:H:82:ASP:OD2	2.67	0.42
1:I:44:ILE:HD12	1:I:44:ILE:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:PRO:HA	1:L:310:MET:SD	2.60	0.42
1:A:16:PRO:HB3	1:A:146:GLN:O	2.19	0.42
1:A:30:ILE:HD11	1:A:242:PHE:CE2	2.55	0.42
1:F:297:ARG:HD3	5:F:505:HOH:O	2.20	0.42
1:J:194:ARG:HB3	1:J:194:ARG:HH11	1.84	0.42
1:C:122:LYS:N	1:C:156:GLU:OE1	2.52	0.42
1:B:179:LEU:HD11	1:B:226:THR:HG22	2.01	0.41
1:E:193:THR:HG23	1:E:199:HIS:CD2	2.55	0.41
1:A:315:MET:SD	1:F:273:LEU:HD13	2.61	0.41
1:G:75:ILE:HG23	1:G:110:THR:HG21	2.02	0.41
1:D:179:LEU:HD11	1:D:226:THR:CG2	2.50	0.41
1:G:203:GLY:HA2	1:G:220:GLN:HG2	2.02	0.41
1:H:330:LEU:O	1:H:330:LEU:HD23	2.20	0.41
1:I:44:ILE:HA	1:I:47:VAL:HG22	2.02	0.41
1:K:41:ARG:HA	1:K:44:ILE:HD13	2.01	0.41
1:A:263:PHE:CD1	1:A:285:PHE:HA	2.56	0.41
1:H:308:VAL:HG13	1:I:61:ALA:O	2.21	0.41
1:D:53:VAL:HG22	1:D:87:ALA:HB3	2.03	0.41
1:G:136:LEU:HD13	1:G:149:ILE:HD11	2.03	0.41
1:I:270:ALA:HB2	1:I:285:PHE:CE2	2.56	0.41
1:K:143:HIS:O	1:K:144:GLN:C	2.58	0.41
1:K:72:ALA:O	1:K:75:ILE:HG13	2.21	0.41
1:L:252:GLU:OE2	1:L:276:ASN:HB2	2.21	0.41
1:E:196:GLY:HA3	1:E:246:PHE:HA	2.02	0.41
1:G:152:HIS:ND1	1:G:175:HIS:HD2	2.18	0.41
1:E:62:ILE:O	1:F:310:MET:HE1	2.21	0.41
1:I:64:ILE:HA	1:I:67:LYS:HG2	2.01	0.41
1:I:44:ILE:CG2	1:I:77:VAL:HG13	2.45	0.41
1:L:101:LEU:HA	1:L:101:LEU:HD23	1.86	0.41
1:I:260:ARG:HA	1:I:284:VAL:HG21	2.02	0.41
1:I:63:PRO:CG	1:I:66:ALA:CB	2.93	0.41
1:I:74:PHE:CZ	1:I:90:VAL:HB	2.56	0.41
1:A:302:MET:CE	1:A:317:ASP:N	2.84	0.40
1:C:153:ALA:O	1:C:177:PHE:HA	2.20	0.40
1:L:206:ALA:O	1:L:215:ARG:HD2	2.21	0.40
1:B:24:VAL:HG12	1:B:333:MET:CE	2.49	0.40
1:E:182:ALA:HB2	1:E:195:VAL:HG13	2.04	0.40
1:E:60:ASP:O	1:E:61:ALA:HB3	2.21	0.40
1:H:179:LEU:HD11	1:H:226:THR:HG22	2.03	0.40
1:F:288:ASP:HB3	1:F:291:GLU:HB2	2.04	0.40
1:K:286:SER:HA	1:K:287:PRO:HD3	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/347 (92%)	308 (97%)	11 (3%)	0	100	100
1	B	343/347 (99%)	331 (96%)	12 (4%)	0	100	100
1	C	339/347 (98%)	329 (97%)	10 (3%)	0	100	100
1	D	322/347 (93%)	315 (98%)	7 (2%)	0	100	100
1	E	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
1	F	338/347 (97%)	325 (96%)	13 (4%)	0	100	100
1	G	315/347 (91%)	299 (95%)	16 (5%)	0	100	100
1	H	306/347 (88%)	295 (96%)	11 (4%)	0	100	100
1	I	343/347 (99%)	321 (94%)	22 (6%)	0	100	100
1	J	342/347 (99%)	331 (97%)	11 (3%)	0	100	100
1	K	321/347 (92%)	299 (93%)	22 (7%)	0	100	100
1	L	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
All	All	3971/4164 (95%)	3812 (96%)	159 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/276 (95%)	254 (97%)	8 (3%)	40	58
1	B	274/276 (99%)	263 (96%)	11 (4%)	31	47
1	C	273/276 (99%)	268 (98%)	5 (2%)	59	75
1	D	261/276 (95%)	248 (95%)	13 (5%)	24	38
1	E	276/276 (100%)	270 (98%)	6 (2%)	52	70
1	F	272/276 (99%)	268 (98%)	4 (2%)	65	79
1	G	256/276 (93%)	247 (96%)	9 (4%)	36	53
1	H	249/276 (90%)	242 (97%)	7 (3%)	43	61
1	I	274/276 (99%)	263 (96%)	11 (4%)	31	47
1	J	276/276 (100%)	270 (98%)	6 (2%)	52	70
1	K	259/276 (94%)	244 (94%)	15 (6%)	20	31
1	L	272/276 (99%)	262 (96%)	10 (4%)	34	51
All	All	3204/3312 (97%)	3099 (97%)	105 (3%)	38	55

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	122	LYS
1	A	207	ASP
1	A	250	LYS
1	A	303	PRO
1	A	304	ASP
1	A	318	ASP
1	A	336	LYS
1	B	4	PRO
1	B	39	LYS
1	B	49	LYS
1	B	68	GLU
1	B	76	GLU
1	B	82	ASP
1	B	179	LEU
1	B	183	ASP
1	B	194	ARG
1	B	308	VAL
1	B	314	LYS
1	C	38	GLU
1	C	68	GLU
1	C	215	ARG

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Mol	Chain	Res	Type
1	C	288	ASP
1	C	291	GLU
1	D	1	MET
1	D	5	ILE
1	D	38	GLU
1	D	122	LYS
1	D	154	LEU
1	D	213	GLU
1	D	256	GLU
1	D	310	MET
1	D	312	ASP
1	D	318	ASP
1	D	332	ARG
1	D	336	LYS
1	D	343	GLN
1	E	39	LYS
1	E	155	LEU
1	E	256	GLU
1	E	260	ARG
1	E	288	ASP
1	E	337	LYS
1	F	59	GLU
1	F	288	ASP
1	F	318	ASP
1	F	336	LYS
1	G	28	ARG
1	G	45	PRO
1	G	103	ASP
1	G	106	ASP
1	G	149	ILE
1	G	183	ASP
1	G	215	ARG
1	G	318	ASP
1	G	327	ILE
1	H	114	LYS
1	H	154	LEU
1	H	302	MET
1	H	303	PRO
1	H	308	VAL
1	H	314	LYS
1	H	318	ASP
1	I	38	GLU

