WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:51 PM EDT

PDB ID	:	7RS7
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-30
Authors	:	Min, J.; Nwachukwu, J.C.; Min, C.K.; Njeri, J.W.; Srinivasan, S.; Rangarajan, E.S.; Nettles, C.C.; Yan, S.; Houtman, R.; Griffin, P.R.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2021-08-11
Resolution	:	1.58 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 ①) were used in the production of this report:

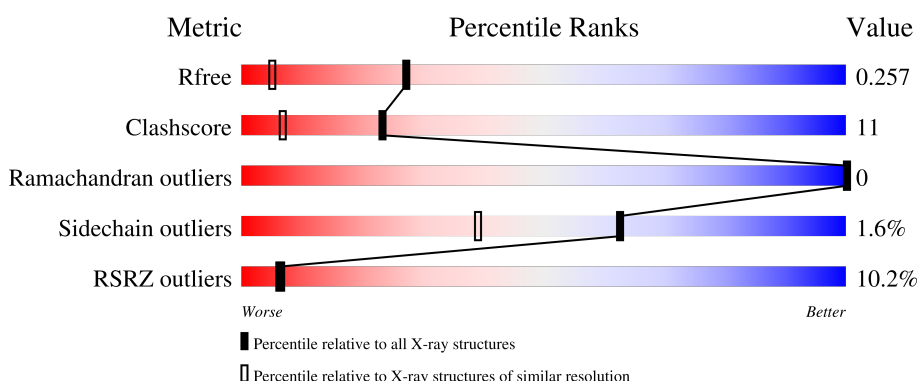|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.58 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.257
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		10.2%

Worse　　　　　*Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	257	10% / 79% 15% · 5%
1	B	257	8% / 77% 12% 11%
1	C	257	9% / 80% 14% 5%
1	D	257	10% / 79% 13% 7%

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	73I	A	601[A]	-	-	X	-
2	73I	A	601[B]	-	-	X	-

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8171 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1955	1249	334	355	17			
1	B	228	Total	C	N	O	S	0	0	0
			1825	1170	308	330	17			
1	C	244	Total	C	N	O	S	0	1	0
			1959	1252	334	355	18			
1	D	239	Total	C	N	O	S	0	0	0
			1903	1217	323	345	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (1S,2R,4S,5S,6S)-N,5,6-tris(4-hydroxyphenyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonamide (three-letter code: 73I) (formula: $C_{26}H_{22}F_3NO_6S$) (labeled as "Ligand of Interest" by depositor).
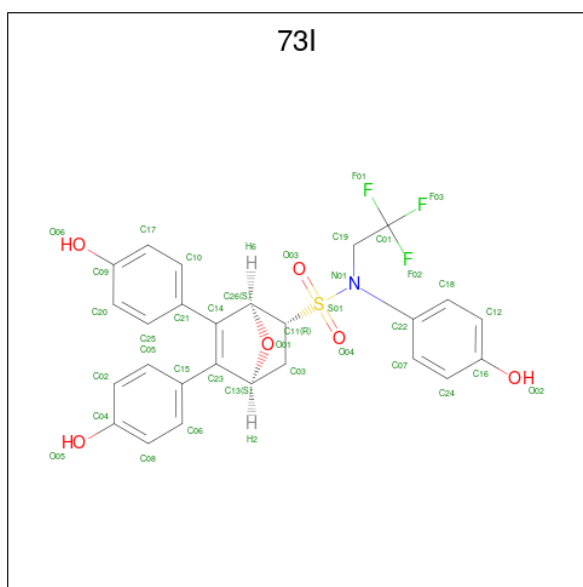
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	1
			71	52	3	2	12	2		
2	B	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	C	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	D	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	80	Total	O	0	0
			80	80		
3	C	88	Total	O	0	0
			88	88		
3	D	88	Total	O	0	0
			88	88		

3 Residue-property plots ⓘ

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

• Molecule 1: Estrogen receptor

Chain A:
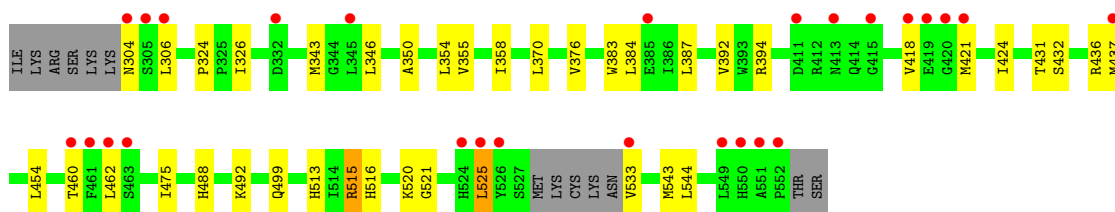
• Molecule 1: Estrogen receptor

