



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:12 PM EDT

PDB ID : 7RB1
Title : Isocitrate Lyase-1 from Mycobacterium tuberculosis covalently modified by 5
-descarboxy-5-nitro-D-isocitric acid
Authors : Krieger, I.V.; Mellott, D.; Meek, T.; Sacchetti, J.C.
Deposited on : 2021-07-05
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

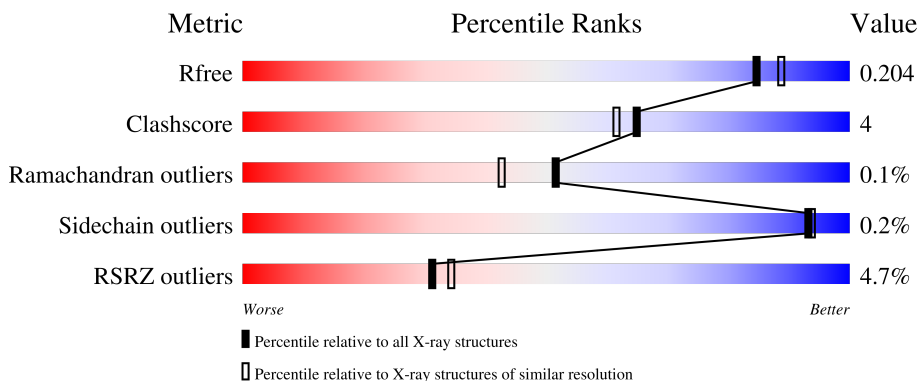
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	428	4% 92% 8%
1	B	428	2% 91% 9%
1	C	428	5% 89% 10%
1	D	428	8% 89% 10%

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
5	GOL	A	507	-	-	X	-
5	GOL	B	506	-	-	X	-

2 Entry composition [i](#)

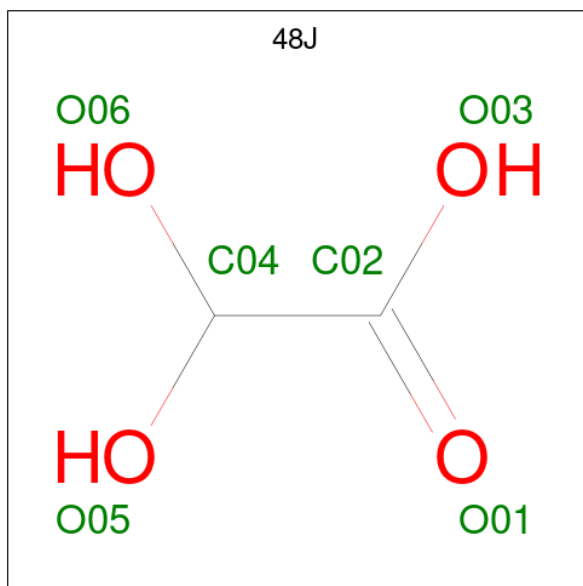
There are 7 unique types of molecules in this entry. The entry contains 14201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	Total 3330	C 2092	N 581	O 648	S 9	0	3	0
1	B	427	Total 3322	C 2087	N 578	O 648	S 9	0	2	0
1	C	427	Total 3324	C 2088	N 581	O 646	S 9	0	2	0
1	D	427	Total 3308	C 2078	N 575	O 646	S 9	0	0	0

- Molecule 2 is dihydroxyacetic acid (three-letter code: 48J) (formula: C₂H₄O₄).



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

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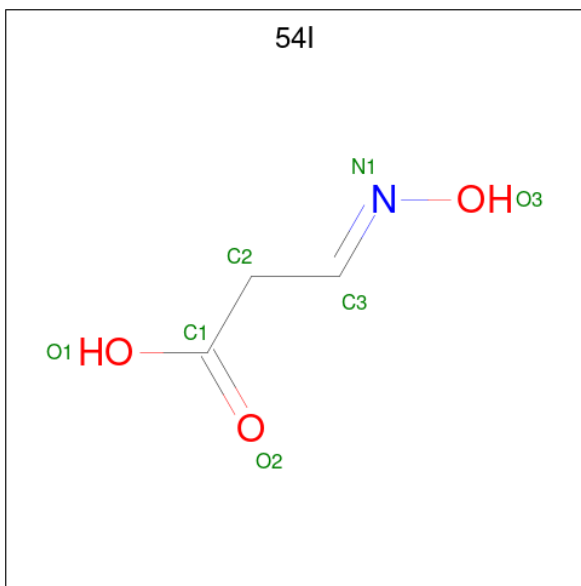
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	2	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is (3E)-3-(hydroxyimino)propanoic acid (three-letter code: 54I) (formula: C₃H₅NO₃) (labeled as "Ligand of Interest" by depositor).



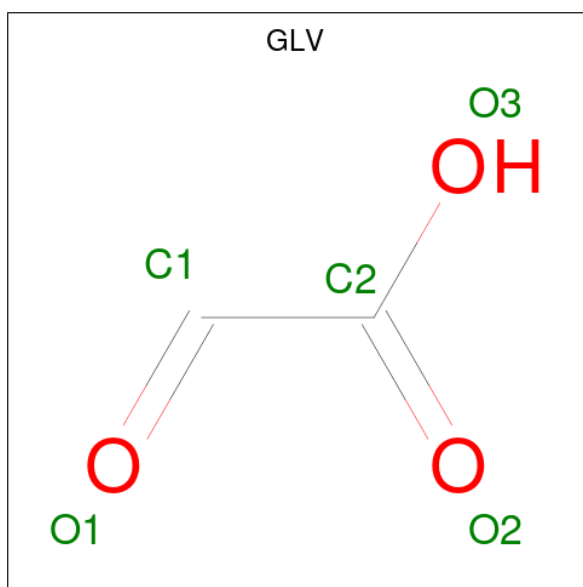
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	3	1	3		
4	B	1	Total	C	N	O	0	0
			7	3	1	3		
4	C	1	Total	C	N	O	0	0
			7	3	1	3		
4	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is GLYOXYLIC ACID (three-letter code: GLV) (formula: $C_2H_2O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			5	2	3		