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Mol	Chain	Res	Type
1	I	59	GLU
1	I	65	ASP
1	I	68	GLU
1	I	183	ASP
1	I	248	ASP
1	I	304	ASP
1	I	323	GLN
1	I	333	MET
1	I	337	LYS
1	I	341	LEU
1	J	21	GLU
1	J	43	ARG
1	J	88	LEU
1	J	179	LEU
1	J	194	ARG
1	J	207	ASP
1	K	17	GLN
1	K	44	ILE
1	K	49	LYS
1	K	59	GLU
1	K	65	ASP
1	K	115	LEU
1	K	154	LEU
1	K	210	GLU
1	K	232	ASP
1	K	268	THR
1	K	317	ASP
1	K	323	GLN
1	K	325	LYS
1	K	332	ARG
1	K	333	MET
1	L	4	PRO
1	L	28	ARG
1	L	43	ARG
1	L	59	GLU
1	L	65	ASP
1	L	147	LYS
1	L	154	LEU
1	L	155	LEU
1	L	192	THR
1	L	300	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	B	159	GLN
1	F	17	GLN
1	F	258	GLN
1	G	175	HIS
1	G	316	GLN
1	H	219	GLN
1	H	323	GLN
1	I	93	ASN
1	I	152	HIS
1	I	316	GLN
1	J	159	GLN
1	K	134	GLN
1	K	323	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	C	401	-	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	I	401	4	0,5,5	0.00	-	0,6,6	0.00	-
2	TRS	J	401	-	7,7,7	0.65	0	9,9,9	5.08	6 (66%)
3	OXL	F	401	4	0,5,5	0.00	-	0,6,6	0.00	-
2	TRS	B	401	-	7,7,7	0.35	0	9,9,9	0.26	0
2	TRS	G	401	-	7,7,7	0.80	0	9,9,9	0.80	0
2	TRS	A	401	-	7,7,7	0.29	0	9,9,9	0.32	0
3	OXL	L	401	-	0,5,5	0.00	-	0,6,6	0.00	-

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	C	401	-	-	0/0/4/4	-
3	OXL	I	401	4	-	0/0/4/4	-
2	TRS	J	401	-	-	6/9/9/9	-
3	OXL	F	401	4	-	0/0/4/4	-
2	TRS	B	401	-	-	3/9/9/9	-
2	TRS	G	401	-	-	0/9/9/9	-
2	TRS	A	401	-	-	0/9/9/9	-
3	OXL	L	401	-	-	0/0/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	TRS	C3-C-N	-9.39	79.95	107.98
2	J	401	TRS	C2-C-N	-8.52	82.55	107.98
2	J	401	TRS	C1-C-N	-7.15	86.62	107.98
2	J	401	TRS	C2-C-C1	2.69	119.16	110.81
2	J	401	TRS	C3-C-C2	2.46	118.44	110.81
2	J	401	TRS	C3-C-C1	2.34	118.06	110.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	401	TRS	C2-C-C1-O1

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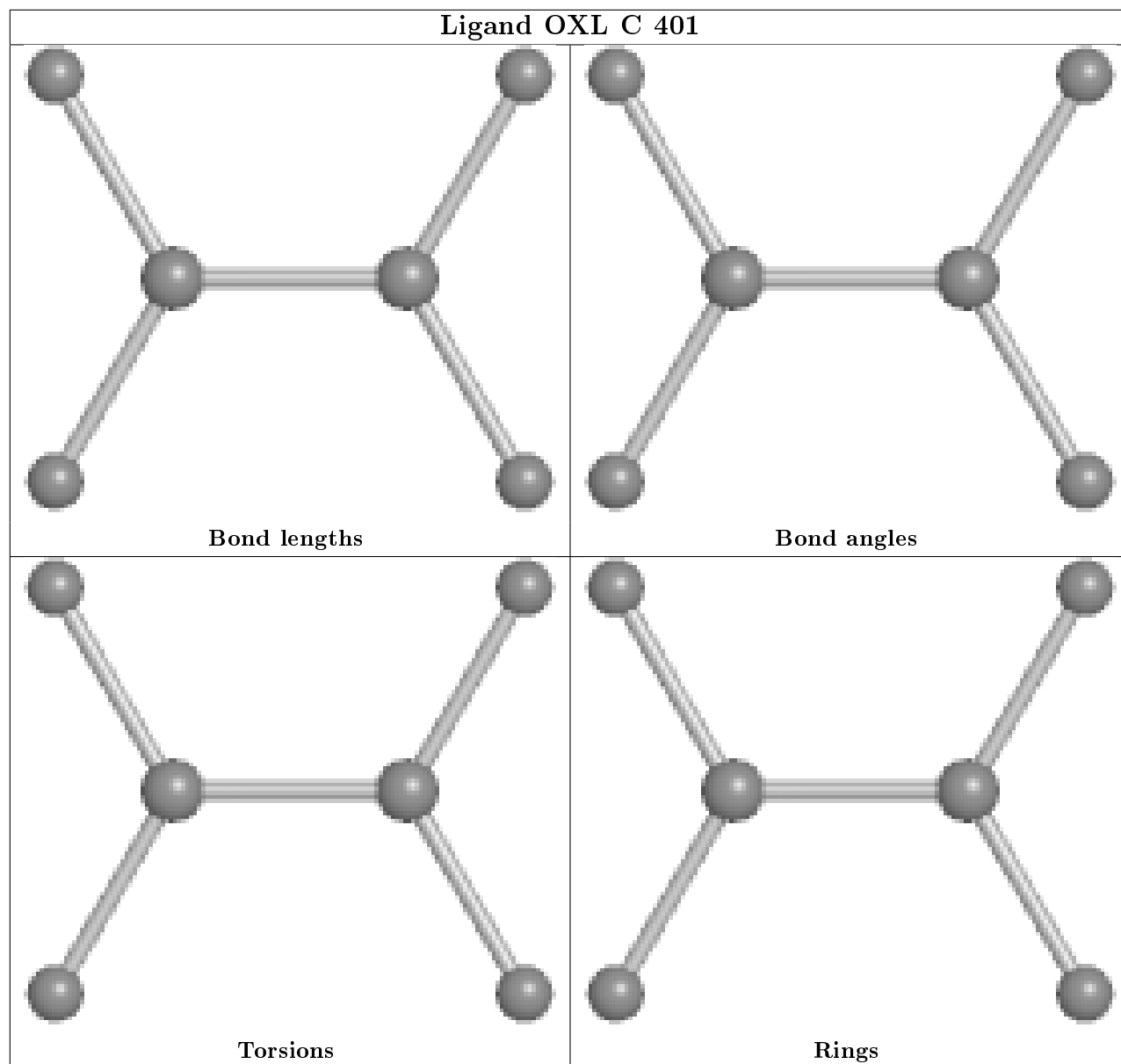
Mol	Chain	Res	Type	Atoms
2	J	401	TRS	N-C-C1-O1
2	J	401	TRS	C3-C-C2-O2
2	J	401	TRS	N-C-C2-O2
2	J	401	TRS	C1-C-C3-O3
2	J	401	TRS	N-C-C3-O3
2	B	401	TRS	N-C-C3-O3
2	B	401	TRS	C2-C-C3-O3
2	B	401	TRS	C1-C-C3-O3