Chain B:
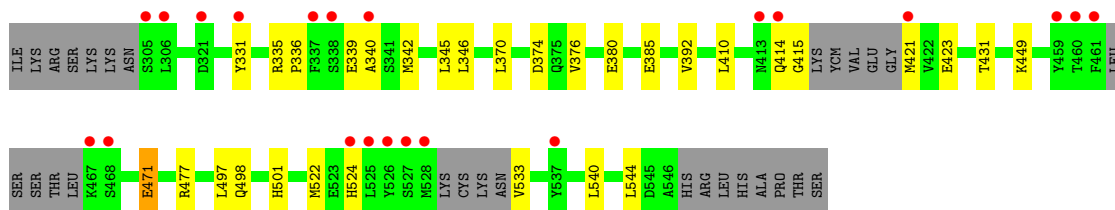
• Molecule 1: Estrogen receptor

Chain C:
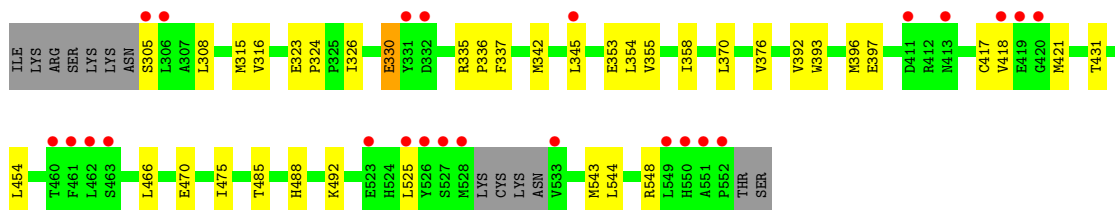
• Molecule 1: Estrogen receptor

Chain D:
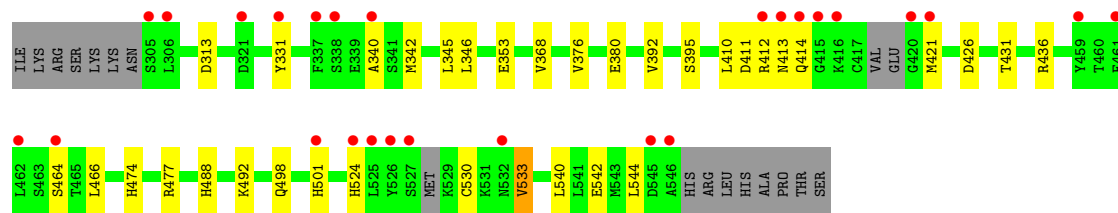
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.66Å　58.62Å　93.93Å 87.27°　74.87°　62.91°	Depositor
Resolution (Å)	90.37　–　1.58 90.36　–　1.58	Depositor EDS
% Data completeness (in resolution range)	70.1 (90.37-1.58) 70.1 (90.36-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.223　,　0.251 0.230　,　0.257	Depositor DCC
R_{free} test set	4633 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.156 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8171	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 73I, YCM

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	0.66	0/1975	0.72	0/2669
1	B	0.66	0/1847	0.73	0/2493
1	C	0.66	0/1975	0.71	0/2668
1	D	0.67	0/1920	0.74	0/2591
All	All	0.66	0/7717	0.72	0/10421

