



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:10 PM EDT

PDB ID : 6KKH / pdb_00006khh
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 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

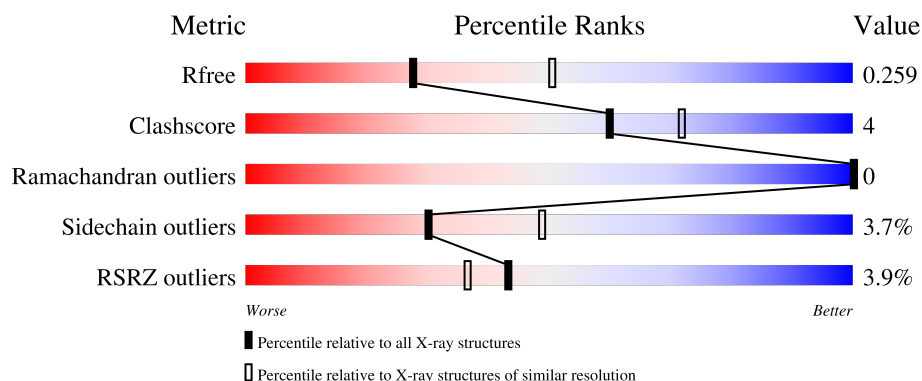
1 Overall quality at a glance

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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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 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	347	5% 82% 11% • 5%
1	B	347	4% 88% 10% ••
1	C	347	2% 93% 6% •
1	D	347	3% 82% 12% • 5%
1	E	347	89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	347	
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	-	-
3	OXL	C	401	-	X	-	-
3	OXL	F	401	-	X	-	-
3	OXL	I	401	-	X	-	-
3	OXL	L	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.

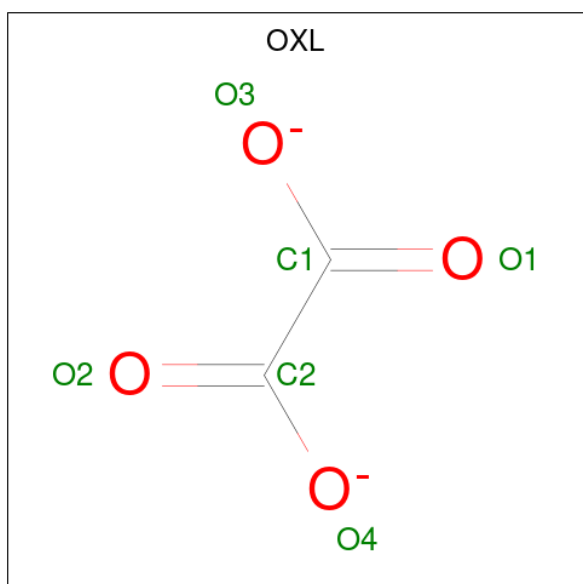
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2547	1640	444	449	14			
1	B	345	Total	C	N	O	S	0	0	0
			2679	1721	468	476	14			
1	C	343	Total	C	N	O	S	0	0	0
			2664	1714	464	471	15			
1	D	328	Total	C	N	O	S	0	0	0
			2555	1645	447	449	14			
1	E	347	Total	C	N	O	S	0	0	0
			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 (CCD ID: 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 (CCD ID: OXL) (formula: C₂O₄) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

Continued on next page...

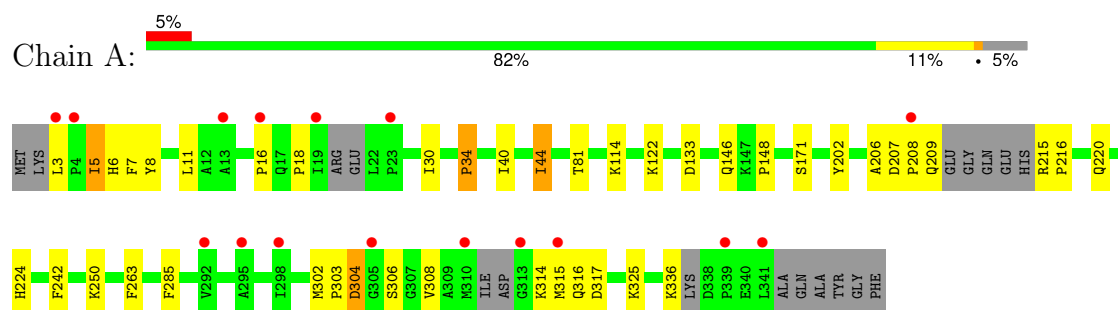
Continued from previous page...

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

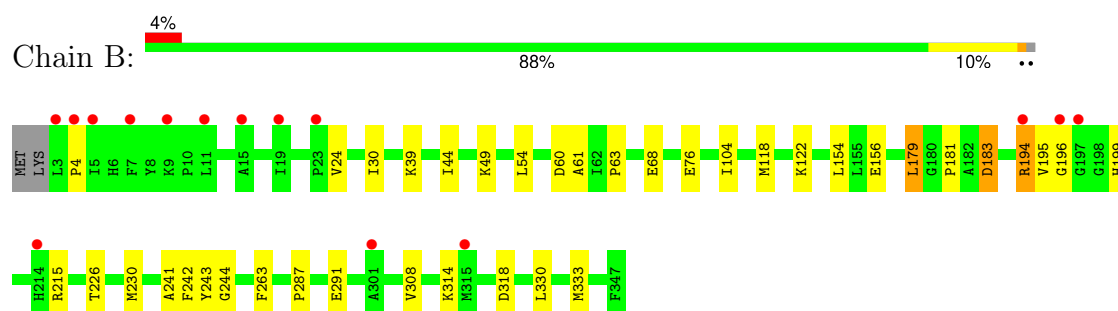
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

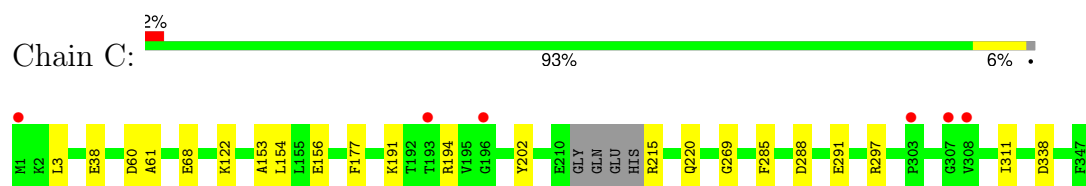
• Molecule 1: HpcH/HpaI aldolase



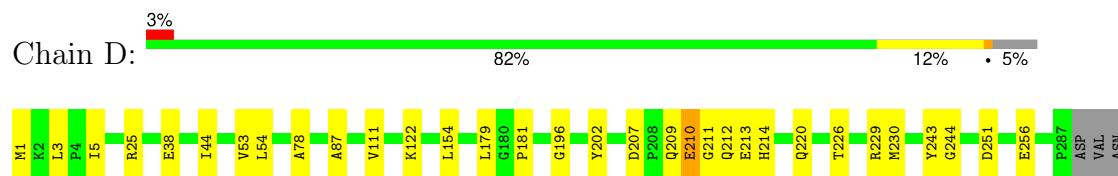
• Molecule 1: HpcH/HpaI aldolase

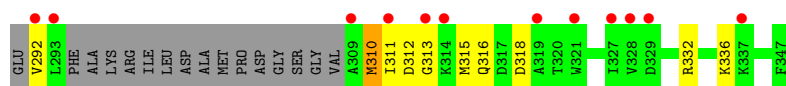


• Molecule 1: HpcH/HpaI aldolase

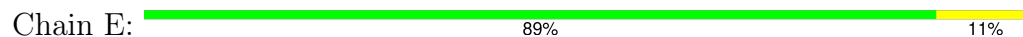


• Molecule 1: HpcH/HpaI aldolase

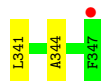
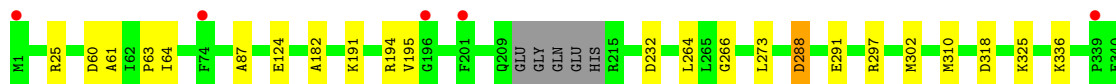




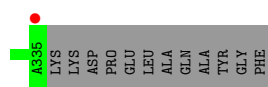
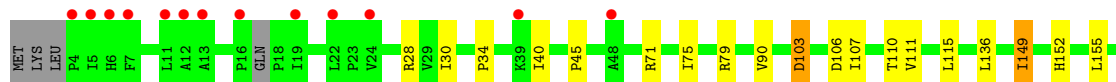
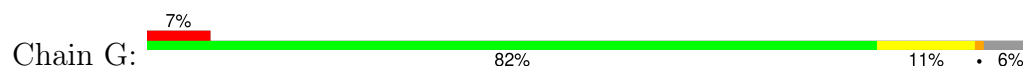
- Molecule 1: HpcH/HpaI aldolase



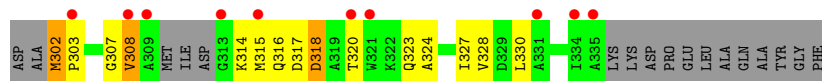
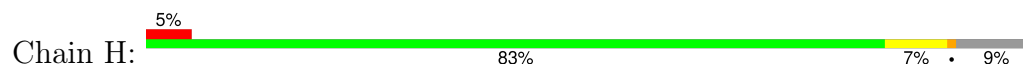
- Molecule 1: HpcH/HpaI aldolase