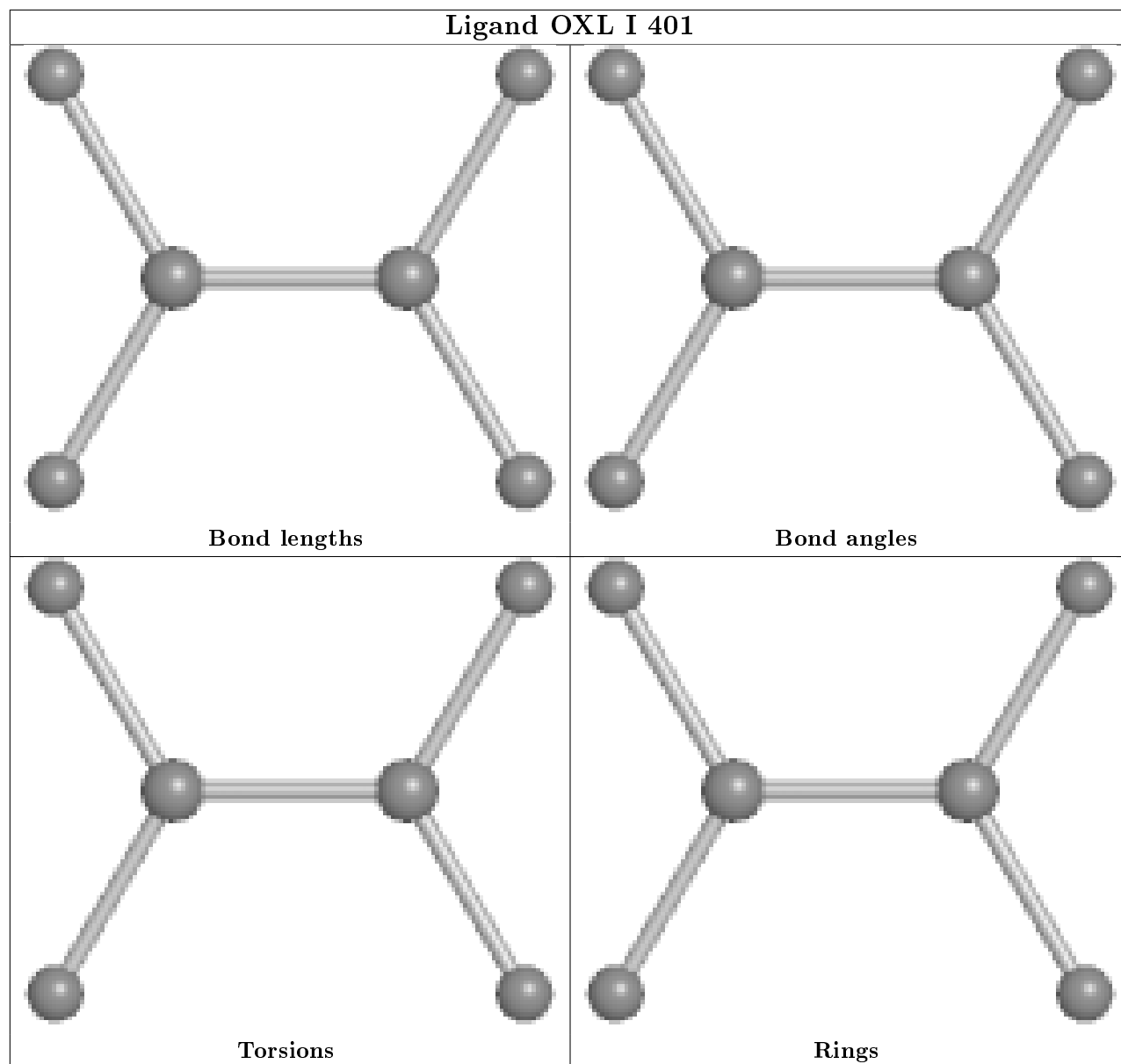
There are no ring outliers.