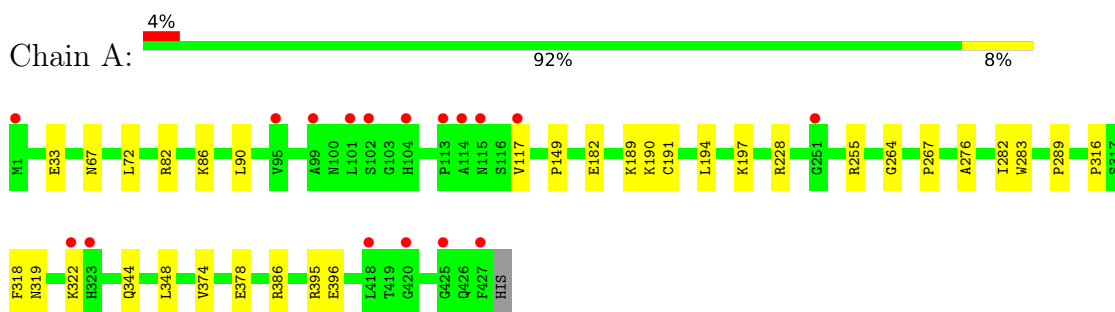
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	208	Total	O	0	0
			208	208		
7	C	190	Total	O	0	0
			190	190		
7	D	201	Total	O	0	0
			201	201		

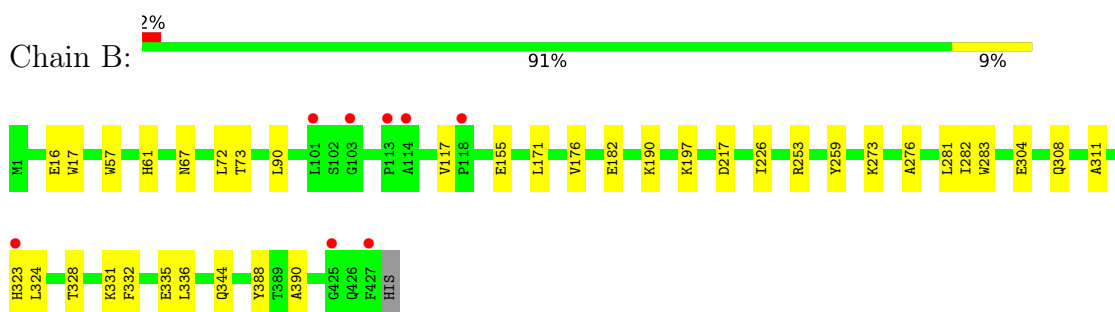
3 Residue-property plots [i](#)

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.

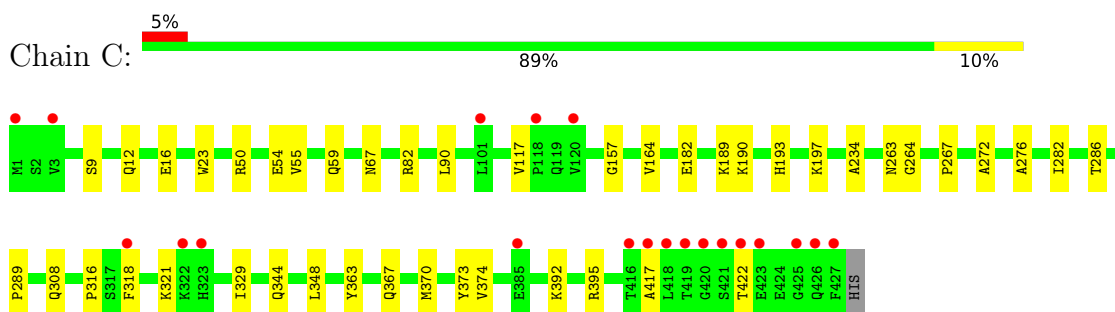
- Molecule 1: Isocitrate lyase



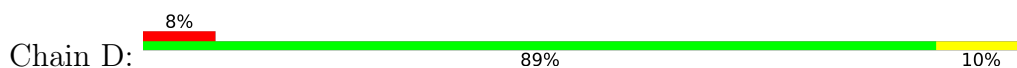
- Molecule 1: Isocitrate lyase

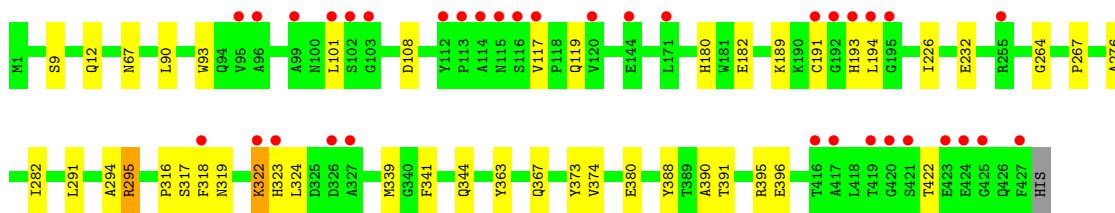


- Molecule 1: Isocitrate lyase



- Molecule 1: Isocitrate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.07Å 140.30Å 160.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 1.90 43.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.57-1.90) 94.7 (43.60-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.171 , 0.204 0.171 , 0.204	Depositor DCC
R_{free} test set	6645 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14201	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: 48J, MG, 54I, GOL, GLV

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	0.49	0/3410	0.66	0/4635
1	B	0.47	0/3399	0.61	0/4621
1	C	0.47	0/3401	0.64	0/4623
1	D	0.46	0/3379	0.62	0/4595
All	All	0.47	0/13589	0.63	0/18474