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	ASN	Peptide
1	A	460	THR	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1955	0	1984	86	0
1	B	1825	0	1857	24	0
1	C	1959	0	1992	35	0
1	D	1903	0	1944	30	0
2	A	71	0	0	55	0
2	B	37	0	0	0	0
2	C	37	0	0	1	0
2	D	37	0	0	0	0
3	A	91	0	0	6	0
3	B	80	0	0	5	0
3	C	88	0	0	13	1
3	D	88	0	0	9	1
All	All	8171	0	7777	176	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (176) 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:387:LEU:HB3	2:A:601[B]:73I:C04	1.24	1.62
1:A:384:LEU:HD11	2:A:601[B]:73I:C13	1.56	1.35
1:A:387:LEU:HD13	2:A:601[B]:73I:C08	1.67	1.24
1:A:387:LEU:HB3	2:A:601[B]:73I:C02	1.71	1.20
1:A:387:LEU:CB	2:A:601[B]:73I:C04	2.21	1.16
1:A:525:LEU:HB2	2:A:601[A]:73I:C12	1.73	1.16
1:C:485:THR:HG21	3:C:704:HOH:O	1.45	1.15
1:A:384:LEU:CD1	2:A:601[B]:73I:C23	2.30	1.10
1:A:387:LEU:HD13	2:A:601[B]:73I:C06	1.84	1.08
1:A:384:LEU:CD1	2:A:601[B]:73I:C13	2.32	1.07
1:A:343:MET:SD	2:A:601[B]:73I:C22	2.46	1.04
1:D:421:MET:HG2	1:D:524:HIS:ND1	1.77	0.98
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.41	0.98
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.43	0.97
1:D:542:GLU:OE2	3:D:701:HOH:O	1.82	0.96
1:A:387:LEU:CB	2:A:601[B]:73I:C02	2.44	0.94
1:C:396:MET:HG3	3:C:703:HOH:O	1.69	0.91
1:A:383:TRP:HH2	2:A:601[B]:73I:C10	1.85	0.89
1:A:387:LEU:HB3	2:A:601[B]:73I:C08	2.01	0.89
1:A:384:LEU:HD13	2:A:601[B]:73I:C23	2.04	0.88
1:A:387:LEU:CD1	2:A:601[B]:73I:C08	2.50	0.86
1:C:305:SER:OG	3:C:701:HOH:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HB3	2:A:601[A]:73I:C10	2.09	0.82
1:B:370:LEU:HD22	1:B:471:GLU:HG3	1.61	0.82
1:A:387:LEU:HB3	2:A:601[B]:73I:O05	1.80	0.82
1:D:412:ARG:HD3	1:D:426:ASP:OD1	1.80	0.81
1:C:397[B]:GLU:HA	1:C:397[B]:GLU:OE1	1.79	0.81
1:A:346:LEU:HB2	2:A:601[A]:73I:C17	2.10	0.81
1:A:387:LEU:CD1	2:A:601[B]:73I:C06	2.59	0.80
1:C:355:VAL:HG22	1:C:543:MET:CE	2.11	0.80
1:C:485:THR:CG2	3:C:704:HOH:O	2.10	0.79
1:D:413:ASN:OD1	1:D:414:GLN:HG3	1.83	0.77
1:A:355:VAL:HG22	1:A:543:MET:CE	2.16	0.75
1:A:346:LEU:CB	2:A:601[A]:73I:C10	2.64	0.75
1:A:421:MET:SD	2:A:601[A]:73I:C01	2.75	0.75
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.69	0.74
1:A:383:TRP:CH2	2:A:601[B]:73I:C10	2.70	0.74
1:A:343:MET:SD	2:A:601[B]:73I:C19	2.77	0.73
1:A:343:MET:HE1	2:A:601[B]:73I:C24	2.17	0.73
1:D:477:ARG:NH2	3:D:703:HOH:O	2.16	0.73
1:A:343:MET:HE1	2:A:601[B]:73I:C07	2.19	0.73
1:A:462:LEU:HD22	3:B:714:HOH:O	1.89	0.72
1:A:521:GLY:C	2:A:601[A]:73I:C07	2.61	0.69
1:A:525:LEU:C	1:A:525:LEU:HD12	2.13	0.69
1:B:449:LYS:NZ	3:B:701:HOH:O	2.18	0.68
1:A:525:LEU:CB	2:A:601[A]:73I:C12	2.64	0.68
1:C:355:VAL:HG22	1:C:543:MET:HE1	1.75	0.68
1:C:323:GLU:O	3:C:702:HOH:O	2.12	0.68
1:C:316:VAL:N	3:C:704:HOH:O	2.27	0.68
1:A:525:LEU:HB2	2:A:601[A]:73I:C16	2.22	0.67
1:D:395:SER:O	3:D:702:HOH:O	2.12	0.66
1:A:350:ALA:HB3	2:A:601[B]:73I:C20	2.25	0.66
1:B:423:GLU:OE1	1:B:524:HIS:CE1	2.49	0.66
1:C:355:VAL:HG22	1:C:543:MET:HE2	1.77	0.66
1:A:499:GLN:NE2	1:D:464:SER:O	2.28	0.65
1:A:343:MET:SD	2:A:601[B]:73I:N01	2.69	0.65
1:A:346:LEU:CB	2:A:601[A]:73I:C17	2.76	0.64
1:A:525:LEU:C	1:A:525:LEU:CD1	2.68	0.62
1:A:355:VAL:HA	1:A:543:MET:CE	2.29	0.62
1:A:350:ALA:CB	2:A:601[B]:73I:C25	2.79	0.61
1:B:335:ARG:HB3	1:B:339:GLU:OE1	2.00	0.61
1:A:515:ARG:NE	3:A:704:HOH:O	2.34	0.61
1:C:316:VAL:HG23	3:C:704:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:SD	2:A:601[B]:73I:C18	2.89	0.60
1:B:336:PRO:HD2	1:B:339:GLU:OE1	2.02	0.59
1:A:418:VAL:O	1:A:421:MET:HG2	2.02	0.59
1:B:342:MET:HE1	1:B:410:LEU:HD11	1.85	0.59
1:B:342:MET:HE3	1:B:346:LEU:HG	1.85	0.59
2:A:601[A]:73I:C01	2:A:601[A]:73I:C18	2.80	0.58
1:D:474:HIS:ND1	3:D:703:HOH:O	2.32	0.58
1:A:384:LEU:HD12	2:A:601[B]:73I:C05	2.34	0.58
1:B:370:LEU:CD2	1:B:471:GLU:HG3	2.32	0.58
1:D:342:MET:CE	1:D:410:LEU:HD11	2.35	0.57
1:D:353:GLU:OE1	3:D:704:HOH:O	2.17	0.57
1:A:525:LEU:CB	2:A:601[A]:73I:C16	2.81	0.56
1:B:477:ARG:NH2	3:B:703:HOH:O	2.25	0.56
1:B:376:VAL:CG2	1:B:544:LEU:HD12	2.36	0.55
1:A:350:ALA:CB	2:A:601[B]:73I:C20	2.84	0.55
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.36	0.55
1:B:342:MET:CE	1:B:410:LEU:HD11	2.36	0.55
1:A:436:ARG:NH1	3:A:701:HOH:O	2.26	0.54
1:A:343:MET:CE	2:A:601[B]:73I:C07	2.85	0.54
1:A:346:LEU:HB2	2:A:601[A]:73I:C10	2.34	0.54