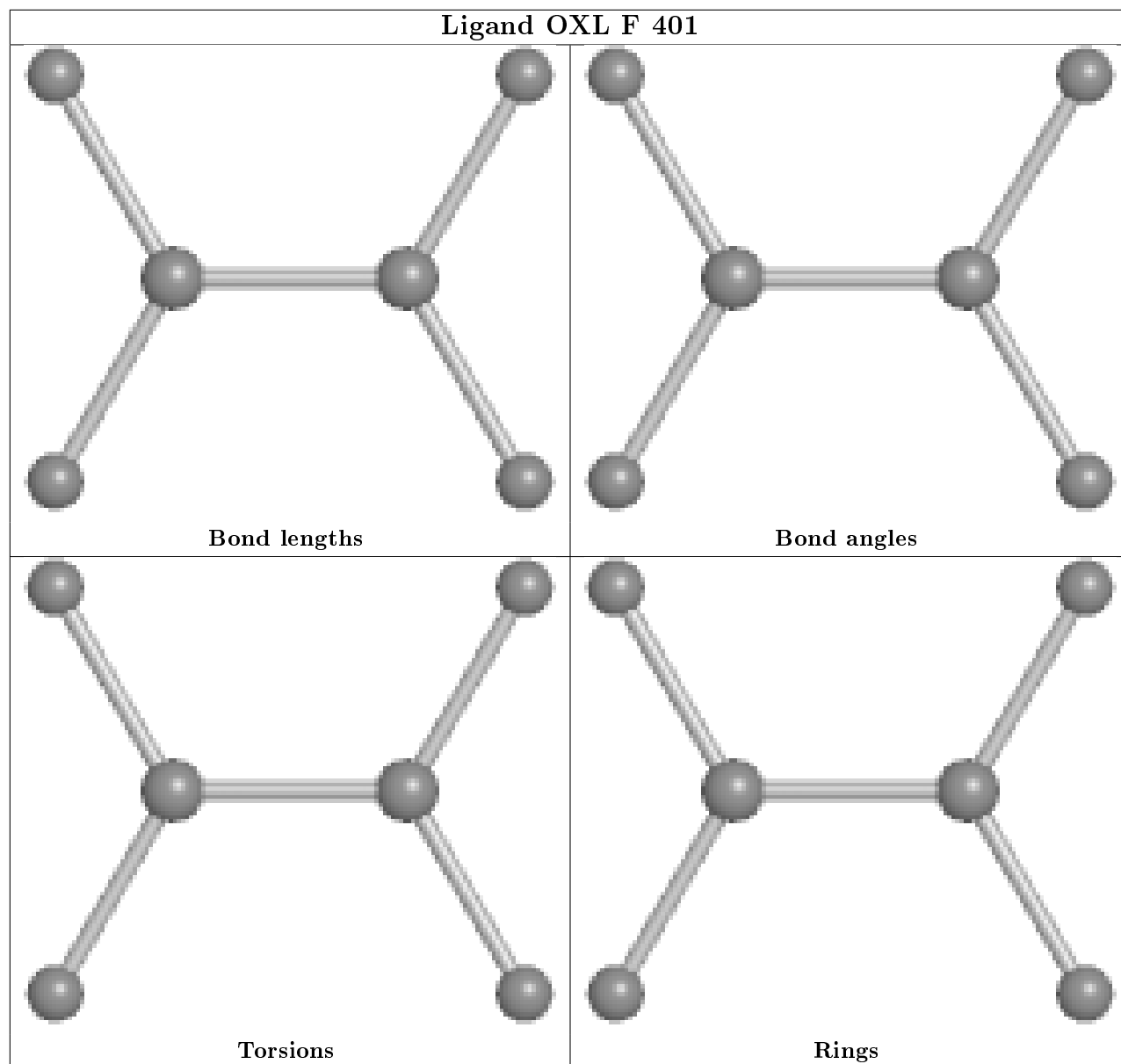
4 monomers are involved in 5 short contacts:

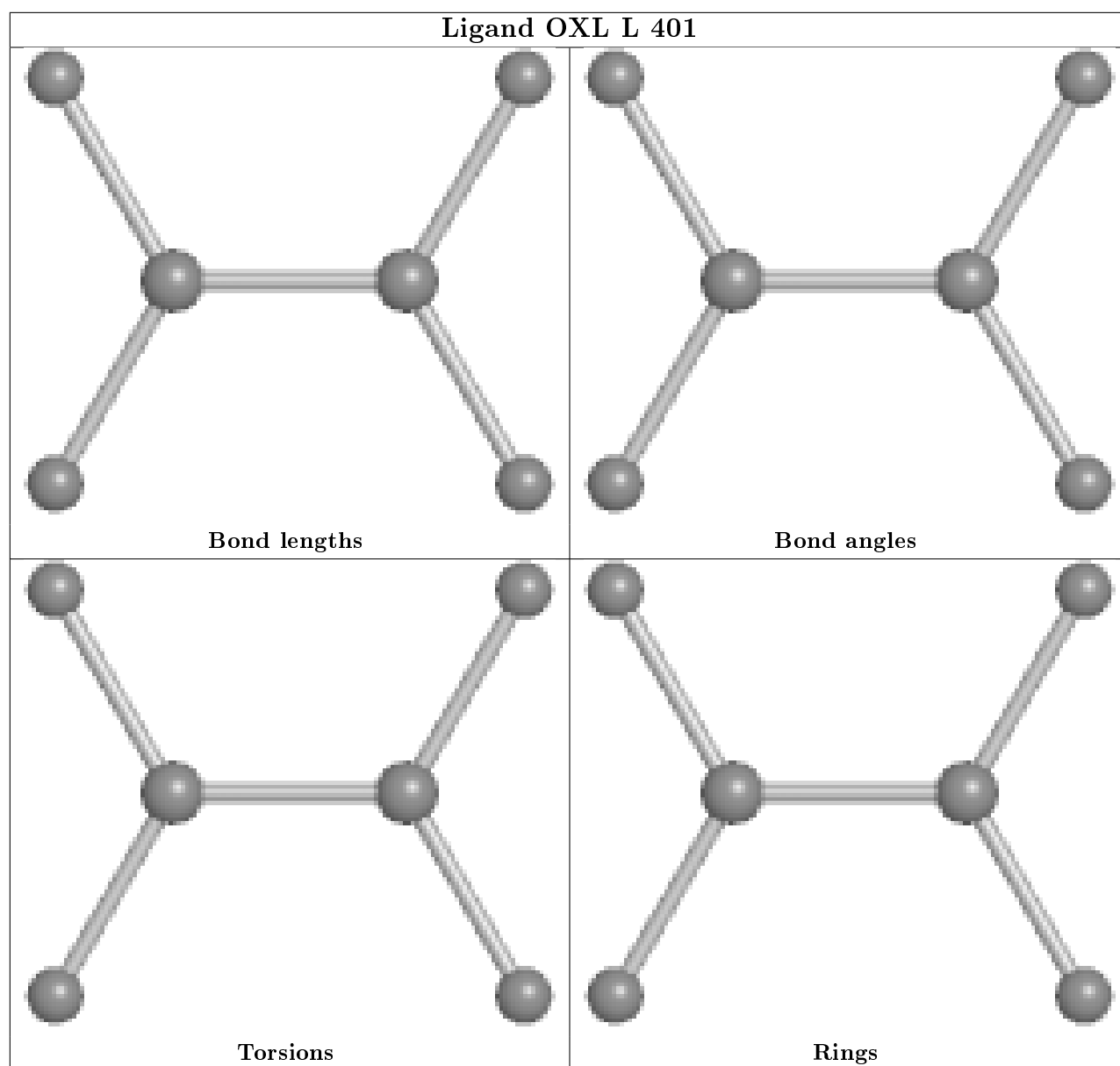
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	OXL	1	0
3	F	401	OXL	1	0
2	G	401	TRS	1	0
2	A	401	TRS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	329/347 (94%)	0.00	11 (3%)	46	43	22, 40, 93, 109	0
1	B	345/347 (99%)	0.02	18 (5%)	27	24	24, 42, 97, 127	0
1	C	343/347 (98%)	-0.29	2 (0%)	89	88	21, 37, 74, 96	0
1	D	328/347 (94%)	-0.04	14 (4%)	35	31	26, 45, 93, 109	0
1	E	347/347 (100%)	-0.14	5 (1%)	75	73	27, 47, 76, 106	0
1	F	342/347 (98%)	0.03	3 (0%)	84	83	30, 52, 75, 99	0
1	G	325/347 (93%)	0.71	43 (13%)	3	2	42, 72, 109, 130	0
1	H	316/347 (91%)	0.26	27 (8%)	10	8	31, 47, 100, 118	0
1	I	345/347 (99%)	0.38	16 (4%)	32	28	41, 74, 104, 120	0
1	J	346/347 (99%)	0.38	16 (4%)	32	28	36, 64, 93, 111	0
1	K	327/347 (94%)	0.71	48 (14%)	2	1	45, 71, 109, 123	0
1	L	342/347 (98%)	0.29	13 (3%)	40	36	31, 55, 90, 105	0
All	All	4035/4164 (96%)	0.19	216 (5%)	25	22	21, 54, 98, 130	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	19	ILE	7.7
1	D	321	TRP	7.1
1	G	14	GLY	7.1
1	G	18	PRO	5.9
1	B	23	PRO	5.8
1	K	345	TYR	5.8
1	K	1	MET	5.8
1	B	3	LEU	5.5
1	H	331	ALA	5.4
1	G	293	LEU	5.4
1	K	321	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	11	LEU	5.0
1	L	1	MET	5.0
1	A	16	PRO	4.9
1	K	328	VAL	4.9
1	B	211	GLY	4.9
1	D	309	ALA	4.8
1	J	347	PHE	4.8
1	F	347	PHE	4.7
1	G	15	ALA	4.7
1	K	324	ALA	4.7
1	D	319	ALA	4.6
1	J	1	MET	4.6
1	G	330	LEU	4.4
1	G	193	THR	4.4
1	G	300	ASP	4.3
1	G	20	ARG	4.3
1	K	209	GLN	4.3
1	H	294	PHE	4.3
1	G	12	ALA	4.2
1	K	344	ALA	4.1
1	K	325	LYS	4.1
1	K	333	MET	4.1
1	K	327	ILE	4.0
1	H	296	LYS	4.0
1	H	293	LEU	3.9
1	K	335	ALA	3.9
1	K	339	PRO	3.8
1	K	336	LYS	3.8
1	B	20	ARG	3.8
1	I	213	GLU	3.8
1	G	16	PRO	3.7
1	G	289	VAL	3.7
1	H	324	ALA	3.7
1	H	332	ARG	3.7
1	C	1	MET	3.6
1	K	42	ALA	3.6
1	H	308	VAL	3.6
1	D	328	VAL	3.6
1	K	334	ILE	3.6
1	K	346	GLY	3.6
1	L	209	GLN	3.5
1	A	13	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	322	LYS	3.5
1	K	43	ARG	3.5
1	G	24	VAL	3.5
1	L	347	PHE	3.5
1	G	23	PRO	3.5
1	H	16	PRO	3.4
1	I	44	ILE	3.4
1	I	1	MET	3.4
1	G	303	PRO	3.4
1	I	308	VAL	3.3
1	B	19	ILE	3.3
1	D	336	LYS	3.3
1	H	289	VAL	3.2
1	G	4	PRO	3.2
1	F	1	MET	3.2
1	G	333	MET	3.2
1	K	40	ILE	3.2
1	G	54	LEU	3.2
1	J	339	PRO	3.2
1	B	13	ALA	3.2
1	A	305	GLY	3.2
1	G	48	ALA	3.1
1	B	21	GLU	3.1
1	L	309	ALA	3.1
1	G	6	HIS	3.1
1	H	334	ILE	3.1
1	K	318	ASP	3.1
1	D	347	PHE	3.0
1	H	321	TRP	3.0
1	A	23	PRO	3.0
1	L	308	VAL	3.0
1	B	208	PRO	3.0
1	I	309	ALA	3.0
1	H	290	ASN	3.0
1	D	345	TYR	2.9
1	H	14	GLY	2.9
1	D	332	ARG	2.9
1	G	13	ALA	2.9
1	K	288	ASP	2.9
1	H	17	GLN	2.9
1	L	304	ASP	2.9
1	B	9	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	214	HIS	2.9
1	I	46	GLU	2.8
1	D	318	ASP	2.8
1	I	211	GLY	2.8
1	H	330	LEU	2.8
1	B	15	ALA	2.8
1	I	210	GLU	2.8
1	K	46	GLU	2.8
1	H	15	ALA	2.8
1	K	332	ARG	2.8
1	G	5	ILE	2.8
1	D	322	LYS	2.8
1	K	249	ILE	2.8
1	H	320	THR	2.8
1	E	42	ALA	2.7
1	F	209	GLN	2.7
1	I	63	PRO	2.7
1	K	35	PRO	2.7
1	J	194	ARG	2.7
1	H	19	ILE	2.7
1	K	323	GLN	2.7
1	G	309	ALA	2.7
1	K	307	GLY	2.7
1	G	331	ALA	2.7
1	K	61	ALA	2.7
1	A	332	ARG	2.7
1	D	329	ASP	2.7
1	K	329	ASP	2.7
1	H	23	PRO	2.6
1	E	213	GLU	2.6
1	C	210	GLU	2.6
1	K	306	SER	2.6
1	G	10	PRO	2.6
1	G	297	ARG	2.6
1	K	37	VAL	2.5
1	H	288	ASP	2.5
1	G	334	ILE	2.5
1	L	303	PRO	2.5
1	A	3	LEU	2.5
1	B	14	GLY	2.5
1	K	337	LYS	2.5
1	G	299	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	21	GLU	2.5
1	J	299	LEU	2.5
1	G	8	TYR	2.5
1	G	296	LYS	2.5
1	K	39	LYS	2.5
1	K	308	VAL	2.5
1	D	324	ALA	2.4
1	G	51	VAL	2.4
1	J	304	ASP	2.4
1	K	305	GLY	2.4
1	J	305	GLY	2.4
1	J	79	ARG	2.4
1	H	213	GLU	2.4
1	L	313	GLY	2.4
1	L	299	LEU	2.4
1	K	338	ASP	2.4
1	B	310	MET	2.3
1	K	343	GLN	2.3
1	G	329	ASP	2.3
1	H	304	ASP	2.3
1	J	13	ALA	2.3
1	B	196	GLY	2.3
1	L	44	ILE	2.3
1	H	24	VAL	2.3
1	D	323	GLN	2.3
1	K	85	ASP	2.3
1	K	341	LEU	2.3
1	K	114	LYS	2.3
1	E	210	GLU	2.3
1	D	325	LYS	2.3
1	J	345	TYR	2.3
1	I	209	GLN	2.3
1	K	47	VAL	2.3
1	J	306	SER	2.2
1	B	12	ALA	2.2
1	A	297	ARG	2.2
1	L	85	ASP	2.2
1	G	112	GLY	2.2
1	A	14	GLY	2.2
1	K	38	GLU	2.2
1	K	26	PRO	2.2
1	J	337	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	83	PHE	2.2
1	H	303	PRO	2.2
1	G	46	GLU	2.2
1	J	336	LYS	2.2
1	I	13	ALA	2.2
1	I	64	ILE	2.2
1	I	298	ILE	2.2
1	B	10	PRO	2.2
1	L	146	GLN	2.2
1	H	328	VAL	2.1
1	I	291	GLU	2.1
1	G	141	ALA	2.1
1	G	213	GLU	2.1
1	K	24	VAL	2.1
1	K	316	GLN	2.1
1	J	83	PHE	2.1
1	I	38	GLU	2.1
1	B	212	GLN	2.1
1	G	201	PHE	2.1
1	A	293	LEU	2.1
1	E	39	LYS	2.1
1	K	340	GLU	2.1
1	A	298	ILE	2.1
1	K	45	PRO	2.1
1	A	15	ALA	2.1
1	K	22	LEU	2.0
1	B	16	PRO	2.0
1	L	328	VAL	2.0
1	J	43	ARG	2.0
1	G	21	GLU	2.0
1	J	14	GLY	2.0
1	G	147	LYS	2.0
1	G	301	ALA	2.0
1	H	329	ASP	2.0
1	G	25	ARG	2.0
1	I	327	ILE	2.0
1	B	209	GLN	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 carbohydrates in this entry.