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	3330	0	3221	24	0
1	B	3322	0	3208	25	0
1	C	3324	0	3215	32	0
1	D	3308	0	3189	32	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	1	0
5	A	18	0	24	5	0
5	B	12	0	16	5	0
5	C	12	0	16	1	0
5	D	6	0	7	0	0
6	D	5	0	1	0	0
7	A	211	0	0	5	0
7	B	208	0	0	1	0
7	C	190	0	0	3	0
7	D	201	0	0	0	0
All	All	14201	0	12897	107	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 (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HH21	5:A:507:GOL:H11	1.30	0.95
1:B:17:TRP:HE1	5:B:506:GOL:H32	1.38	0.86
1:C:373:TYR:OH	1:D:316:PRO:HB3	1.96	0.66
1:D:395:ARG:NH1	1:D:396:GLU:OE1	2.25	0.65
1:A:319:ASN:HB3	7:B:605:HOH:O	1.96	0.65
1:B:273:LYS:HE2	1:B:304:GLU:HG3	1.76	0.65
1:C:316:PRO:HG2	1:C:348:LEU:HB2	1.79	0.65
1:A:182[B]:GLU:OE2	1:A:189:LYS:NZ	2.22	0.65
1:C:289:PRO:HD3	1:C:318:PHE:CG	2.32	0.64
1:C:189:LYS:NZ	7:C:602:HOH:O	2.30	0.64
1:A:191:CYS:HB3	1:A:194:LEU:HG	1.79	0.64
1:C:276:ALA:HA	1:C:282:ILE:HD11	1.80	0.64
1:B:90:LEU:HD22	1:B:117:VAL:HG13	1.79	0.64
1:D:380:GLU:HB3	1:D:391:THR:HG22	1.80	0.63
1:A:264:GLY:O	1:A:267:PRO:HD2	1.99	0.62
1:A:82:ARG:HH21	5:A:507:GOL:C1	2.08	0.62
1:B:276:ALA:HA	1:B:282:ILE:HD11	1.82	0.61
1:D:264:GLY:O	1:D:267:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16[B]:GLU:OE1	5:B:506:GOL:O2	2.21	0.58
1:D:295:ARG:HA	1:D:339:MET:HE3	1.84	0.58
1:C:9:SER:OG	1:C:12:GLN:HG3	2.03	0.58
1:C:82:ARG:NH2	7:C:605:HOH:O	2.31	0.58
1:C:23:TRP:HZ2	5:C:506:GOL:H31	1.68	0.57
1:A:255:ARG:HG2	7:A:744:HOH:O	2.04	0.57
1:C:55:VAL:O	1:C:59:GLN:HG3	2.05	0.56
1:C:182:GLU:OE1	1:C:189:LYS:HE2	2.04	0.56
1:C:316:PRO:HB3	1:D:373:TYR:OH	2.05	0.55
1:A:386[B]:ARG:NH2	7:A:603:HOH:O	2.40	0.55
1:C:50:ARG:O	1:C:54:GLU:HG3	2.08	0.54
1:B:388:TYR:CZ	1:B:390:ALA:HB3	2.42	0.54
1:C:190:LYS:HB2	1:C:197:LYS:HG2	1.89	0.54
1:A:276:ALA:HA	1:A:282:ILE:HD11	1.90	0.54
1:C:90:LEU:HD22	1:C:117:VAL:HG13	1.91	0.53
1:D:323:HIS:HB2	1:D:324:LEU:HG	1.92	0.52
1:A:82:ARG:NH2	5:A:507:GOL:H11	2.12	0.51
1:A:318:PHE:HB3	7:A:674:HOH:O	2.10	0.51
1:D:339:MET:HE2	1:D:341:PHE:HE2	1.76	0.51
1:A:33:GLU:HG3	7:A:752:HOH:O	2.11	0.51
1:C:422:THR:OG1	1:D:193:HIS:HB3	2.11	0.51
1:D:317:SER:OG	4:D:504:54I:O1	2.28	0.51
1:D:67:ASN:HA	1:D:344:GLN:O	2.11	0.50
1:D:90:LEU:HD22	1:D:117:VAL:HG13	1.92	0.50
1:A:90:LEU:HD22	1:A:117:VAL:HG13	1.93	0.50
1:C:289:PRO:HD3	1:C:318:PHE:CD2	2.46	0.50
1:D:388:TYR:CZ	1:D:390:ALA:HB3	2.47	0.50
1:C:395:ARG:HH11	1:C:395:ARG:HG3	1.78	0.49
1:D:93:TRP:CD1	1:D:108:ASP:HB2	2.48	0.49
1:B:190:LYS:HB2	1:B:197:LYS:HG2	1.95	0.49
1:A:396:GLU:OE1	5:A:507:GOL:H12	2.12	0.49
1:B:282:ILE:HD12	1:B:308:GLN:HG2	1.94	0.49
1:D:191:CYS:HB3	1:D:194:LEU:HG	1.94	0.48
1:C:370:MET:O	1:C:374:VAL:HG23	2.13	0.48
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.28	0.48
1:C:67:ASN:HA	1:C:344:GLN:O	2.14	0.47
1:B:282:ILE:HD12	1:B:308:GLN:CG	2.45	0.47
1:D:276:ALA:HA	1:D:282:ILE:HD11	1.95	0.47
1:B:331:LYS:O	1:B:335:GLU:HG2	2.14	0.47
1:D:191:CYS:H	1:D:194:LEU:HD12	1.79	0.47
1:B:57:TRP:CE2	1:B:61:HIS:HE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:SER:OG	1:D:12:GLN:HG3	2.15	0.47
1:D:295:ARG:HA	1:D:339:MET:CE	2.44	0.47
1:C:264:GLY:O	1:C:267:PRO:HD2	2.14	0.46
1:A:289:PRO:HD3	1:A:318:PHE:CG	2.49	0.46
1:B:155:GLU:O	1:B:182:GLU:HG2	2.15	0.46
1:A:316:PRO:HG2	1:A:348:LEU:HB2	1.98	0.46
1:B:331:LYS:HD2	1:B:335:GLU:OE2	2.16	0.46
1:C:329:ILE:HD13	1:D:374:VAL:HG21	1.97	0.46
1:A:67:ASN:HA	1:A:344:GLN:O	2.17	0.45
1:D:191:CYS:O	1:D:194:LEU:HB2	2.16	0.45
1:A:190:LYS:HB2	1:A:197:LYS:HG2	1.98	0.45
1:B:328:THR:HA	1:B:331:LYS:HE2	1.97	0.45
1:D:182:GLU:OE2	1:D:189:LYS:HE2	2.16	0.45
1:D:363:TYR:O	1:D:367:GLN:HG2	2.16	0.45
1:B:72:LEU:HD12	1:B:73:THR:HG23	1.98	0.45
1:B:17:TRP:NE1	5:B:506:GOL:H32	2.19	0.45
1:B:67:ASN:HA	1:B:344:GLN:O	2.16	0.45
1:B:171:LEU:HB3	1:B:176:VAL:HG11	1.99	0.44
1:C:272:ALA:HB1	1:C:282:ILE:HG21	1.99	0.44
1:B:217:ASP:OD1	5:B:506:GOL:H31	2.18	0.43
1:B:283:TRP:HB2	1:B:311:ALA:HB3	2.01	0.43
1:D:316:PRO:C	1:D:318:PHE:H	2.22	0.43
1:C:193:HIS:HB3	1:D:422:THR:OG1	2.17	0.43
1:D:319:ASN:O	1:D:322:LYS:HB3	2.19	0.43
1:D:339:MET:HE2	1:D:341:PHE:CE2	2.53	0.43
1:B:226:ILE:HG12	1:B:281:LEU:HB2	2.02	0.42
1:A:374:VAL:O	1:A:378:GLU:HG2	2.20	0.42
1:C:157:GLY:HA3	1:C:164:VAL:HG22	2.02	0.42
1:C:234:ALA:O	1:C:263:ASN:HB3	2.19	0.42
1:D:101:LEU:HD11	1:D:119:GLN:HG3	2.01	0.42
1:C:392:LYS:HE3	1:C:395:ARG:HD3	2.01	0.42
1:A:86:LYS:O	1:A:149:PRO:HD2	2.19	0.41
1:A:395:ARG:HH12	5:A:507:GOL:H31	1.85	0.41
1:B:308:GLN:HA	5:B:505:GOL:H2	2.02	0.41
1:C:321:LYS:HB3	1:C:321:LYS:HE3	1.84	0.41
1:D:291:LEU:HD23	1:D:291:LEU:HA	1.88	0.41
1:A:228:ARG:HA	1:A:283:TRP:O	2.21	0.41
1:C:417:ALA:HB1	1:D:194:LEU:HD13	2.02	0.41
1:D:294:ALA:C	1:D:339:MET:HE1	2.41	0.41
1:B:323:HIS:O	1:B:324:LEU:HD23	2.20	0.41
1:B:332:PHE:CE2	1:B:336:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HD3	1:B:259:TYR:CZ	2.56	0.41
1:C:286:THR:HG22	7:C:607:HOH:O	2.21	0.41
1:A:72:LEU:HD22	7:A:781:HOH:O	2.21	0.40
1:A:322:LYS:HG2	1:A:322:LYS:O	2.20	0.40
1:C:282:ILE:HD12	1:C:308:GLN:HG2	2.03	0.40
1:C:363:TYR:O	1:C:367:GLN:HG2	2.21	0.40
1:D:180:HIS:HB3	1:D:226:ILE:HB	2.03	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	428/428 (100%)	418 (98%)	10 (2%)	0	100	100
1	B	427/428 (100%)	419 (98%)	8 (2%)	0	100	100
1	C	427/428 (100%)	417 (98%)	10 (2%)	0	100	100
1	D	425/428 (99%)	416 (98%)	8 (2%)	1 (0%)	47	38
All	All	1707/1712 (100%)	1670 (98%)	36 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	322	LYS