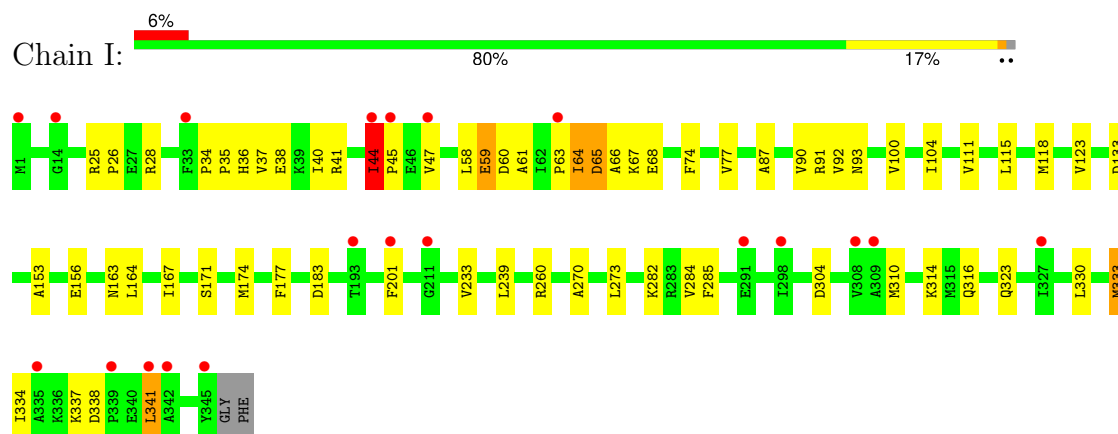
- Molecule 1: HpcH/HpaI aldolase



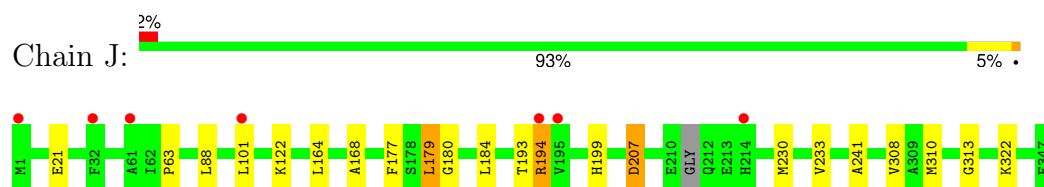
- Molecule 1: HpcH/HpaI aldolase



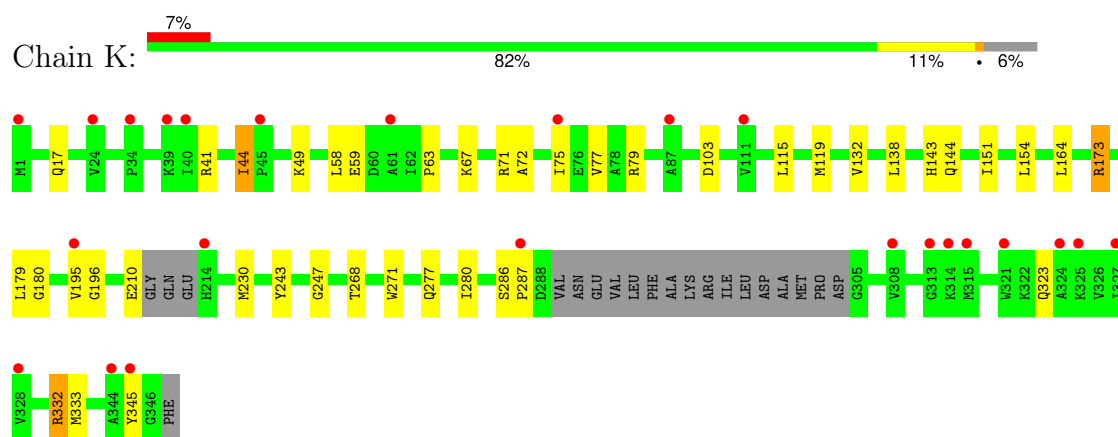
• Molecule 1: HpcH/HpaI aldolase



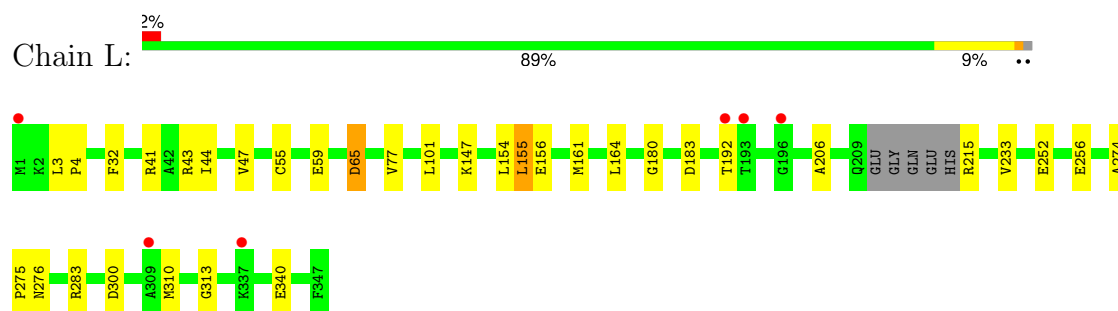
• Molecule 1: HpcH/HpaI aldolase



• 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 49.48 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.48-2.64) 98.8 (49.48-2.64)	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 (5.00%)	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 , 42.2	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TRS, 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	0.73	1/2610 (0.0%)	0.98	2/3546 (0.1%)
1	B	0.66	0/2749	0.93	2/3738 (0.1%)
1	C	0.69	0/2732	0.92	4/3712 (0.1%)
1	D	0.61	0/2621	0.90	3/3560 (0.1%)
1	E	0.63	0/2765	0.88	0/3757
1	F	0.57	0/2723	0.86	2/3700 (0.1%)
1	G	0.59	0/2577	0.88	2/3500 (0.1%)
1	H	0.60	0/2494	0.88	0/3388
1	I	0.64	0/2744	0.93	1/3731 (0.0%)
1	J	0.57	0/2761	0.85	2/3751 (0.1%)
1	K	0.59	0/2601	0.86	2/3533 (0.1%)
1	L	0.59	0/2723	0.89	6/3700 (0.2%)
All	All	0.62	1/32100 (0.0%)	0.90	26/43616 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	PRO	C-O	-6.23	1.17	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	HIS	CA-C-N	7.58	127.46	119.05
1	B	199	HIS	C-N-CA	7.58	127.46	119.05
1	D	210	GLU	CB-CA-C	-7.09	107.58	117.23
1	L	274	ALA	CA-C-N	6.56	127.08	119.47
1	L	274	ALA	C-N-CA	6.56	127.08	119.47
1	C	338	ASP	CA-C-N	6.22	126.41	119.32
1	C	338	ASP	C-N-CA	6.22	126.41	119.32
1	K	180	GLY	CA-C-N	5.94	126.36	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	180	GLY	C-N-CA	5.94	126.36	119.47
1	L	3	LEU	CA-C-N	5.83	127.13	119.84
1	L	3	LEU	C-N-CA	5.83	127.13	119.84
1	J	180	GLY	CA-C-N	5.23	124.85	119.05
1	J	180	GLY	C-N-CA	5.23	124.85	119.05
1	A	34	PRO	CA-C-N	5.23	124.73	119.19
1	A	34	PRO	C-N-CA	5.23	124.73	119.19
1	D	3	LEU	CA-C-N	5.22	125.27	119.32
1	D	3	LEU	C-N-CA	5.22	125.27	119.32
1	I	44	ILE	O-C-N	5.13	123.71	120.07
1	F	302	MET	CA-C-N	5.08	126.19	119.84
1	F	302	MET	C-N-CA	5.08	126.19	119.84
1	G	180	GLY	CA-C-N	5.06	124.84	119.28
1	G	180	GLY	C-N-CA	5.06	124.84	119.28
1	L	180	GLY	CA-C-N	5.04	124.65	119.05
1	L	180	GLY	C-N-CA	5.04	124.65	119.05
1	C	3	LEU	CA-C-N	5.01	125.28	119.47
1	C	3	LEU	C-N-CA	5.01	125.28	119.47