6.4 Ligands ⓘ

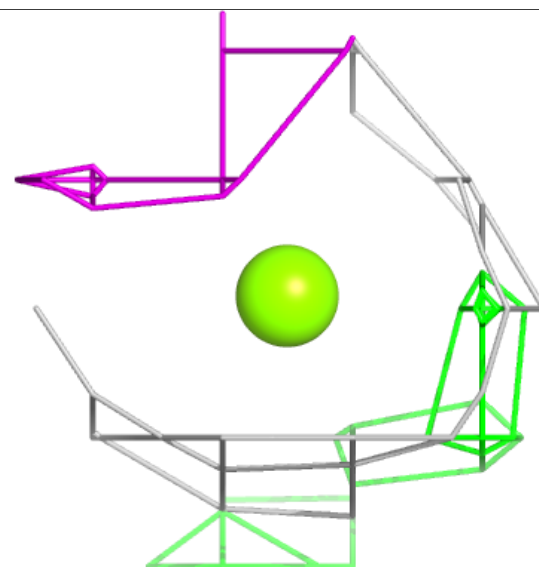
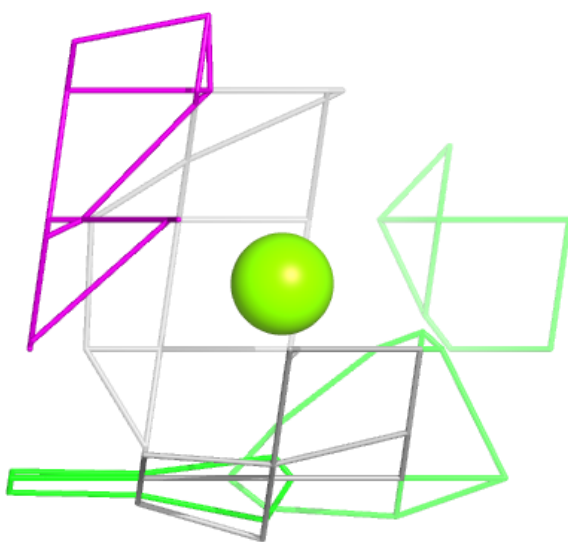
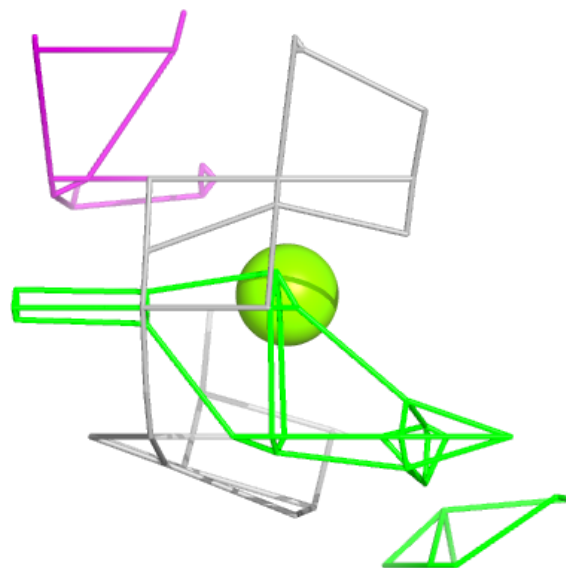
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	F	402	1/1	0.80	0.15	59,59,59,59	0
3	OXL	I	401	6/6	0.83	0.21	78,84,87,91	0
3	OXL	C	401	6/6	0.85	0.23	39,44,45,47	0
3	OXL	L	401	6/6	0.87	0.17	67,67,69,70	0
3	OXL	F	401	6/6	0.88	0.27	48,49,50,50	0
2	TRS	A	401	8/8	0.89	0.20	40,40,41,42	0
2	TRS	B	401	8/8	0.91	0.20	34,35,35,36	0
4	MG	I	402	1/1	0.92	0.09	78,78,78,78	0
2	TRS	G	401	8/8	0.94	0.20	57,58,58,60	0
2	TRS	J	401	8/8	0.97	0.14	49,50,51,52	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.