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	340/339 (100%)	340 (100%)	0	100	100
1	B	339/339 (100%)	339 (100%)	0	100	100
1	C	339/339 (100%)	338 (100%)	1 (0%)	92	93
1	D	337/339 (99%)	335 (99%)	2 (1%)	86	87
All	All	1355/1356 (100%)	1352 (100%)	3 (0%)	93	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	GLU
1	D	232	GLU
1	D	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	119	GLN
1	B	367	GLN
1	C	59	GLN
1	D	129	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
4	54I	B	504	-	5,6,6	0.61	0	5,6,6	3.40	1 (20%)
2	48J	C	501	3	5,5,5	0.91	0	4,6,6	1.56	1 (25%)
5	GOL	A	506	-	5,5,5	0.30	0	5,5,5	0.46	0
2	48J	B	501	3	5,5,5	0.97	0	4,6,6	2.03	1 (25%)
4	54I	C	504	1	5,6,6	1.09	0	5,6,6	5.90	2 (40%)
4	54I	D	504	1	5,6,6	0.67	0	5,6,6	5.13	2 (40%)
5	GOL	C	505	3	5,5,5	0.50	0	5,5,5	0.97	0
5	GOL	C	506	-	5,5,5	0.40	0	5,5,5	0.48	0
5	GOL	B	505	3	5,5,5	0.59	0	5,5,5	0.48	0
2	48J	A	501	3	5,5,5	1.11	0	4,6,6	1.77	2 (50%)
5	GOL	A	505	3	5,5,5	0.62	0	5,5,5	0.64	0
4	54I	A	504	1	5,6,6	0.94	0	5,6,6	5.75	3 (60%)
5	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.55	0
6	GLV	D	501	3	4,4,4	2.31	1 (25%)	3,4,4	1.72	1 (33%)
5	GOL	B	506	-	5,5,5	0.42	0	5,5,5	0.52	0
5	GOL	D	505	3	5,5,5	0.80	0	5,5,5	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	54I	B	504	-	-	2/2/4/4	-
2	48J	C	501	3	-	2/4/4/4	-
5	GOL	A	506	-	-	2/4/4/4	-
2	48J	B	501	3	-	2/4/4/4	-
4	54I	C	504	1	-	2/2/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	54I	D	504	1	-	1/2/4/4	-
5	GOL	C	505	3	-	4/4/4/4	-
5	GOL	C	506	-	-	2/4/4/4	-
5	GOL	B	505	3	-	1/4/4/4	-
2	48J	A	501	3	-	2/4/4/4	-
5	GOL	A	505	3	-	0/4/4/4	-
4	54I	A	504	1	-	2/2/4/4	-
5	GOL	A	507	-	-	4/4/4/4	-
6	GLV	D	501	3	-	0/0/2/2	-
5	GOL	B	506	-	-	0/4/4/4	-
5	GOL	D	505	3	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	501	GLV	C1-C2	4.03	1.53	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	54I	O3-N1-C3	12.61	123.52	111.70
4	A	504	54I	O3-N1-C3	12.25	123.18	111.70
4	D	504	54I	O3-N1-C3	10.96	121.98	111.70
4	B	504	54I	O3-N1-C3	7.21	118.46	111.70
2	B	501	48J	O03-C02-C04	3.21	122.05	113.30
4	D	504	54I	C3-C2-C1	-2.98	107.85	113.70
4	C	504	54I	C3-C2-C1	-2.89	108.03	113.70
2	A	501	48J	O03-C02-C04	2.60	120.39	113.30
2	C	501	48J	O03-C02-C04	2.52	120.16	113.30
4	A	504	54I	C3-C2-C1	-2.51	108.78	113.70
4	A	504	54I	O1-C1-C2	2.21	123.12	114.40
2	A	501	48J	O03-C02-O01	-2.19	119.11	124.09
6	D	501	GLV	O3-C2-C1	2.19	120.26	113.52