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	2547	0	2552	34	0
1	B	2679	0	2672	24	0
1	C	2664	0	2672	11	0
1	D	2555	0	2559	35	0
1	E	2695	0	2695	20	0
1	F	2655	0	2666	17	0
1	G	2514	0	2499	19	0
1	H	2435	0	2425	27	0
1	I	2675	0	2674	61	0
1	J	2692	0	2693	10	0
1	K	2536	0	2537	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2655	0	2666	14	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	269	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 (269) 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:H:315:MET:C	1:H:316:GLN:OE1	2.09	0.94
1:L:155:LEU:HD11	1:L:161:MET:SD	2.09	0.93
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:OE1	1:H:316:GLN:N	2.08	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:K:173:ARG:HH11	1.42	0.84
1:B:63:PRO:HA	1:D:310:MET:HE3	1.60	0.83
1:A:302:MET:HE1	1:A:317:ASP:N	1.93	0.82
1:I:63:PRO:HG2	1:I:66:ALA:HB3	1.60	0.81
1:H:302:MET:HE1	1:H:317:ASP:HA	1.64	0.80
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:302:MET:HE1	1:A:317:ASP:CA	2.17	0.74
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:H:302:MET:HE1	1:H:317:ASP:CA	2.20	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:O	1:A:209:GLN:HG3	1.94	0.67
1:B:215:ARG:HH22	1:D:251:ASP:CG	2.04	0.66
1:H:302:MET:HE1	1:H:317:ASP:C	2.21	0.66
1:B:194:ARG:HA	1:B:194:ARG:NE	2.11	0.66
1:I:310:MET:HE1	1:J:63:PRO:HA	1.78	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: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:E:188:ARG:HD3	1:F:232:ASP:OD1	2.01	0.61
1:E:310:MET:HE3	1:E:313:GLY:HA2	1.81	0.61
1:G:136:LEU:HD22	1:G:149:ILE:HD11	1.81	0.60
1:H:302:MET:CE	1:H:317:ASP:C	2.74	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:324:ALA:O	1:H:327:ILE:HG22	2.02	0.59
1:I:92:VAL:HG11	1:I:118:MET:HE2	1.83	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:A:302:MET:HE1	1:A:317:ASP:HA	1.85	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:A:302:MET:HE3	1:A:316:GLN:HB3	1.86	0.56
1:D:1:MET:HE1	1:E:1:MET:HE1	1.86	0.56
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:B:24:VAL:HG12	1:B:333:MET:HE3	1.87	0.56
1:D:1:MET:HE1	1:E:1:MET:CE	2.36	0.55
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:E:193:THR:C	1:E:194:ARG:HD3	2.31	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:K:119:MET:HE1	1:K:271:TRP:CZ2	2.44	0.53
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:I:25:ARG:CZ	1:I:87:ALA:HB2	2.39	0.53
1:H:318:ASP:N	1:H:318:ASP:OD1	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: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:J:207:ASP:N	1:J:207:ASP:OD2	2.43	0.51
1:A:133:ASP:OD2	1:A:171:SER:OG	2.25	0.51
1:G:28:ARG:NH1	1:G:286:SER:OG	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:173:ARG:CG	1:K:173:ARG:NH1	2.70	0.51
1:J:230:MET:HE3	1:J:241:ALA:HB1	1.93	0.51
1:E:63:PRO:HA	1:F:310:MET:HE3	1.93	0.51
1:A:34:PRO:HG2	1:A:40:ILE:HD13	1.93	0.51
1:I:111:VAL:HG22	1:I:111:VAL:O	2.11	0.51
1:D:229:ARG:HG3	1:D:229:ARG:HH11	1.76	0.50
1:D:310:MET:SD	1:D:310:MET:C	2.94	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:A:302:MET:HE1	1:A:316:GLN:C	2.36	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: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: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:I:133:ASP:OD2	1:I:171:SER:OG	2.27	0.48
1:G:155:LEU:HD12	1:G:230:MET:HE2	1.96	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:30:ILE:HD11	1:B:242:PHE:CD2	2.49	0.48
1:B:194:ARG:NE	1:B:194:ARG:CA	2.72	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:K:287:PRO:HD2	1:K:345:TYR:HH	1.78	0.47
1:C:202:TYR:CE2	1:C:220:GLN:HB2	2.49	0.47
1:I:104:ILE:HG12	1:I:118:MET:HE1	1.96	0.47
1:K:332:ARG:CG	1:K:332:ARG:HH11	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:ARG:HH11	1:K:332:ARG:HG2	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:B:194:ARG:HA	1:B:194:ARG:HE	1.77	0.47
1:C:297:ARG:NH2	1:C:311:ILE:HG23	2.30	0.47
1:G:278:ILE:HB	1:G:279:PRO:HD3	1.96	0.47
1:I:34:PRO:HD2	1:I:40:ILE:HD13	1.97	0.47
1:I:164:LEU:HG	1:I:233:VAL:HG11	1.96	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: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:B:230:MET:HE3	1:B:241:ALA:HB1	1.97	0.46
1:A:224:HIS:CD2	2:A:401:TRS:H22	2.51	0.46
1:I:26:PRO:CD	1:I:333:MET:HE2	2.46	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: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:I:26:PRO:HD2	1:I:333:MET:HE2	1.98	0.45
1:K:143:HIS:O	1:K:144:GLN:C	2.58	0.45
1:A:308:VAL:CG2	1:F:61:ALA:O	2.65	0.45
1:B:194:ARG:HH21	1:B:195:VAL:H	1.63	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:G:179:LEU:HB2	1:G:230:MET:HE1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:179:LEU:HB2	1:K:230:MET:HE1	1.97	0.44
1:K:195:VAL:HB	1:K:247:GLY:HA3	2.00	0.44
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:B:104:ILE:HG23	1:B:118:MET:HE1	1.99	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:D:310:MET:HE1	1:D:313:GLY:HA2	2.00	0.43
1:G:221:ASP:O	2:G:401:TRS:O1	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:VAL:HG12	1:K:151:ILE:HD11	2.02	0.42
1:A:263:PHE:CZ	1:F:191:LYS:HG2	2.55	0.42
1:C:60:ASP:O	1:C:61:ALA:HB3	2.19	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:30:ILE:HD11	1:G:242:PHE:CD2	2.54	0.42
1:G:152:HIS:HE2	1:G:178:SER:CB	2.32	0.42
1:L:44:ILE:HA	1:L:47:VAL:HG22	2.01	0.42
1:L:310:MET:HE2	1:L:313:GLY:C	2.44	0.42
1:A:114:LYS:CE	1:H:82:ASP:OD2	2.67	0.42
1:B:24:VAL:HG12	1:B:333:MET:CE	2.49	0.42
1:I:44:ILE:HD12	1:I:44:ILE:HA	1.79	0.42
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:HH11	1:J:194:ARG:HB3	1.84	0.42
1:C:122:LYS:N	1:C:156:GLU:OE1	2.52	0.42
1:A:315:MET:SD	1:F:273:LEU:HD13	2.61	0.41
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:G:75:ILE:HG23	1:G:110:THR:HG21	2.02	0.41
1:J:310:MET:HE3	1:J:313:GLY:HA2	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:315:MET:HE3	1:I:273:LEU:HD12	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: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:B:318:ASP:HB2	1:C:60:ASP:CG	2.46	0.41
1:I:44:ILE:CG2	1:I:77:VAL:HG13	2.45	0.41
1:I:64:ILE:HA	1:I:67:LYS:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:LEU:HD23	1:L:101:LEU:HA	1.86	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:I:260:ARG:HA	1:I:284:VAL:HG21	2.02	0.41
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:E:60:ASP:O	1:E:61:ALA:HB3	2.21	0.40
1:E:182:ALA:HB2	1:E:195:VAL:HG13	2.04	0.40
1:H:179:LEU:HD11	1:H:226:THR:HG22	2.03	0.40
1:E:207:ASP:CG	1:F:194:ARG:HH12	2.30	0.40
1:F:288:ASP:HB3	1:F:291:GLU:HB2	2.04	0.40
1:H:302:MET:HE2	1:H:317:ASP:C	2.46	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 ⓘ

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	253 (97%)	9 (3%)	32	52
1	B	274/276 (99%)	261 (95%)	13 (5%)	23	38
1	C	273/276 (99%)	268 (98%)	5 (2%)	51	71
1	D	261/276 (95%)	249 (95%)	12 (5%)	24	39
1	E	276/276 (100%)	266 (96%)	10 (4%)	31	50
1	F	272/276 (99%)	267 (98%)	5 (2%)	51	71
1	G	256/276 (93%)	244 (95%)	12 (5%)	23	38
1	H	249/276 (90%)	238 (96%)	11 (4%)	25	41
1	I	274/276 (99%)	263 (96%)	11 (4%)	28	45
1	J	276/276 (100%)	268 (97%)	8 (3%)	37	57
1	K	259/276 (94%)	247 (95%)	12 (5%)	24	39
1	L	272/276 (99%)	261 (96%)	11 (4%)	28	45
All	All	3204/3312 (97%)	3085 (96%)	119 (4%)	30	49