1:A:355:VAL:HA	1:A:543:MET:HE2	1.89	0.54
1:A:437:MET:HG2	3:A:740:HOH:O	2.07	0.54
1:A:384:LEU:CD1	2:A:601[B]:73I:C15	2.85	0.54
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.90	0.54
1:C:335:ARG:HD3	1:C:337:PHE:CZ	2.44	0.53
1:A:533:VAL:O	2:A:601[B]:73I:O06	2.26	0.53
1:A:355:VAL:CG2	1:A:543:MET:HE1	2.38	0.53
1:A:324:PRO:HG2	3:A:786:HOH:O	2.07	0.53
1:C:330:GLU:HG2	1:C:345:LEU:HD21	1.89	0.53
1:A:355:VAL:HA	1:A:543:MET:HE1	1.91	0.53
1:B:376:VAL:HG22	1:B:544:LEU:HD12	1.91	0.52
2:A:601[B]:73I:C07	2:A:601[B]:73I:C11	2.88	0.52
1:A:521:GLY:HA2	2:A:601[A]:73I:C19	2.41	0.51
1:A:513:HIS:HD2	3:B:705:HOH:O	1.92	0.51
1:C:342:MET:CE	1:C:418:VAL:HG23	2.41	0.50
1:C:315:MET:HB3	3:C:704:HOH:O	2.12	0.50
1:C:326:ILE:HD12	1:C:326:ILE:N	2.27	0.50
1:B:342:MET:HE3	1:B:346:LEU:CG	2.41	0.50
1:C:335:ARG:NH2	3:C:707:HOH:O	2.45	0.49
1:C:393:TRP:HA	3:C:703:HOH:O	2.11	0.49
1:A:387:LEU:CB	2:A:601[B]:73I:C08	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:MET:SD	1:D:524:HIS:HB3	2.51	0.49
1:A:354:LEU:O	1:A:358:ILE:HD13	2.13	0.49
1:A:306:LEU:HD12	1:A:306:LEU:C	2.34	0.49
1:A:387:LEU:CG	2:A:601[B]:73I:C08	2.91	0.49
1:C:354:LEU:O	1:C:358:ILE:HD13	2.13	0.49
1:A:355:VAL:HG22	1:A:543:MET:HE3	1.95	0.48
1:A:355:VAL:CA	1:A:543:MET:HE1	2.43	0.48
1:D:411:ASP:OD1	1:D:413:ASN:OD1	2.31	0.48
1:A:383:TRP:HH2	2:A:601[B]:73I:C17	2.26	0.48
1:D:342:MET:HE3	1:D:346:LEU:HD11	1.96	0.48
1:B:415:GLY:HA2	1:B:421:MET:SD	2.54	0.48
1:A:326:ILE:HD12	1:A:394:ARG:HD3	1.96	0.48
1:A:384:LEU:CD1	2:A:601[B]:73I:C05	2.92	0.48
1:D:342:MET:HE3	1:D:346:LEU:HG	1.95	0.47
1:C:397[B]:GLU:OE1	1:C:397[B]:GLU:CA	2.56	0.47
1:A:343:MET:SD	2:A:601[B]:73I:C07	3.01	0.46
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.50	0.46
1:D:340:ALA:HB1	1:D:345:LEU:HD11	1.97	0.46
1:C:336:PRO:HB2	1:C:417:YCM:HZ22	1.79	0.46
1:B:374:ASP:OD2	1:B:471:GLU:HG2	2.15	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.51	0.46
1:A:454:LEU:HD22	1:A:475:ILE:HD12	1.97	0.46
1:D:342:MET:HE3	1:D:346:LEU:CG	2.46	0.46
1:A:521:GLY:O	2:A:601[A]:73I:C22	2.64	0.46
1:B:340:ALA:HB1	1:B:345:LEU:HD11	1.98	0.45
1:C:525:LEU:C	1:C:525:LEU:HD13	2.37	0.45
1:B:415:GLY:CA	1:B:421:MET:SD	3.04	0.45
1:D:380:GLU:HG3	1:D:540:LEU:HD12	1.99	0.45
1:B:370:LEU:HD22	1:B:471:GLU:CG	2.41	0.44
1:D:392:VAL:HG11	1:D:431:THR:HG22	2.00	0.44
1:D:342:MET:HE3	1:D:346:LEU:CD1	2.48	0.44
1:D:413:ASN:OD1	1:D:414:GLN:N	2.50	0.44
1:C:454:LEU:HD22	1:C:475:ILE:HD12	1.99	0.44
1:A:432:SER:HB3	3:A:701:HOH:O	2.18	0.43
1:C:466:LEU:O	1:C:470:GLU:HG3	2.18	0.43
1:C:392:VAL:HG11	1:C:431:THR:HG22	2.01	0.43
1:D:488:HIS:CE1	1:D:492:LYS:HD3	2.53	0.43
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.30	0.43
1:A:387:LEU:HB2	2:A:601[B]:73I:C02	2.42	0.43
1:B:374:ASP:OD2	1:B:471:GLU:CD	2.57	0.43
1:A:384:LEU:HD12	2:A:601[B]:73I:C15	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:HIS:NE2	1:A:492:LYS:HD2	2.33	0.43
1:A:525:LEU:HA	2:A:601[B]:73I:C12	2.49	0.43
1:C:324:PRO:HG2	3:C:786:HOH:O	2.19	0.43
1:C:353:GLU:OE1	2:C:601:73I:O05	2.36	0.43
1:B:385:GLU:OE2	3:B:702:HOH:O	2.21	0.42
1:A:392:VAL:HG11	1:A:431:THR:HG22	2.02	0.42
1:B:392:VAL:HG11	1:B:431:THR:HG22	2.01	0.42
1:C:488:HIS:NE2	1:C:492:LYS:HD2	2.34	0.42
1:A:432:SER:CB	3:A:701:HOH:O	2.68	0.42
1:B:374:ASP:OD2	1:B:471:GLU:CG	2.67	0.42
1:D:342:MET:HE1	1:D:410:LEU:HD11	2.01	0.42
1:C:396:MET:CG	3:C:703:HOH:O	2.48	0.41
1:C:342:MET:HE1	1:C:418:VAL:HG23	2.02	0.41
1:A:516:HIS:CE1	1:A:520:LYS:HE2	2.54	0.41
1:D:313:ASP:HA	3:D:756:HOH:O	2.20	0.41
1:D:436:ARG:NH2	3:D:702:HOH:O	2.41	0.41
1:A:343:MET:HE3	1:A:343:MET:HB3	1.82	0.41
1:D:412:ARG:HB2	3:D:713:HOH:O	2.20	0.41
1:C:418:VAL:HG11	1:C:421:MET:CE	2.51	0.41
1:D:530:CYS:O	1:D:533:VAL:HB	2.21	0.41
1:A:376:VAL:HG22	1:A:544:LEU:HD12	2.02	0.41
1:D:368:VAL:HG22	3:D:741:HOH:O	2.20	0.41
1:A:343:MET:CE	2:A:601[B]:73I:C22	2.99	0.41
1:A:376:VAL:CG2	1:A:544:LEU:HD12	2.51	0.41
1:A:383:TRP:CH2	2:A:601[B]:73I:C17	3.02	0.40
1:C:485:THR:HG23	3:C:704:HOH:O	2.03	0.40
1:B:380:GLU:HG3	1:B:540:LEU:HD12	2.03	0.40
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.32	0.40
1:A:424:ILE:HG21	2:A:601[A]:73I:O04	2.20	0.40
1:C:376:VAL:HG22	1:C:544:LEU:HD12	2.03	0.40
1:A:418:VAL:HB	1:A:421:MET:CG	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:782:HOH:O	3:D:757:HOH:O[1_645]	2.11	0.09