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	54I	O2-C1-C2-C3
5	A	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	507	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	C	505	GOL	C1-C2-C3-O3
5	D	505	GOL	O1-C1-C2-C3
5	D	505	GOL	C1-C2-C3-O3
5	D	505	GOL	O2-C2-C3-O3
2	C	501	48J	O03-C02-C04-O05
2	C	501	48J	O01-C02-C04-O05
4	A	504	54I	O1-C1-C2-C3
2	A	501	48J	O01-C02-C04-O06
2	A	501	48J	O03-C02-C04-O06
5	A	506	GOL	O1-C1-C2-O2
2	B	501	48J	O03-C02-C04-O05
2	B	501	48J	O01-C02-C04-O05
5	B	505	GOL	O1-C1-C2-C3
5	C	505	GOL	O1-C1-C2-C3
5	C	506	GOL	C1-C2-C3-O3
5	A	507	GOL	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
5	C	505	GOL	O1-C1-C2-O2
5	D	505	GOL	O1-C1-C2-O2
4	C	504	54I	O1-C1-C2-C3
5	C	505	GOL	O2-C2-C3-O3
4	B	504	54I	O1-C1-C2-C3
4	D	504	54I	O1-C1-C2-C3
5	C	506	GOL	O2-C2-C3-O3
4	B	504	54I	O2-C1-C2-C3
4	C	504	54I	O2-C1-C2-C3

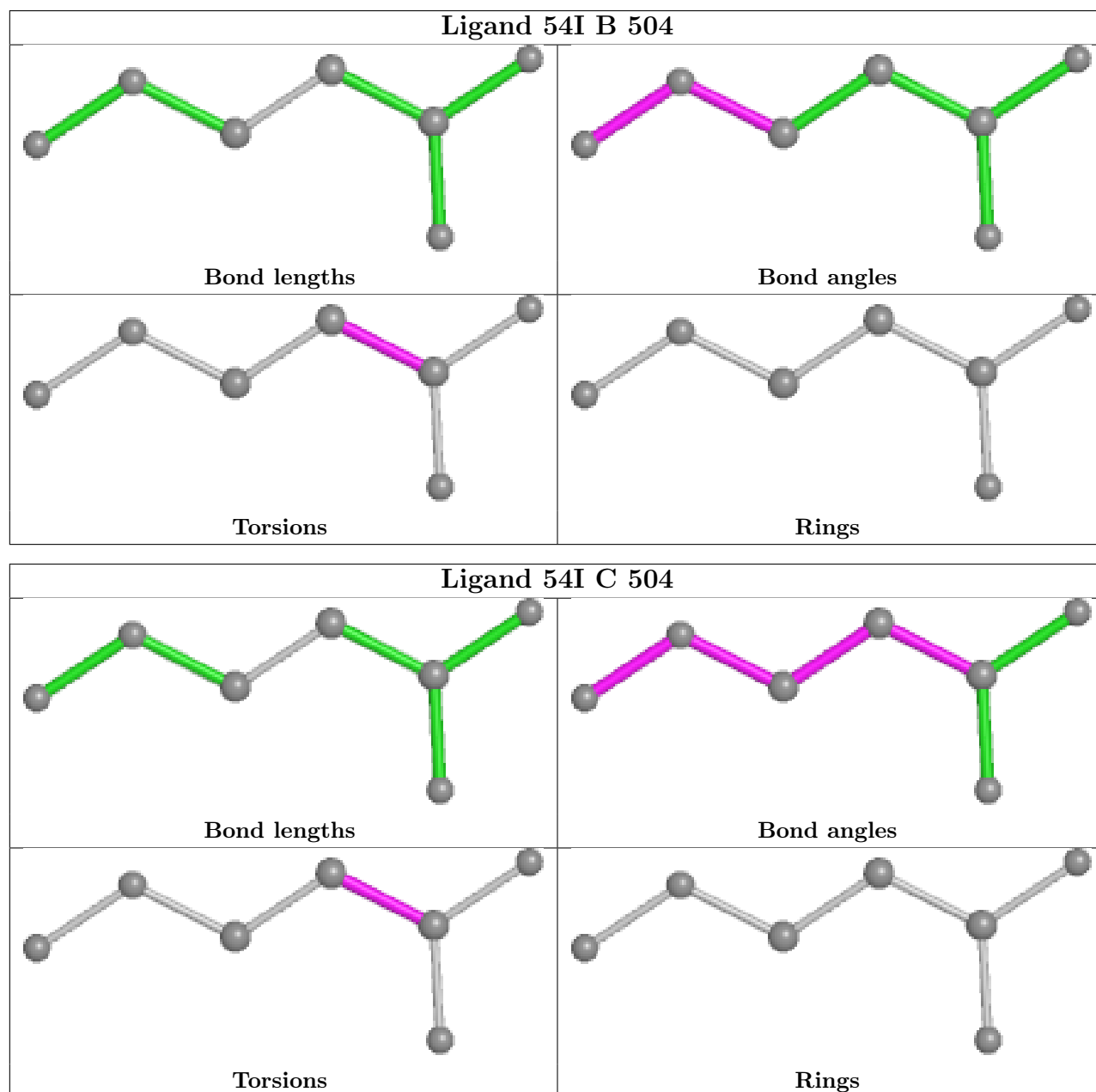
There are no ring outliers.