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	44	ILE
1	A	122	LYS
1	A	207	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	LYS
1	A	303	PRO
1	A	304	ASP
1	A	325	LYS
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	122	LYS
1	B	154	LEU
1	B	179	LEU
1	B	183	ASP
1	B	194	ARG
1	B	291	GLU
1	B	308	VAL
1	B	314	LYS
1	C	38	GLU
1	C	68	GLU
1	C	215	ARG
1	C	288	ASP
1	C	291	GLU
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	311	ILE
1	D	312	ASP
1	D	318	ASP
1	D	332	ARG
1	D	336	LYS
1	E	11	LEU
1	E	38	GLU
1	E	39	LYS
1	E	155	LEU
1	E	256	GLU
1	E	260	ARG
1	E	288	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	308	VAL
1	E	318	ASP
1	E	337	LYS
1	F	124	GLU
1	F	288	ASP
1	F	318	ASP
1	F	325	LYS
1	F	336	LYS
1	G	45	PRO
1	G	79	ARG
1	G	103	ASP
1	G	106	ASP
1	G	107	ILE
1	G	149	ILE
1	G	183	ASP
1	G	208	PRO
1	G	215	ARG
1	G	327	ILE
1	G	328	VAL
1	G	330	LEU
1	H	38	GLU
1	H	40	ILE
1	H	114	LYS
1	H	154	LEU
1	H	179	LEU
1	H	195	VAL
1	H	302	MET
1	H	303	PRO
1	H	308	VAL
1	H	314	LYS
1	H	318	ASP
1	I	38	GLU
1	I	44	ILE
1	I	59	GLU
1	I	64	ILE
1	I	65	ASP
1	I	68	GLU
1	I	304	ASP
1	I	323	GLN
1	I	333	MET
1	I	337	LYS
1	I	341	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	21	GLU
1	J	88	LEU
1	J	122	LYS
1	J	179	LEU
1	J	194	ARG
1	J	207	ASP
1	J	308	VAL
1	J	322	LYS
1	K	17	GLN
1	K	44	ILE
1	K	49	LYS
1	K	59	GLU
1	K	115	LEU
1	K	154	LEU
1	K	173	ARG
1	K	210	GLU
1	K	268	THR
1	K	323	GLN
1	K	332	ARG
1	K	333	MET
1	L	4	PRO
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	275	PRO
1	L	300	ASP
1	L	340	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	323	GLN
1	B	316	GLN
1	C	316	GLN
1	D	17	GLN
1	D	159	GLN
1	E	199	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	17	GLN
1	F	258	GLN
1	G	6	HIS
1	G	36	HIS
1	G	80	ASN
1	G	113	ASN
1	G	134	GLN
1	G	159	GLN
1	G	175	HIS
1	G	199	HIS
1	G	316	GLN
1	H	219	GLN
1	H	323	GLN
1	I	31	HIS
1	I	36	HIS
1	I	93	ASN
1	I	130	HIS
1	I	143	HIS
1	I	152	HIS
1	I	316	GLN
1	J	36	HIS
1	J	159	GLN
1	J	199	HIS
1	K	323	GLN
1	L	159	GLN
1	L	316	GLN
1	L	343	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 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	-	5,5,5	2.78	1 (20%)	6,6,6	2.46	2 (33%)
3	OXL	L	401	-	5,5,5	2.42	2 (40%)	6,6,6	2.02	2 (33%)
3	OXL	I	401	4	5,5,5	2.40	1 (20%)	6,6,6	1.89	2 (33%)
3	OXL	F	401	4	5,5,5	2.55	1 (20%)	6,6,6	1.95	2 (33%)
2	TRS	B	401	-	7,7,7	0.36	0	9,9,9	0.26	0
2	TRS	A	401	-	7,7,7	0.29	0	9,9,9	0.32	0
2	TRS	G	401	-	7,7,7	0.89	0	9,9,9	0.92	0
2	TRS	J	401	-	7,7,7	0.72	0	9,9,9	5.99	6 (66%)

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	-	-	4/4/4/4	-
3	OXL	L	401	-	-	4/4/4/4	-
3	OXL	I	401	4	-	4/4/4/4	-
3	OXL	F	401	4	-	4/4/4/4	-
2	TRS	B	401	-	-	3/9/9/9	-
2	TRS	A	401	-	-	2/9/9/9	-
2	TRS	G	401	-	-	1/9/9/9	-
2	TRS	J	401	-	-	7/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	OXL	C2-C1	-5.44	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	OXL	C2-C1	-4.76	1.46	1.54
3	L	401	OXL	C2-C1	-4.38	1.47	1.54
3	I	401	OXL	C2-C1	-4.36	1.47	1.54
3	L	401	OXL	O4-C2	-2.05	1.25	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	TRS	C3-C-N	-11.06	79.95	108.17
2	J	401	TRS	C2-C-N	-10.05	82.55	108.17
2	J	401	TRS	C1-C-N	-8.45	86.62	108.17
3	C	401	OXL	O4-C2-C1	4.71	121.97	112.83
3	L	401	OXL	O3-C1-C2	3.47	119.57	112.83
3	F	401	OXL	O4-C2-C1	3.19	119.03	112.83
2	J	401	TRS	C2-C-C1	3.19	119.16	110.66
3	F	401	OXL	O3-C1-C2	3.19	119.01	112.83
3	I	401	OXL	O4-C2-C1	3.10	118.84	112.83
3	L	401	OXL	O4-C2-C1	3.03	118.70	112.83
3	I	401	OXL	O3-C1-C2	2.98	118.61	112.83
2	J	401	TRS	C3-C-C2	2.92	118.44	110.66
2	J	401	TRS	C3-C-C1	2.78	118.06	110.66
3	C	401	OXL	O3-C1-C2	2.34	117.36	112.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	401	TRS	C2-C-C1-O1
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
3	L	401	OXL	O1-C1-C2-O2
3	I	401	OXL	O1-C1-C2-O4
3	L	401	OXL	O1-C1-C2-O4
3	L	401	OXL	O3-C1-C2-O2
3	I	401	OXL	O1-C1-C2-O2
3	I	401	OXL	O3-C1-C2-O4
3	L	401	OXL	O3-C1-C2-O4
3	I	401	OXL	O3-C1-C2-O2
3	C	401	OXL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

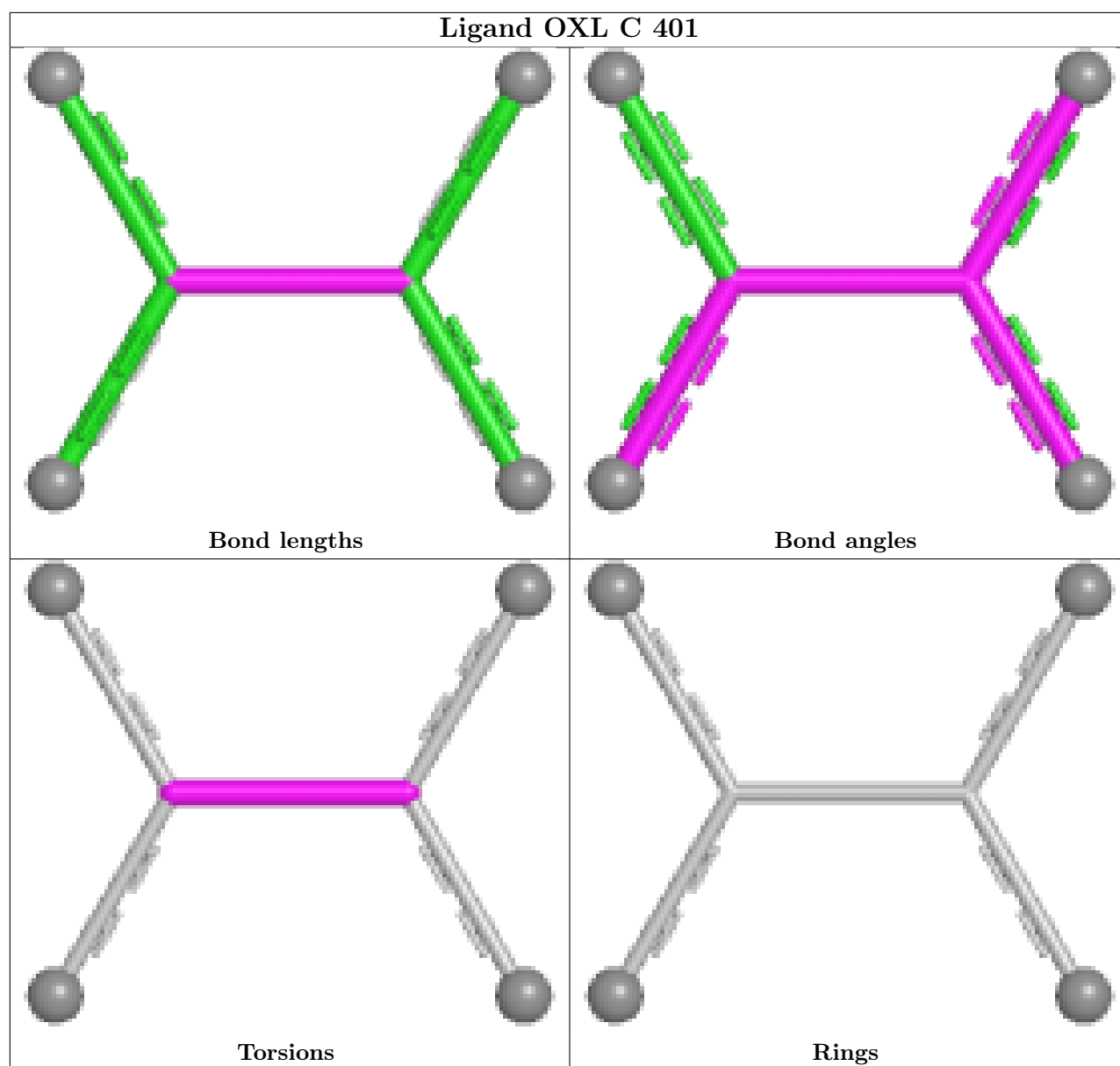
Mol	Chain	Res	Type	Atoms
3	C	401	OXL	O3-C1-C2-O4
3	C	401	OXL	O1-C1-C2-O4
3	C	401	OXL	O3-C1-C2-O2
3	F	401	OXL	O1-C1-C2-O2
3	F	401	OXL	O3-C1-C2-O4
3	F	401	OXL	O1-C1-C2-O4
3	F	401	OXL	O3-C1-C2-O2
2	B	401	TRS	N-C-C3-O3
2	B	401	TRS	C2-C-C3-O3
2	B	401	TRS	C1-C-C3-O3
2	A	401	TRS	C1-C-C3-O3
2	G	401	TRS	C3-C-C2-O2
2	J	401	TRS	C3-C-C1-O1
2	A	401	TRS	N-C-C3-O3