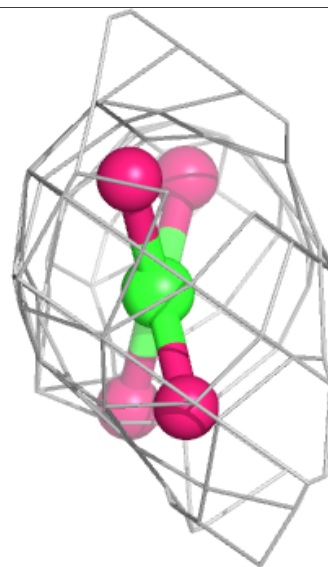
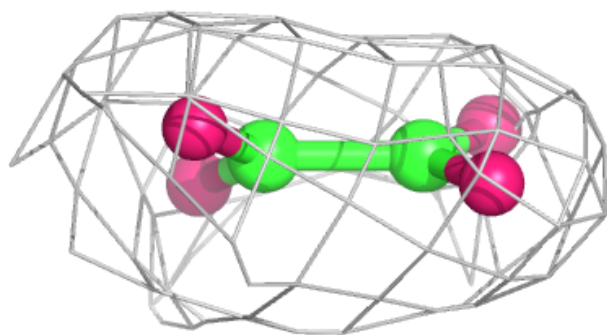
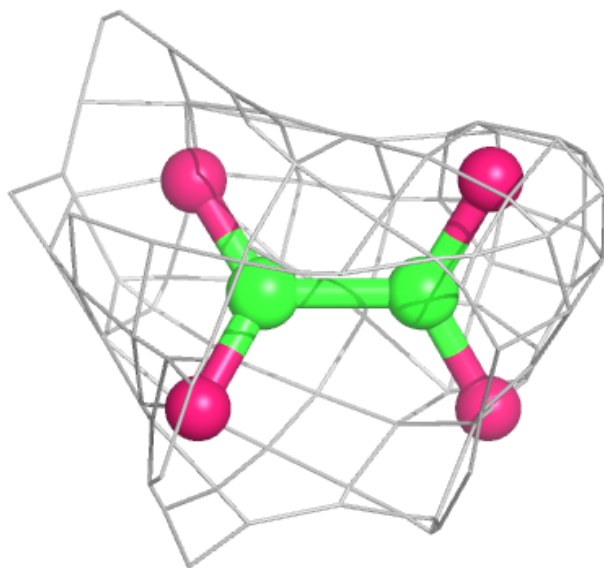
Electron density around MG F 402:

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



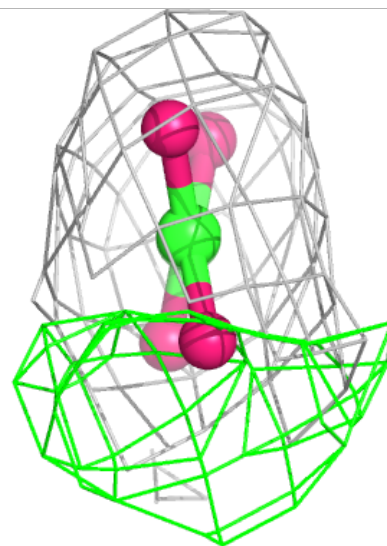
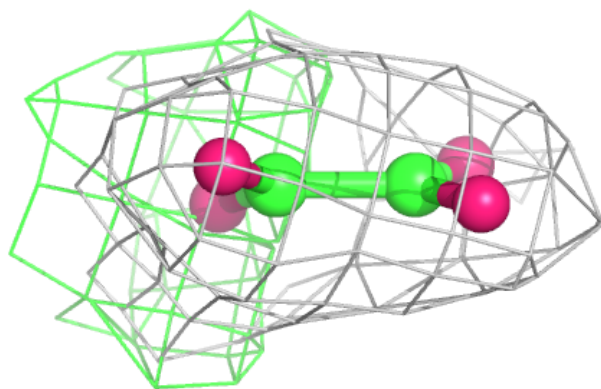
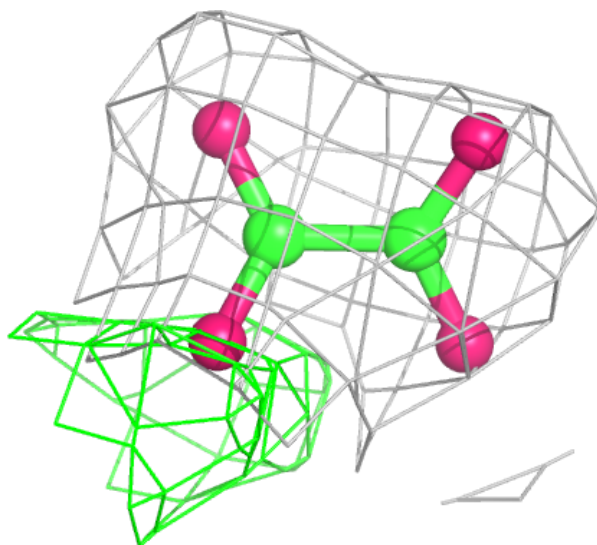
Electron density around OXL I 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



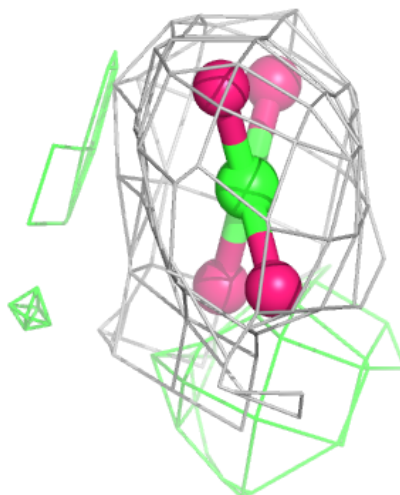
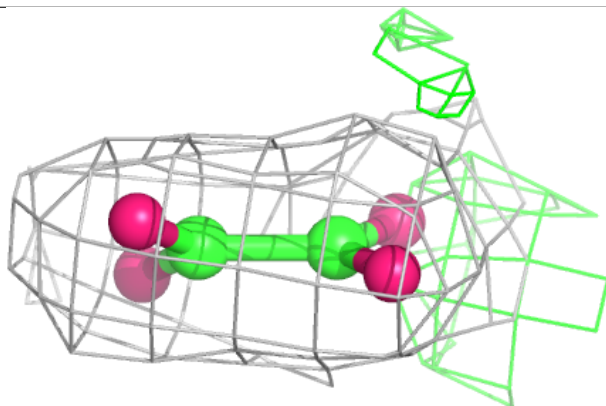
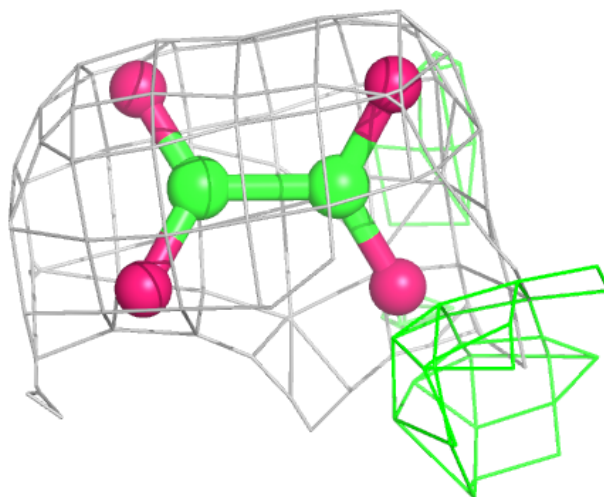
Electron density around OXL C 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