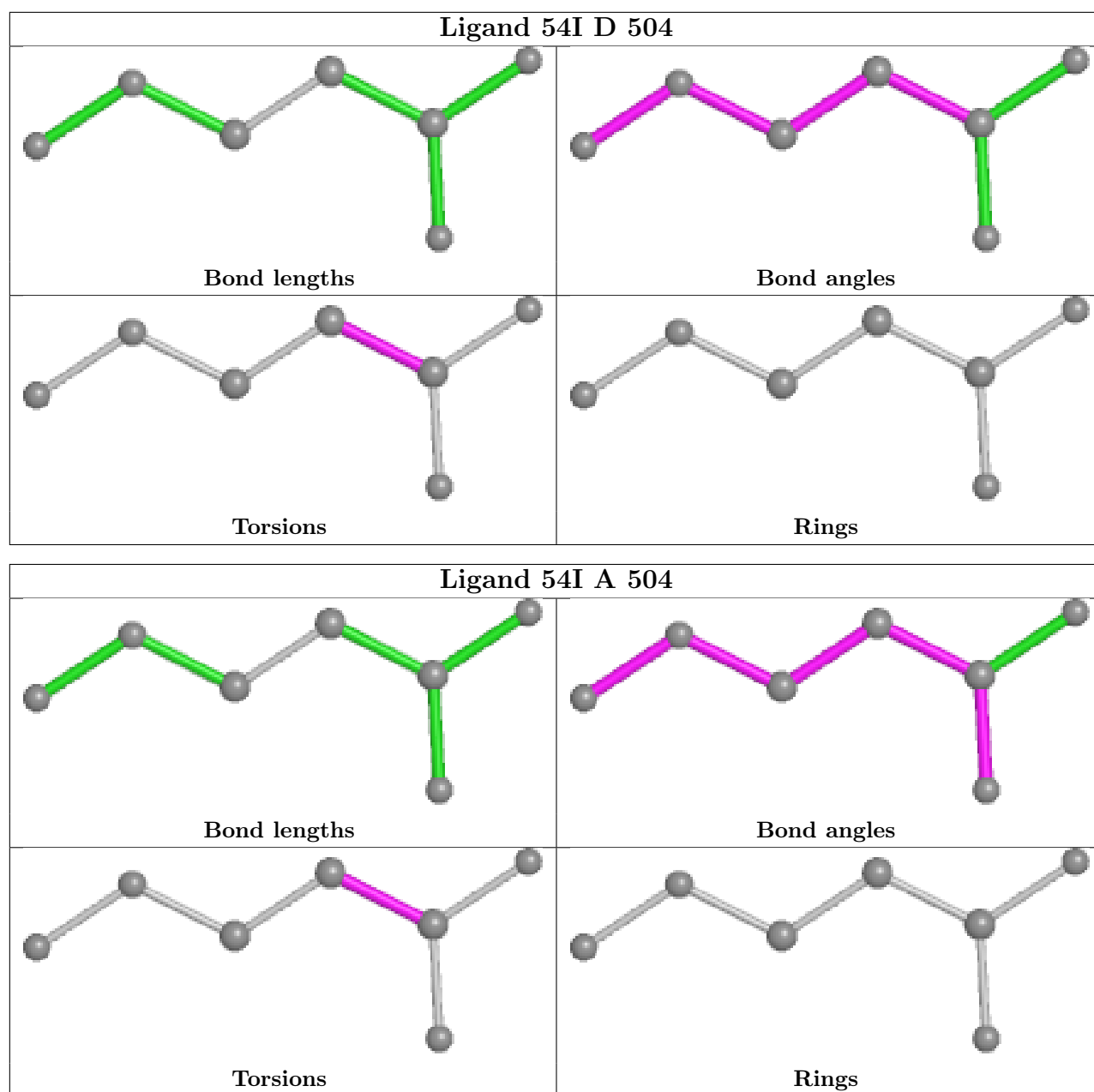
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	54I	1	0
5	C	506	GOL	1	0
5	B	505	GOL	1	0
5	A	507	GOL	5	0
5	B	506	GOL	4	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	427/428 (99%)	0.00	17 (3%) 38 41	18, 28, 46, 61	0
1	B	427/428 (99%)	-0.02	8 (1%) 66 69	19, 30, 44, 60	0
1	C	427/428 (99%)	0.17	20 (4%) 31 34	20, 30, 54, 90	0
1	D	427/428 (99%)	0.21	35 (8%) 11 13	19, 31, 56, 72	0
All	All	1708/1712 (99%)	0.09	80 (4%) 31 34	18, 30, 49, 90	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	427	PHE	9.0
1	C	425	GLY	8.1
1	C	418	LEU	7.3
1	C	426	GLN	5.9
1	D	101	LEU	5.5
1	D	194	LEU	5.4
1	C	417	ALA	5.2
1	C	419	THR	5.1
1	C	416	THR	4.8
1	C	422	THR	4.7
1	C	421	SER	4.3
1	C	420	GLY	4.2
1	D	419	THR	4.2
1	A	323	HIS	4.2
1	D	195	GLY	4.2
1	B	323	HIS	4.1
1	D	425	GLY	4.0
1	D	192	GLY	3.9
1	A	418	LEU	3.8
1	C	423	GLU	3.7
1	B	101	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	427	PHE	3.7
1	C	318	PHE	3.6
1	A	101	LEU	3.6
1	D	95	VAL	3.6
1	D	318	PHE	3.5
1	C	323	HIS	3.4
1	C	322	LYS	3.4
1	A	427	PHE	3.3
1	D	420	GLY	3.2
1	D	114	ALA	3.2
1	C	101	LEU	3.2
1	B	427	PHE	3.2
1	A	117	VAL	3.1
1	B	113	PRO	2.9
1	C	118	PRO	2.9
1	D	417	ALA	2.9
1	D	323	HIS	2.8
1	D	117	VAL	2.8
1	A	1	MET	2.8
1	A	425	GLY	2.7
1	B	118	PRO	2.7
1	C	3	VAL	2.7
1	B	114	ALA	2.6
1	D	112	TYR	2.6
1	C	385	GLU	2.6
1	A	99	ALA	2.6
1	C	1	MET	2.6
1	A	113	PRO	2.5
1	D	423	GLU	2.5
1	D	322	LYS	2.5
1	D	193	HIS	2.5
1	C	120	VAL	2.5
1	D	120	VAL	2.5
1	D	424	GLU	2.4
1	D	116	SER	2.4
1	D	96	ALA	2.4
1	D	102	SER	2.4
1	D	255	ARG	2.3
1	B	425	GLY	2.3
1	B	103	GLY	2.3
1	A	114	ALA	2.3
1	D	326	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	115	ASN	2.2
1	A	102	SER	2.2
1	D	115	ASN	2.2
1	D	113	PRO	2.2
1	D	327	ALA	2.2
1	A	95	VAL	2.2
1	D	103	GLY	2.1
1	D	99	ALA	2.1
1	A	251	GLY	2.1
1	D	421	SER	2.1
1	D	191	CYS	2.1
1	A	420	GLY	2.1
1	D	171	LEU	2.1
1	A	322	LYS	2.0
1	D	144	GLU	2.0
1	A	104	HIS	2.0
1	D	416	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	507	6/6	0.77	0.26	31,40,43,46	0
5	GOL	B	506	6/6	0.78	0.21	26,36,43,47	0
5	GOL	C	506	6/6	0.84	0.24	31,34,46,49	0
4	54I	D	504	7/7	0.85	0.14	46,49,54,60	3
4	54I	C	504	7/7	0.87	0.14	38,42,44,45	5
5	GOL	A	506	6/6	0.90	0.16	32,34,44,47	0