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	239/257 (93%)	237 (99%)	2 (1%)	0	100	100
1	B	219/257 (85%)	217 (99%)	2 (1%)	0	100	100
1	C	239/257 (93%)	235 (98%)	4 (2%)	0	100	100
1	D	232/257 (90%)	230 (99%)	2 (1%)	0	100	100
All	All	929/1028 (90%)	919 (99%)	10 (1%)	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	218/230 (95%)	216 (99%)	2 (1%)	78	64
1	B	204/230 (89%)	198 (97%)	6 (3%)	42	16
1	C	218/230 (95%)	215 (99%)	3 (1%)	67	45
1	D	213/230 (93%)	210 (99%)	3 (1%)	67	45
All	All	853/920 (93%)	839 (98%)	14 (2%)	62	39

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	ARG
1	A	525	LEU

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Mol	Chain	Res	Type
1	B	331	TYR
1	B	414	GLN
1	B	471	GLU
1	B	497	LEU
1	B	522	MET
1	B	533	VAL
1	C	308	LEU
1	C	330	GLU
1	C	548	ARG
1	D	331	TYR
1	D	466	LEU
1	D	533	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	513	HIS
1	A	547	HIS
1	B	398	HIS
1	B	414	GLN
1	B	513	HIS
1	C	398	HIS
1	C	474	HIS
1	C	519	ASN
1	C	547	HIS
1	D	488	HIS
1	D	519	ASN
1	D	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	YCM	C	417	1	7,9,10	0.57	0	4,10,12	0.72	0
1	YCM	D	381	1	7,9,10	0.60	0	4,10,12	0.40	0
1	YCM	D	417	1	4,5,10	0.68	0	1,5,12	0.18	0
1	YCM	A	417	1	4,5,10	0.59	0	1,5,12	0.81	0
1	YCM	C	381	1	7,9,10	0.49	0	4,10,12	0.52	0
1	YCM	B	381	1	7,9,10	0.64	0	4,10,12	0.41	0
1	YCM	A	381	1	7,9,10	0.52	0	4,10,12	0.56	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
1	YCM	C	417	1	-	3/6/8/10	-
1	YCM	D	381	1	-	2/6/8/10	-
1	YCM	D	417	1	-	0/1/4/10	-
1	YCM	A	417	1	-	0/1/4/10	-
1	YCM	C	381	1	-	2/6/8/10	-
1	YCM	B	381	1	-	2/6/8/10	-
1	YCM	A	381	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	B	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	SG-CD-CE-NZ2
1	C	417	YCM	CE-CD-SG-CB
1	C	417	YCM	SG-CD-CE-OZ1
1	C	417	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2