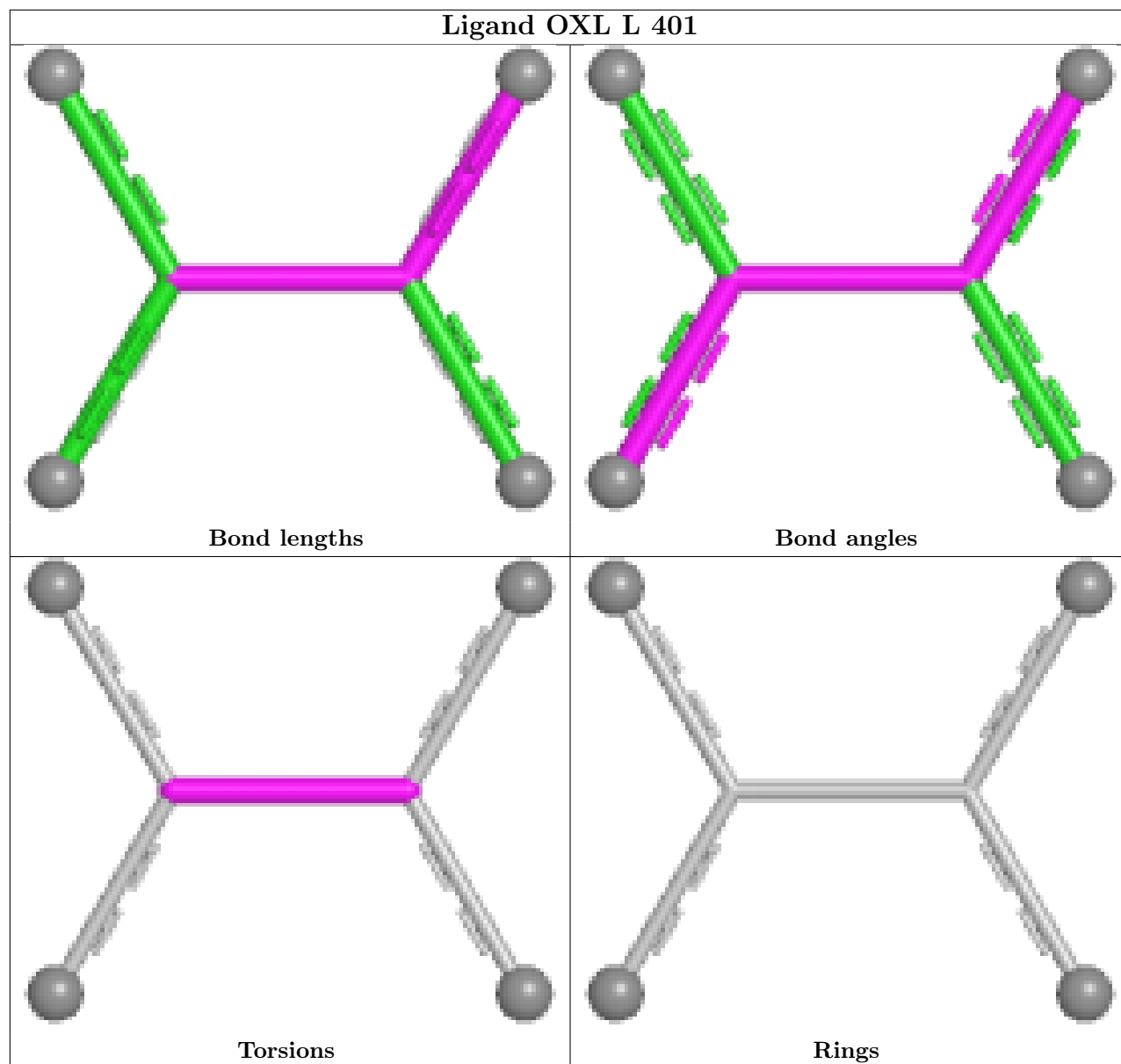
There are no ring outliers.

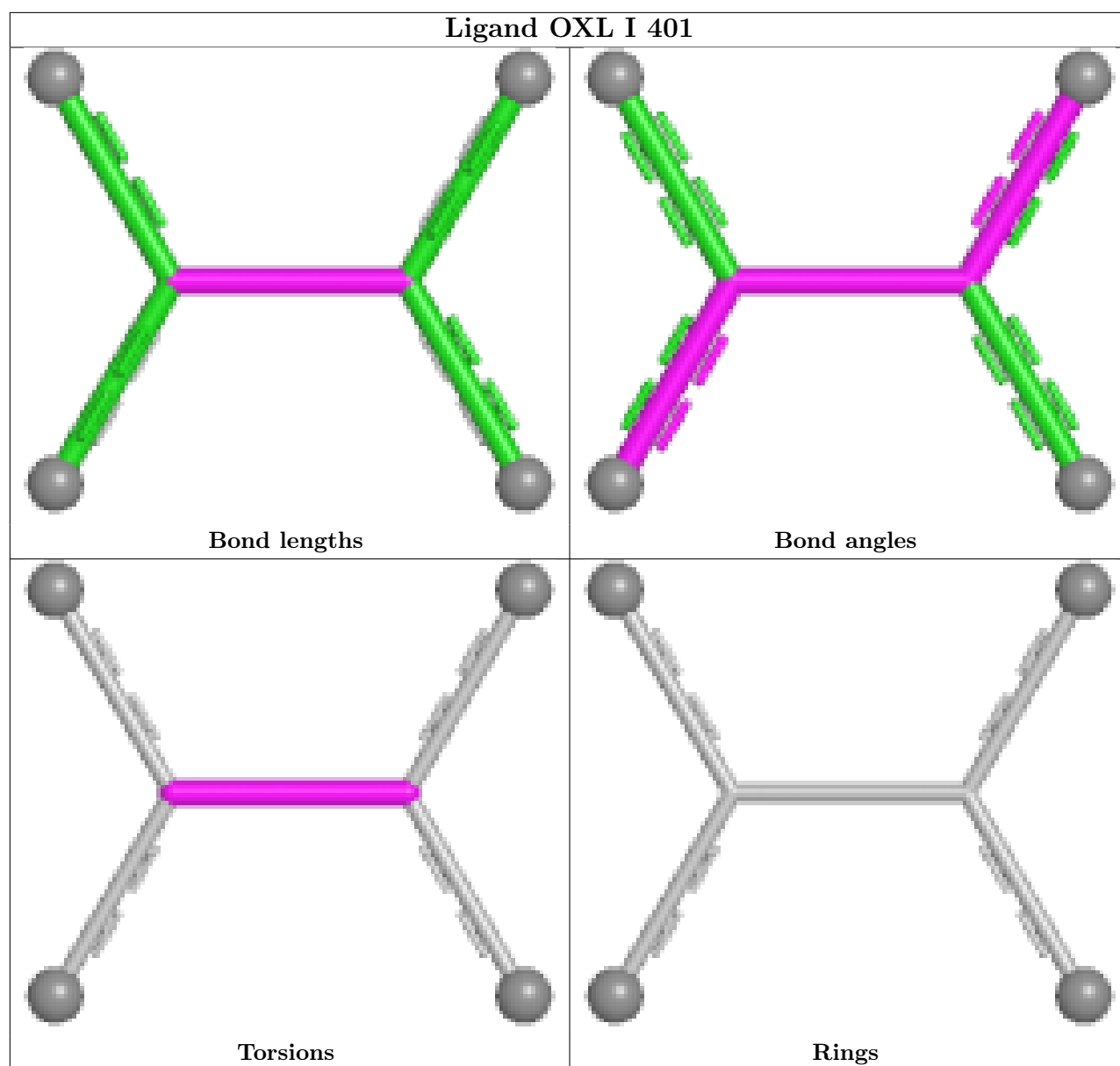
4 monomers are involved in 5 short contacts:

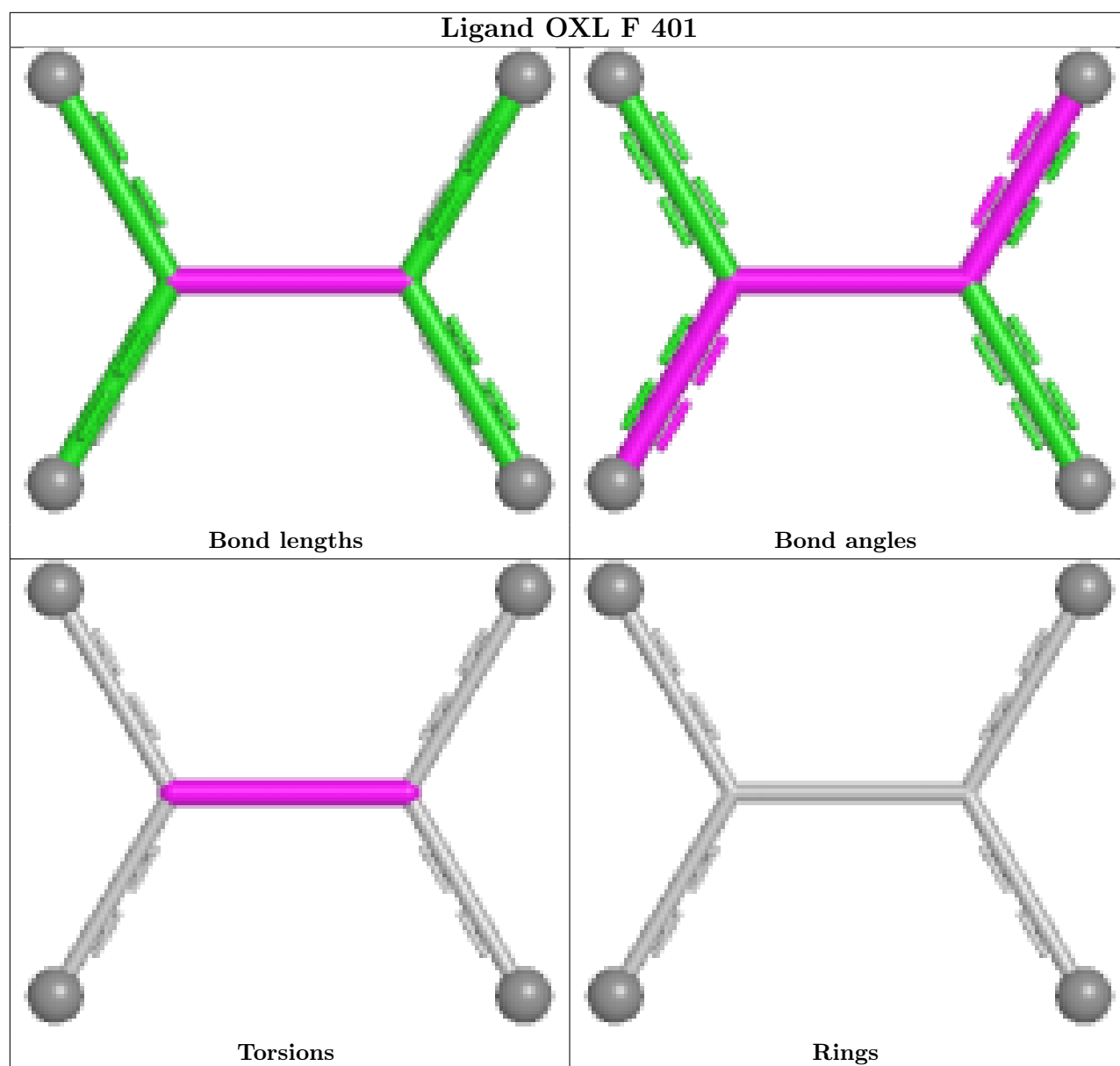
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	OXL	1	0
3	F	401	OXL	1	0
2	A	401	TRS	2	0
2	G	401	TRS	1	0

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









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%)	-0.03	16 (4%)	35	29	22, 40, 93, 109	0
1	B	345/347 (99%)	-0.08	15 (4%)	40	33	24, 42, 97, 127	0
1	C	343/347 (98%)	-0.31	6 (1%)	69	65	21, 37, 74, 96	0
1	D	328/347 (94%)	0.01	12 (3%)	45	39	26, 45, 93, 109	0
1	E	347/347 (100%)	-0.08	1 (0%)	90	89	27, 47, 76, 106	0
1	F	342/347 (98%)	0.12	6 (1%)	67	64	30, 52, 75, 99	0
1	G	325/347 (93%)	0.63	25 (7%)	19	16	42, 72, 109, 130	0
1	H	316/347 (91%)	0.10	18 (5%)	29	24	31, 47, 100, 118	0
1	I	345/347 (99%)	0.72	20 (5%)	29	24	41, 74, 104, 120	0
1	J	346/347 (99%)	0.49	7 (2%)	65	61	36, 64, 93, 111	0
1	K	327/347 (94%)	0.71	24 (7%)	21	17	45, 71, 109, 123	0
1	L	342/347 (98%)	0.15	6 (1%)	67	64	31, 55, 90, 105	0
All	All	4035/4164 (96%)	0.20	156 (3%)	43	36	21, 54, 98, 130	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.2
1	D	311	ILE	5.1
1	G	335	ALA	5.0
1	A	341	LEU	4.9
1	D	319	ALA	4.8
1	G	5	ILE	4.2
1	L	1	MET	4.2
1	B	19	ILE	4.1
1	D	293	LEU	4.1
1	G	4	PRO	4.0
1	G	19	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	11	LEU	3.9
1	A	16	PRO	3.8
1	H	321	TRP	3.8
1	C	1	MET	3.7
1	B	23	PRO	3.7
1	G	314	LYS	3.6
1	F	339	PRO	3.6
1	A	19	ILE	3.6
1	G	12	ALA	3.5
1	B	197	GLY	3.5
1	C	196	GLY	3.5
1	K	1	MET	3.5
1	K	321	TRP	3.4
1	B	196	GLY	3.4
1	G	6	HIS	3.4
1	B	11	LEU	3.4
1	B	301	ALA	3.4
1	I	44	ILE	3.3
1	D	321	TRP	3.3
1	L	309	ALA	3.3
1	G	211	GLY	3.2
1	H	8	TYR	3.2
1	H	335	ALA	3.2
1	I	341	LEU	3.2
1	G	307	GLY	3.2
1	I	308	VAL	3.2
1	J	1	MET	3.1
1	K	314	LYS	3.1
1	H	320	THR	3.1
1	H	308	VAL	3.1
1	K	324	ALA	3.1
1	K	344	ALA	3.1
1	G	22	LEU	3.0
1	I	211	GLY	3.0
1	C	193	THR	3.0
1	A	13	ALA	3.0
1	H	309	ALA	3.0
1	K	328	VAL	3.0
1	I	63	PRO	3.0
1	G	315	MET	3.0
1	G	198	GLY	3.0
1	G	309	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	313	GLY	2.9
1	A	3	LEU	2.9
1	I	339	PRO	2.9
1	I	1	MET	2.9
1	D	309	ALA	2.9
1	C	307	GLY	2.8
1	H	16	PRO	2.8
1	H	313	GLY	2.8
1	G	193	THR	2.8
1	B	5	ILE	2.7
1	K	45	PRO	2.7
1	K	325	LYS	2.7
1	D	292	VAL	2.7
1	K	61	ALA	2.7
1	B	9	LYS	2.7
1	A	339	PRO	2.7
1	G	16	PRO	2.7
1	I	327	ILE	2.7
1	B	315	MET	2.6
1	F	1	MET	2.6
1	D	313	GLY	2.6
1	G	13	ALA	2.6
1	I	345	TYR	2.6
1	F	347	PHE	2.6
1	G	24	VAL	2.6
1	H	331	ALA	2.6
1	A	310	MET	2.6
1	K	327	ILE	2.5
1	H	15	ALA	2.5
1	L	196	GLY	2.5
1	L	193	THR	2.5
1	D	337	LYS	2.5
1	B	7	PHE	2.5
1	I	201	PHE	2.5
1	G	294	PHE	2.4
1	I	342	ALA	2.4
1	L	192	THR	2.4
1	H	11	LEU	2.4
1	B	214	HIS	2.4
1	A	208	PRO	2.4
1	K	287	PRO	2.4
1	K	308	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	295	ALA	2.4
1	G	7	PHE	2.4
1	G	48	ALA	2.4
1	D	314	LYS	2.4
1	H	315	MET	2.4
1	B	15	ALA	2.4
1	I	335	ALA	2.4
1	K	111	VAL	2.3
1	I	309	ALA	2.3
1	A	315	MET	2.3
1	A	305	GLY	2.3
1	K	195	VAL	2.3
1	H	13	ALA	2.3
1	K	40	ILE	2.3
1	K	39	LYS	2.3
1	C	308	VAL	2.3
1	J	101	LEU	2.3
1	A	298	ILE	2.2
1	G	293	LEU	2.2
1	H	195	VAL	2.2
1	J	32	PHE	2.2
1	K	75	ILE	2.2
1	I	193	THR	2.2
1	E	313	GLY	2.2
1	F	196	GLY	2.2
1	H	293	LEU	2.2
1	J	195	VAL	2.2
1	J	194	ARG	2.2
1	B	4	PRO	2.2
1	I	14	GLY	2.2
1	K	315	MET	2.2
1	G	201	PHE	2.2
1	I	33	PHE	2.2
1	I	298	ILE	2.2
1	H	208	PRO	2.2
1	D	328	VAL	2.2
1	A	4	PRO	2.1
1	A	23	PRO	2.1
1	I	291	GLU	2.1
1	D	329	ASP	2.1
1	H	334	ILE	2.1
1	K	214	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	47	VAL	2.1
1	L	337	LYS	2.1
1	H	303	PRO	2.1
1	K	345	TYR	2.1
1	G	39	LYS	2.1
1	J	214	HIS	2.1
1	D	327	ILE	2.1
1	A	292	VAL	2.1
1	K	24	VAL	2.1
1	F	74	PHE	2.1
1	B	194	ARG	2.0
1	J	61	ALA	2.0
1	K	87	ALA	2.0
1	C	303	PRO	2.0
1	I	45	PRO	2.0
1	K	313	GLY	2.0
1	F	201	PHE	2.0
1	K	34	PRO	2.0
1	G	292	VAL	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($\text{\AA}^2$)	Q<0.9
3	OXL	L	401	6/6	0.74	0.14	67,67,69,70	0
4	MG	F	402	1/1	0.77	0.16	59,59,59,59	0
3	OXL	C	401	6/6	0.81	0.14	39,44,45,47	0
3	OXL	F	401	6/6	0.85	0.20	48,49,50,50	0

Continued on next page...