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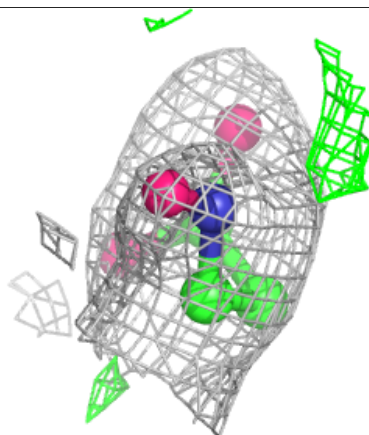
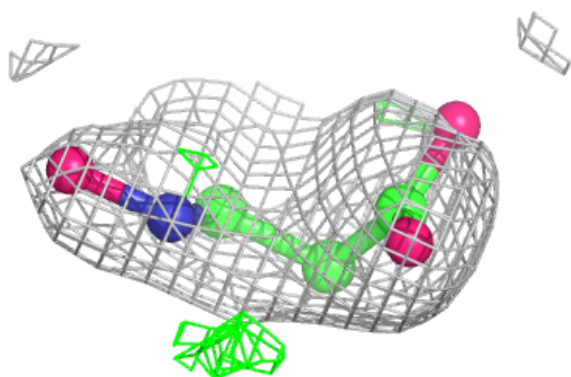
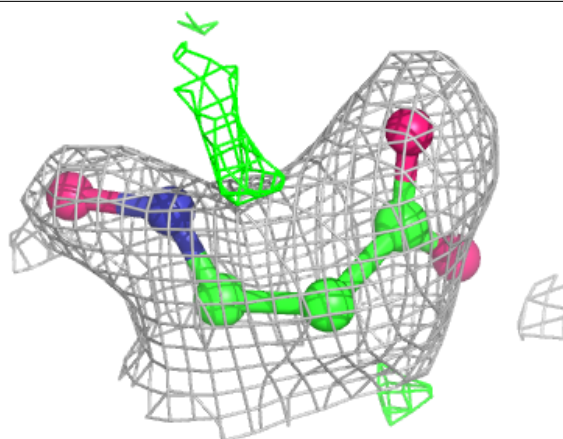
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	54I	A	504	7/7	0.91	0.13	34,35,40,41	5
5	GOL	C	505	6/6	0.92	0.21	26,35,42,46	0
5	GOL	D	505	6/6	0.92	0.16	32,34,40,41	0
4	54I	B	504	7/7	0.93	0.15	35,39,43,44	5
5	GOL	B	505	6/6	0.93	0.17	25,35,39,42	0
3	MG	B	503	1/1	0.95	0.10	31,31,31,31	0
5	GOL	A	505	6/6	0.95	0.15	25,30,36,40	0
2	48J	B	501	6/6	0.95	0.15	26,29,30,34	3
3	MG	B	502	1/1	0.97	0.10	26,26,26,26	0
3	MG	D	502	1/1	0.97	0.12	27,27,27,27	0
3	MG	D	503	1/1	0.97	0.14	29,29,29,29	0
6	GLV	D	501	5/5	0.97	0.12	27,31,35,37	0
3	MG	C	503	1/1	0.98	0.05	26,26,26,26	0
3	MG	A	503	1/1	0.98	0.05	24,24,24,24	0
2	48J	A	501	6/6	0.98	0.09	23,26,27,34	3
2	48J	C	501	6/6	0.98	0.09	26,28,29,37	4
3	MG	A	502	1/1	0.99	0.08	21,21,21,21	0
3	MG	C	502	1/1	0.99	0.06	26,26,26,26	0