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Mol	Chain	Res	Type	Atoms
1	B	381	YCM	SG-CD-CE-OZ1
1	C	381	YCM	SG-CD-CE-OZ1
1	D	381	YCM	SG-CD-CE-OZ1
1	A	381	YCM	SG-CD-CE-OZ1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	417	YCM	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	73I	C	601	-	38,41,41	2.87	15 (39%)	50,63,63	2.90	20 (40%)
2	73I	A	601[B]	-	38,41,41	2.97	18 (47%)	50,63,63	4.01	22 (44%)
2	73I	B	601	-	38,41,41	2.84	13 (34%)	50,63,63	2.76	20 (40%)
2	73I	A	601[A]	-	36,38,41	3.19	19 (52%)	43,57,63	4.47	27 (62%)
2	73I	D	601	-	38,41,41	2.79	13 (34%)	50,63,63	2.88	21 (42%)

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
2	73I	C	601	-	-	8/27/53/53	0/6/5/5
2	73I	A	601[B]	-	-	16/27/53/53	0/6/5/5
2	73I	B	601	-	-	9/27/53/53	0/6/5/5
2	73I	A	601[A]	-	-	9/24/50/53	0/6/5/5
2	73I	D	601	-	-	10/27/53/53	0/6/5/5

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[B]	73I	C22-N01	-10.33	1.30	1.44
2	C	601	73I	C22-N01	-10.13	1.30	1.44
2	B	601	73I	C22-N01	-9.82	1.31	1.44
2	D	601	73I	C22-N01	-9.69	1.31	1.44
2	A	601[A]	73I	C22-N01	-7.25	1.34	1.44
2	A	601[B]	73I	C15-C23	-6.95	1.35	1.48
2	C	601	73I	C21-C14	-6.92	1.35	1.48
2	B	601	73I	O04-S01	6.60	1.49	1.43
2	D	601	73I	C15-C23	-6.45	1.36	1.48
2	B	601	73I	C15-C23	-6.36	1.36	1.48
2	A	601[B]	73I	C21-C14	-6.11	1.37	1.48
2	A	601[A]	73I	C15-C23	-6.02	1.37	1.48
2	A	601[A]	73I	C26-C14	5.92	1.57	1.50
2	D	601	73I	O03-S01	5.67	1.48	1.43
2	A	601[A]	73I	O04-S01	5.65	1.48	1.43
2	A	601[A]	73I	C20-C09	-5.20	1.29	1.38
2	D	601	73I	C21-C14	-4.98	1.39	1.48
2	C	601	73I	O03-S01	4.90	1.47	1.43
2	C	601	73I	C15-C23	-4.76	1.39	1.48
2	B	601	73I	C21-C14	-4.75	1.39	1.48
2	A	601[A]	73I	C18-C12	-4.69	1.30	1.38
2	C	601	73I	C26-C14	4.64	1.55	1.50
2	A	601[A]	73I	C12-C16	-4.34	1.30	1.38
2	A	601[A]	73I	O03-S01	4.31	1.47	1.43
2	A	601[A]	73I	S01-N01	4.19	1.75	1.67
2	A	601[A]	73I	O01-C26	-4.12	1.38	1.43
2	B	601	73I	C26-C14	3.91	1.54	1.50
2	C	601	73I	O04-S01	3.87	1.46	1.43
2	A	601[A]	73I	C19-N01	3.82	1.54	1.48
2	A	601[A]	73I	C18-C22	-3.82	1.31	1.39
2	A	601[B]	73I	O01-C13	-3.76	1.36	1.44
2	D	601	73I	C26-C14	3.34	1.54	1.50
2	A	601[B]	73I	C05-C02	-3.30	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[B]	73I	C20-C09	-3.16	1.32	1.38
2	B	601	73I	O03-S01	3.15	1.46	1.43
2	A	601[B]	73I	C06-C15	-3.10	1.34	1.39
2	A	601[B]	73I	C07-C24	-3.04	1.33	1.38
2	A	601[A]	73I	C17-C09	-2.99	1.33	1.38
2	C	601	73I	C24-C16	-2.96	1.33	1.38
2	A	601[B]	73I	C26-C14	2.95	1.53	1.50
2	A	601[A]	73I	C13-C23	2.94	1.55	1.51
2	B	601	73I	C02-C04	-2.93	1.33	1.38
2	A	601[B]	73I	O01-C26	-2.91	1.39	1.43
2	D	601	73I	C24-C16	-2.90	1.33	1.38
2	D	601	73I	C05-C02	-2.89	1.33	1.38
2	A	601[A]	73I	C10-C21	-2.86	1.34	1.39
2	A	601[B]	73I	C10-C21	-2.75	1.34	1.39
2	B	601	73I	C24-C16	-2.71	1.33	1.38
2	A	601[B]	73I	C24-C16	-2.68	1.33	1.38
2	A	601[B]	73I	C03-C11	2.64	1.57	1.54
2	D	601	73I	C13-C23	2.60	1.55	1.51
2	D	601	73I	C02-C04	-2.59	1.34	1.38
2	B	601	73I	C13-C23	2.54	1.55	1.51
2	A	601[B]	73I	C08-C06	-2.52	1.34	1.38