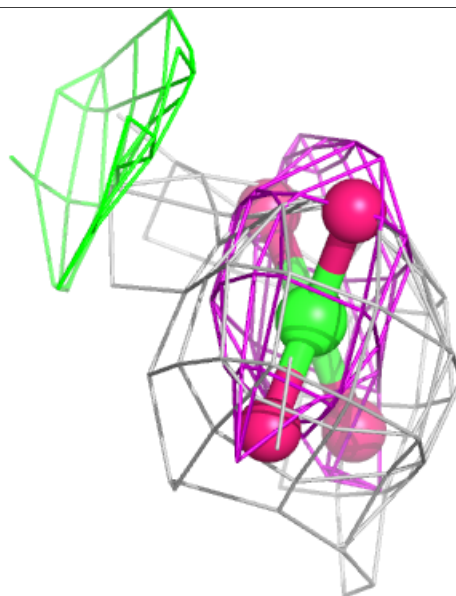
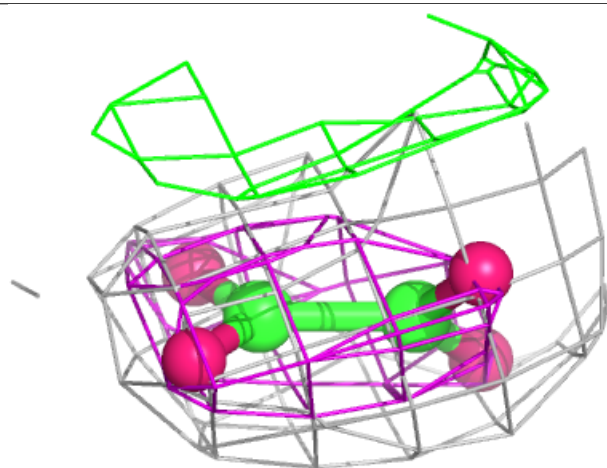
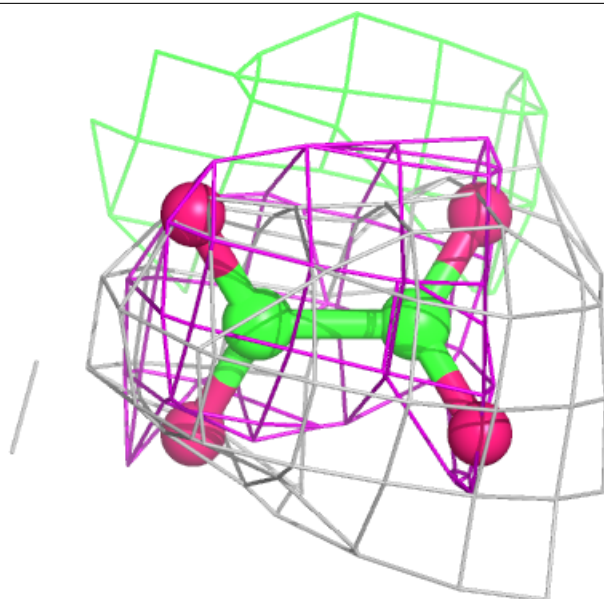
Electron density around OXL L 401:

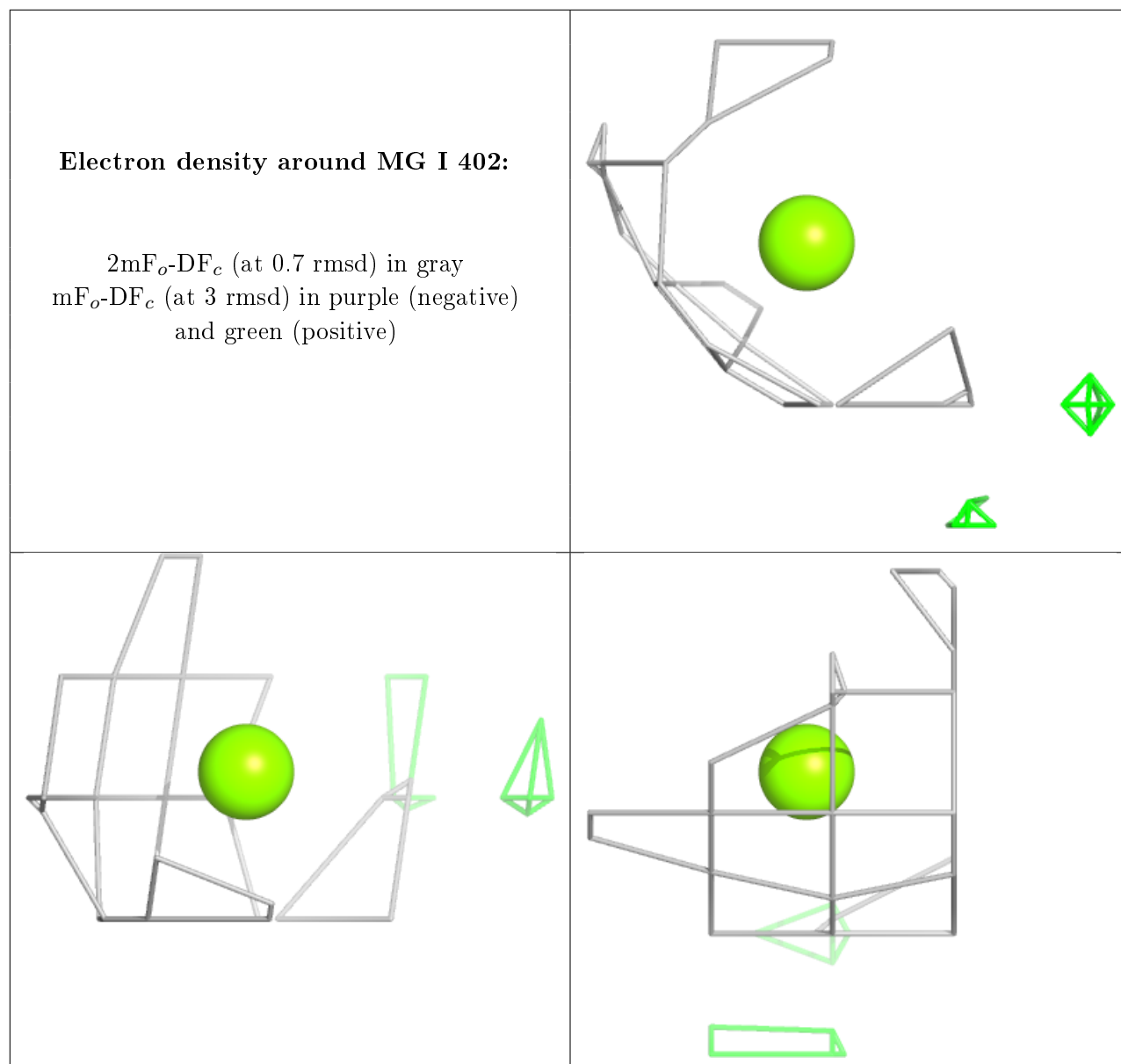
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OXL 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.