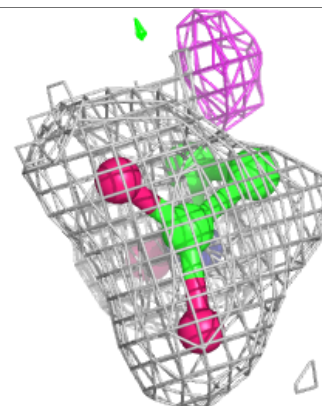
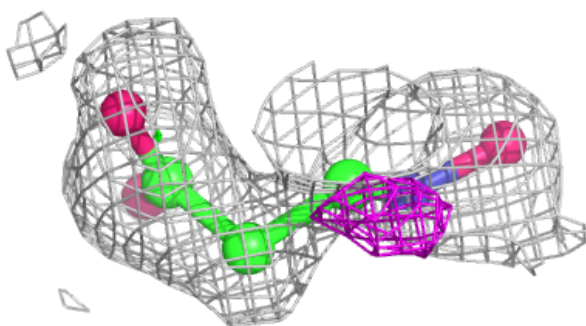
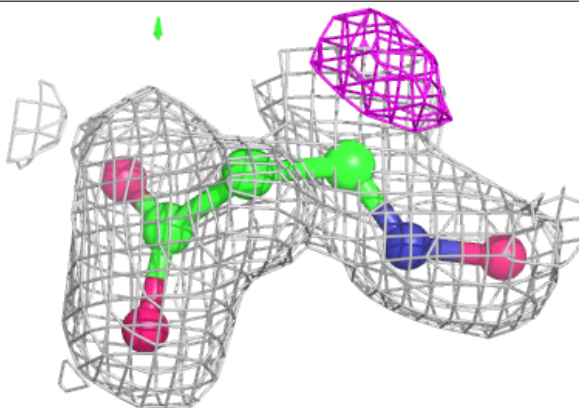
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 54I D 504:

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

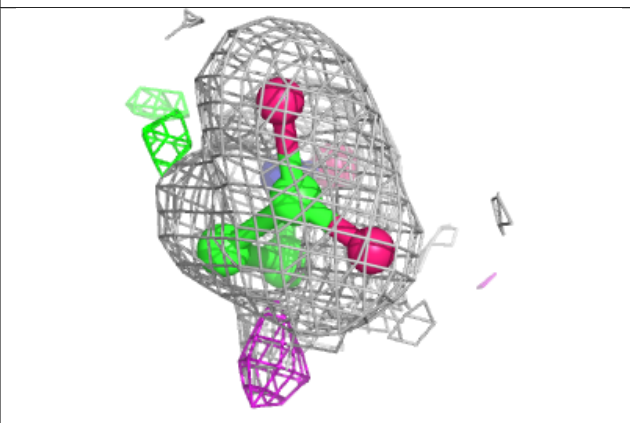
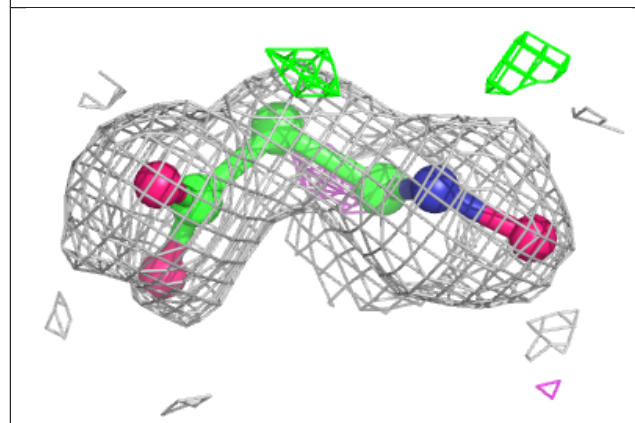
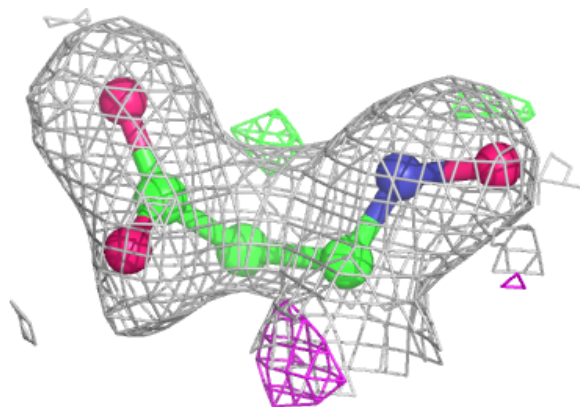
**Electron density around 54I C 504:**

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

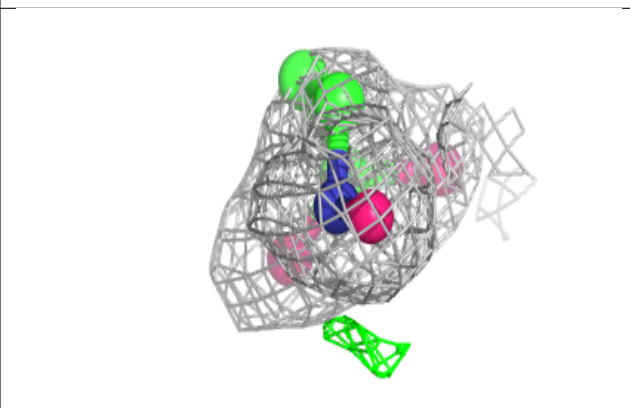
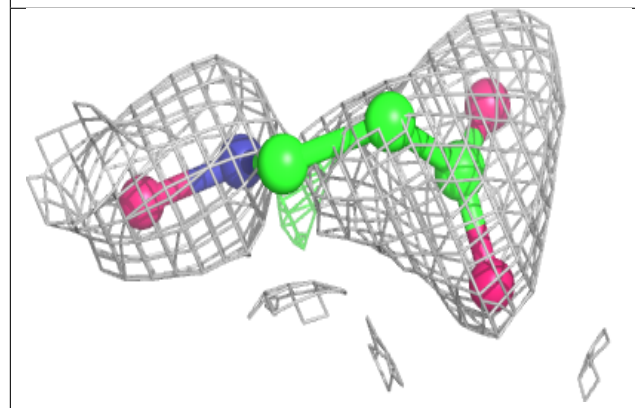
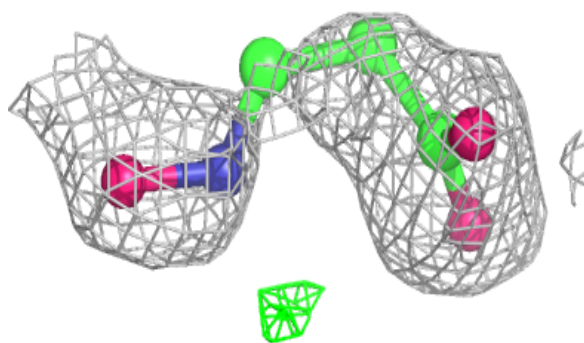


Electron density around 54I A 504:

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

**Electron density around 54I B 504:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.