2	D	601	73I	C08-C04	-2.52	1.34	1.38
2	A	601[A]	73I	C25-C20	-2.50	1.34	1.38
2	C	601	73I	C08-C04	-2.47	1.34	1.38
2	C	601	73I	C07-C24	-2.37	1.34	1.38
2	B	601	73I	S01-N01	2.36	1.72	1.67
2	D	601	73I	C20-C09	-2.35	1.34	1.38
2	C	601	73I	C13-C23	2.33	1.54	1.51
2	C	601	73I	C07-C22	-2.31	1.34	1.39
2	A	601[B]	73I	C19-C01	2.27	1.53	1.50
2	D	601	73I	C12-C16	-2.26	1.34	1.38
2	B	601	73I	C05-C02	-2.22	1.34	1.38
2	A	601[B]	73I	C07-C22	-2.20	1.34	1.39
2	C	601	73I	C25-C21	-2.20	1.35	1.39
2	C	601	73I	C12-C16	-2.20	1.34	1.38
2	B	601	73I	C08-C04	-2.19	1.34	1.38
2	C	601	73I	O01-C26	-2.19	1.40	1.43
2	A	601[B]	73I	C17-C09	-2.14	1.34	1.38
2	A	601[A]	73I	O01-C13	-2.12	1.39	1.44
2	A	601[B]	73I	C25-C21	-2.08	1.35	1.39
2	C	601	73I	C20-C09	-2.05	1.35	1.38
2	B	601	73I	C20-C09	-2.05	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	73I	C24-C16	-2.01	1.35	1.38
2	A	601[A]	73I	C14-C23	2.01	1.38	1.34
2	D	601	73I	C08-C06	-2.00	1.35	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	73I	C07-C22-N01	13.95	140.97	120.16
2	B	601	73I	O03-S01-N01	12.37	122.70	107.56
2	A	601[B]	73I	C19-N01-C22	12.04	133.68	117.59
2	A	601[B]	73I	O04-S01-O03	-11.59	111.77	119.22
2	D	601	73I	O04-S01-N01	10.79	120.77	107.56
2	A	601[B]	73I	O01-C13-C23	-10.50	87.38	101.99
2	A	601[B]	73I	C01-C19-N01	10.16	122.01	112.14
2	C	601	73I	C01-C19-N01	9.77	121.63	112.14
2	A	601[A]	73I	O03-S01-N01	9.60	119.31	107.56
2	D	601	73I	C01-C19-N01	8.68	120.57	112.14
2	A	601[A]	73I	C25-C21-C10	-8.66	106.24	118.59
2	C	601	73I	O04-S01-N01	8.10	117.48	107.56
2	A	601[B]	73I	C18-C22-N01	7.85	131.88	120.16
2	A	601[A]	73I	C18-C12-C16	7.63	128.25	119.88
2	A	601[A]	73I	C20-C25-C21	7.60	129.62	120.78
2	A	601[A]	73I	C25-C21-C14	6.69	129.56	120.91
2	C	601	73I	O03-S01-N01	6.51	115.53	107.56
2	A	601[B]	73I	C13-C03-C11	6.35	106.22	100.61
2	B	601	73I	C01-C19-N01	6.00	117.97	112.14
2	A	601[A]	73I	C18-C22-C07	-5.94	107.08	119.16
2	C	601	73I	O04-S01-O03	5.88	122.99	119.22
2	A	601[B]	73I	C13-C23-C14	-5.87	94.65	106.97
2	A	601[A]	73I	C12-C16-C24	-5.71	110.15	119.77
2	A	601[A]	73I	C21-C14-C23	5.70	143.56	128.81
2	A	601[A]	73I	C18-C22-N01	-5.52	111.94	120.16
2	A	601[A]	73I	C12-C18-C22	5.32	127.32	120.32
2	A	601[B]	73I	C24-C07-C22	5.27	127.25	120.32
2	A	601[A]	73I	O02-C16-C24	5.21	134.87	120.02
2	B	601	73I	C07-C22-N01	5.18	127.89	120.16
2	D	601	73I	C07-C22-N01	5.12	127.79	120.16
2	D	601	73I	O01-C13-C23	-4.58	95.62	101.99
2	B	601	73I	C21-C14-C26	4.42	128.53	121.27
2	A	601[A]	73I	C17-C10-C21	4.06	125.50	120.78
2	D	601	73I	C21-C14-C26	3.99	127.84	121.27
2	D	601	73I	C19-N01-C22	3.98	122.91	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601[A]	73I	C24-C07-C22	3.86	125.41	120.32
2	C	601	73I	C19-N01-C22	3.83	122.71	117.59
2	D	601	73I	C18-C22-C07	-3.63	111.77	119.16
2	A	601[B]	73I	C18-C22-C07	-3.63	111.78	119.16
2	B	601	73I	O01-C13-C23	-3.61	96.96	101.99
2	C	601	73I	C18-C22-C07	-3.60	111.84	119.16
2	C	601	73I	C24-C07-C22	3.60	125.06	120.32
2	D	601	73I	C12-C18-C22	3.59	125.05	120.32
2	A	601[A]	73I	C06-C15-C23	3.58	125.54	120.91