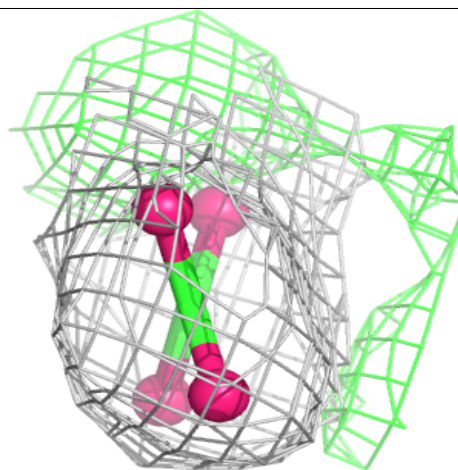
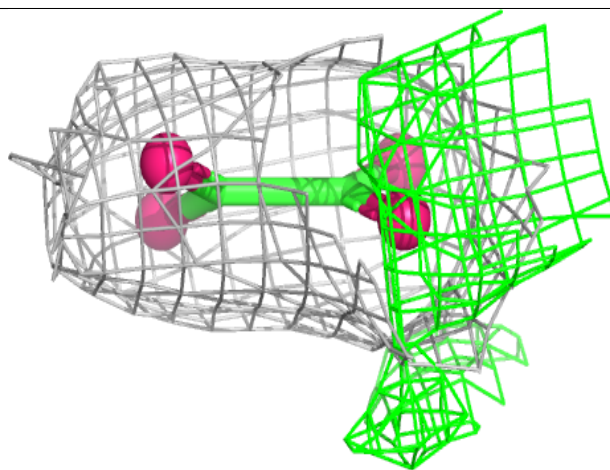
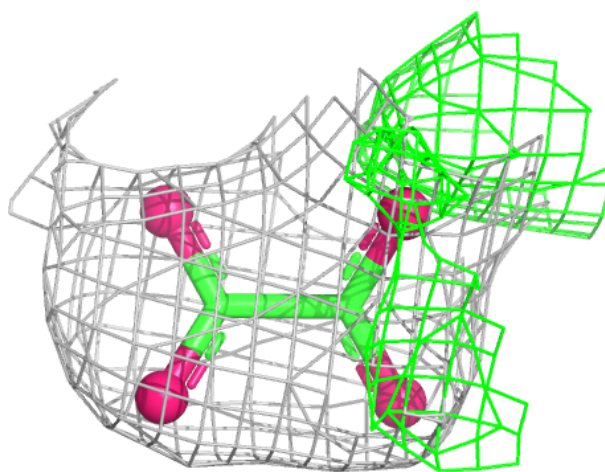
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRS	A	401	8/8	0.86	0.15	40,40,41,42	0
2	TRS	B	401	8/8	0.87	0.12	34,35,35,36	0
3	OXL	I	401	6/6	0.87	0.12	78,84,87,91	0
2	TRS	G	401	8/8	0.92	0.09	57,58,58,60	0
4	MG	I	402	1/1	0.92	0.07	78,78,78,78	0
2	TRS	J	401	8/8	0.96	0.08	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.

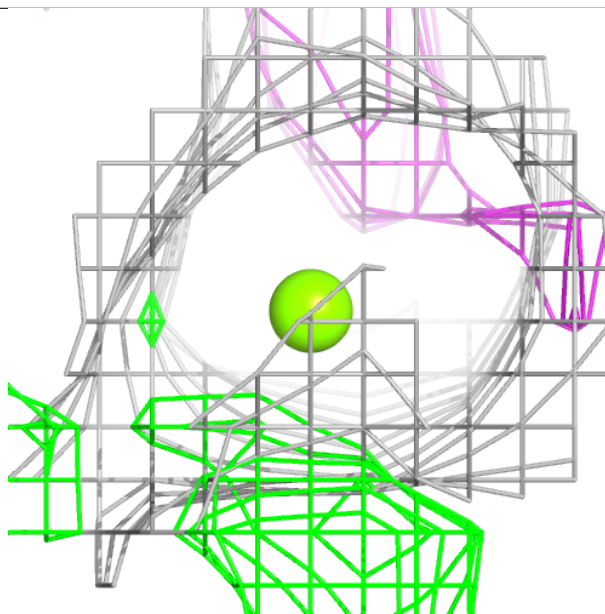
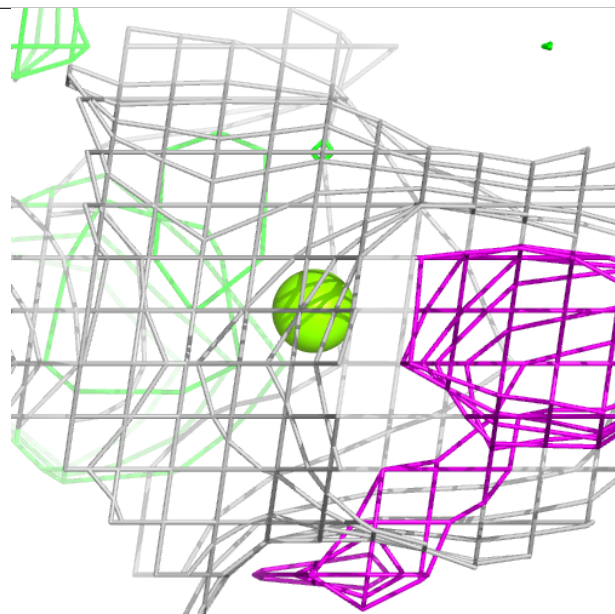
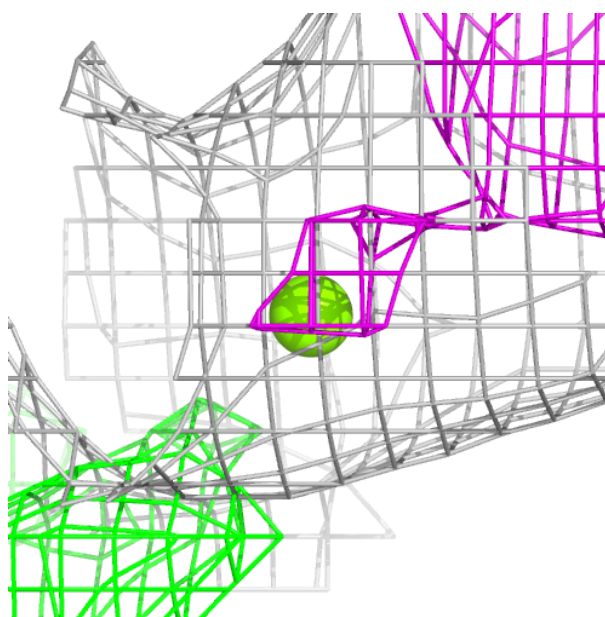
Electron density around OXL L 401:

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



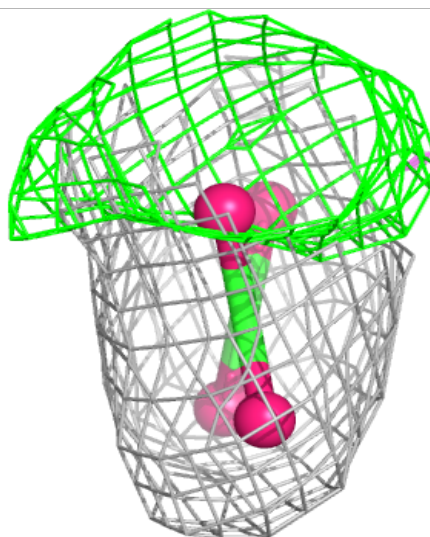
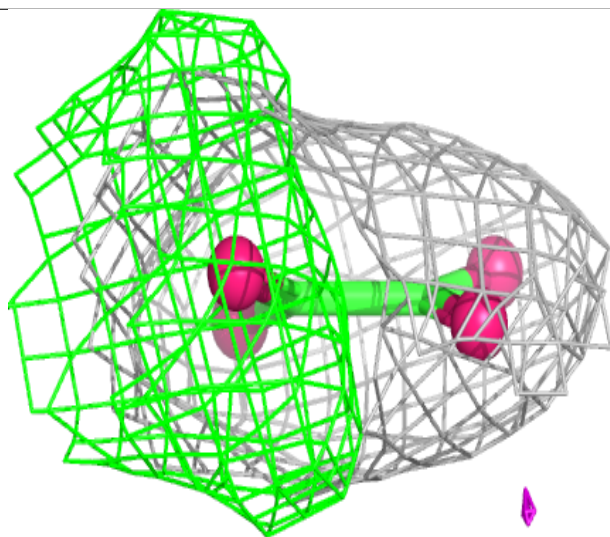
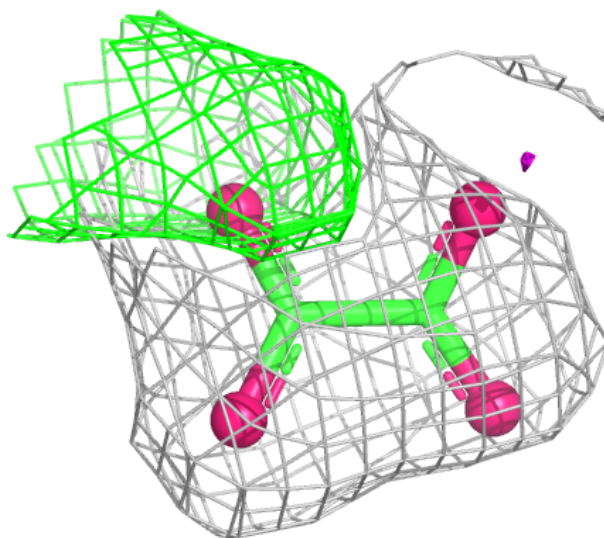
Electron density around MG F 402:

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



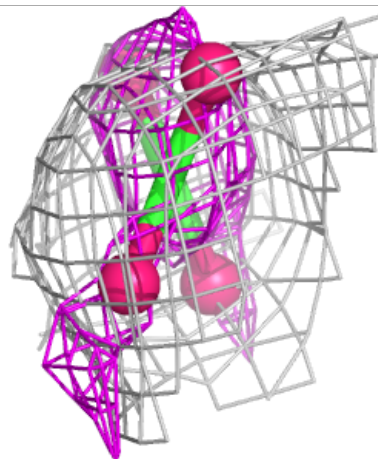
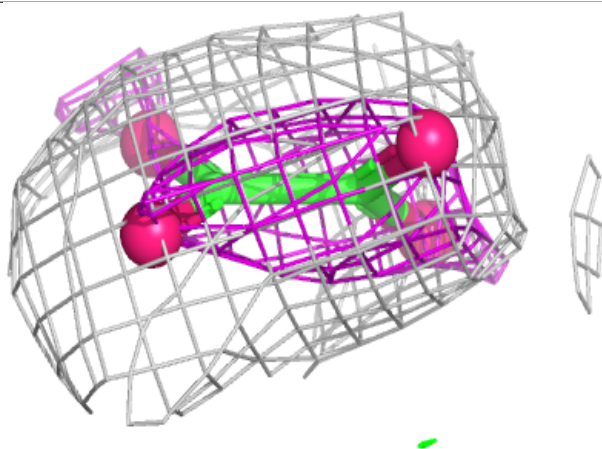
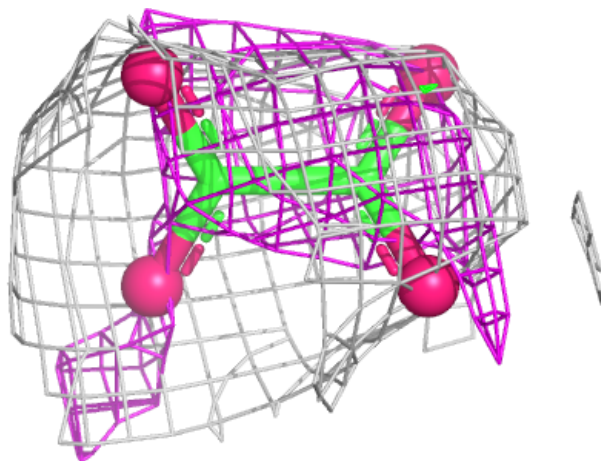
Electron density around OXL C 401:

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



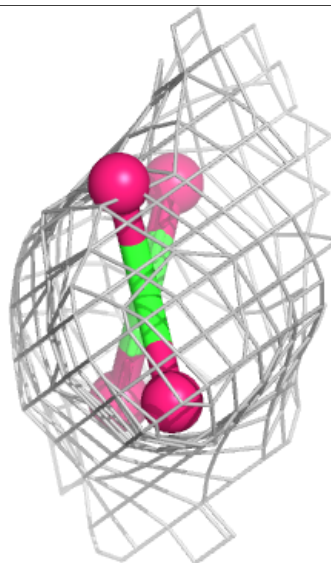
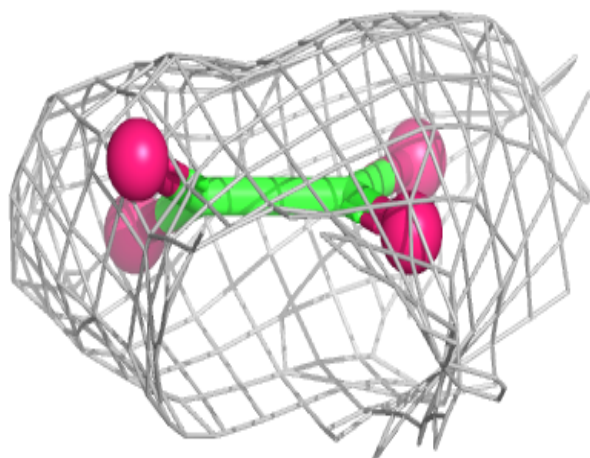
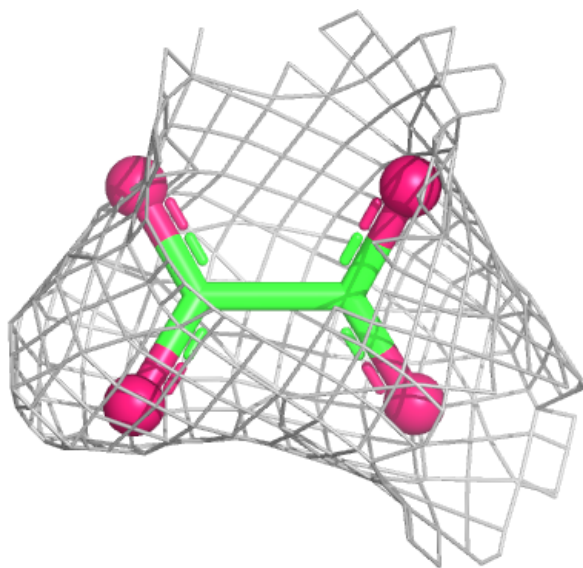
Electron density around OXL F 401:

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



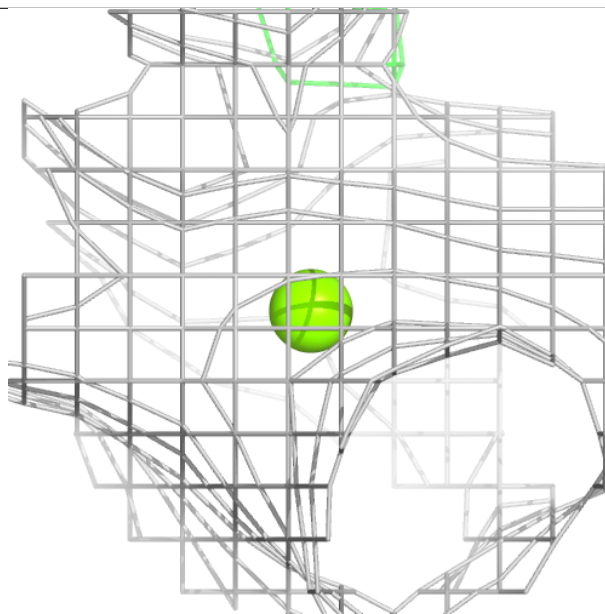
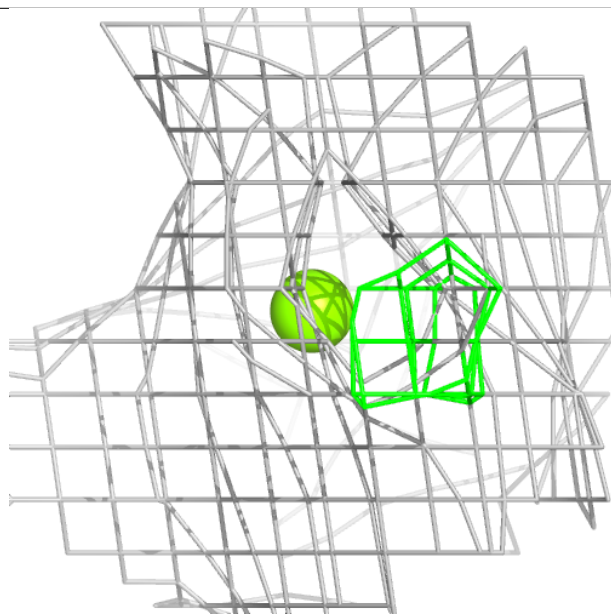
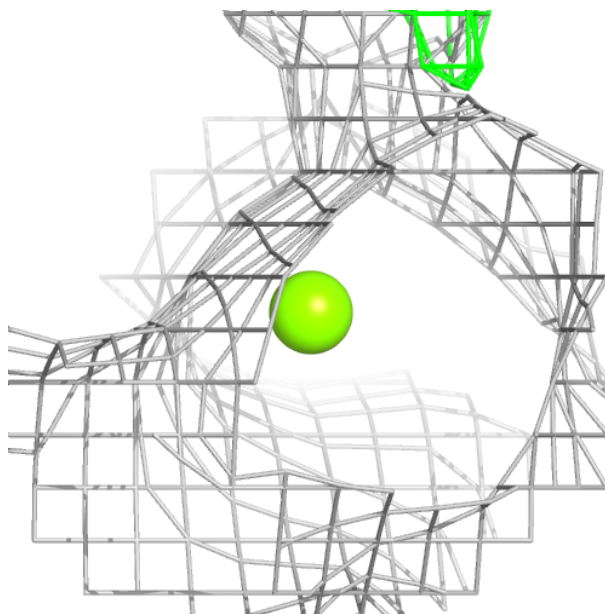
Electron density around OXL I 401:

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



Electron density around MG I 402:

$2mF_o-DF_c$ (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.