2	C	601	73I	O01-C13-C23	3.57	106.96	101.99
2	C	601	73I	C13-C03-C11	-3.38	97.63	100.61
2	D	601	73I	C25-C21-C10	-3.37	113.79	118.59
2	A	601[B]	73I	O02-C16-C12	3.34	129.53	120.02
2	C	601	73I	C06-C15-C05	-3.33	113.84	118.59
2	B	601	73I	C18-C22-C07	-3.26	112.53	119.16
2	A	601[B]	73I	C21-C14-C23	3.20	137.08	128.81
2	B	601	73I	C15-C23-C13	3.17	126.60	121.44
2	A	601[A]	73I	O01-C13-C03	-3.13	98.49	104.64
2	A	601[B]	73I	C12-C16-C24	-3.12	114.51	119.77
2	A	601[B]	73I	C15-C23-C13	-3.10	116.38	121.44
2	A	601[B]	73I	C07-C22-N01	-3.08	115.57	120.16
2	D	601	73I	C25-C20-C09	3.05	123.22	119.88
2	A	601[A]	73I	C21-C14-C26	-2.98	116.36	121.27
2	A	601[B]	73I	C25-C21-C10	-2.96	114.37	118.59
2	A	601[A]	73I	O04-S01-O03	-2.95	117.32	119.22
2	C	601	73I	C07-C22-N01	2.95	124.57	120.16
2	C	601	73I	C02-C05-C15	2.95	124.21	120.78
2	A	601[A]	73I	C10-C17-C09	2.92	123.08	119.88
2	A	601[A]	73I	C15-C23-C14	2.89	136.29	128.81
2	A	601[A]	73I	C20-C09-C17	-2.87	114.93	119.77
2	D	601	73I	C15-C23-C13	2.85	126.09	121.44
2	A	601[B]	73I	F01-C01-C19	2.84	116.78	112.13
2	D	601	73I	C24-C07-C22	2.79	123.99	120.32
2	C	601	73I	C06-C15-C23	2.79	124.52	120.91
2	B	601	73I	C12-C18-C22	2.78	123.98	120.32
2	B	601	73I	C25-C21-C10	-2.76	114.66	118.59
2	B	601	73I	C05-C02-C04	2.73	122.87	119.88
2	C	601	73I	C12-C18-C22	2.70	123.87	120.32
2	B	601	73I	C24-C07-C22	2.67	123.83	120.32
2	D	601	73I	C07-C24-C16	2.67	122.80	119.88
2	D	601	73I	C12-C16-C24	-2.67	115.28	119.77
2	B	601	73I	F01-C01-C19	2.61	116.41	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	73I	C12-C16-C24	-2.51	115.55	119.77
2	B	601	73I	C25-C20-C09	2.50	122.62	119.88
2	C	601	73I	C12-C16-C24	-2.50	115.56	119.77
2	D	601	73I	C20-C09-C17	-2.48	115.59	119.77
2	A	601[B]	73I	C18-C12-C16	2.48	122.59	119.88
2	C	601	73I	C13-C23-C14	-2.45	101.83	106.97
2	C	601	73I	C15-C23-C14	2.40	135.01	128.81
2	A	601[A]	73I	C13-C03-C11	-2.39	98.50	100.61
2	B	601	73I	C06-C15-C05	-2.39	115.18	118.59
2	A	601[A]	73I	C15-C23-C13	-2.39	117.55	121.44
2	A	601[A]	73I	C02-C05-C15	2.36	123.53	120.78
2	D	601	73I	C17-C10-C21	2.34	123.50	120.78
2	D	601	73I	C06-C15-C05	-2.33	115.26	118.59
2	D	601	73I	O03-S01-N01	2.31	110.39	107.56
2	B	601	73I	C07-C24-C16	2.29	122.39	119.88
2	A	601[A]	73I	C10-C21-C14	2.28	123.85	120.91
2	C	601	73I	C18-C22-N01	2.27	123.54	120.16
2	A	601[B]	73I	C20-C25-C21	2.24	123.39	120.78
2	C	601	73I	C25-C21-C10	-2.19	115.47	118.59
2	A	601[B]	73I	F03-C01-F01	-2.18	98.42	106.43
2	B	601	73I	C25-C21-C14	2.17	123.71	120.91
2	A	601[B]	73I	C10-C17-C09	2.15	122.23	119.88
2	D	601	73I	C25-C21-C14	2.15	123.68	120.91
2	C	601	73I	C06-C08-C04	2.13	122.21	119.88
2	A	601[A]	73I	C01-C19-N01	2.10	117.25	111.73
2	A	601[B]	73I	C20-C09-C17	-2.09	116.24	119.77
2	B	601	73I	C13-C23-C14	-2.09	102.58	106.97
2	D	601	73I	C13-C23-C14	-2.09	102.58	106.97
2	B	601	73I	C20-C09-C17	-2.09	116.25	119.77
2	B	601	73I	C17-C10-C21	2.08	123.20	120.78
2	A	601[B]	73I	O03-S01-N01	2.08	110.10	107.56
2	A	601[A]	73I	C06-C15-C05	-2.06	115.65	118.59
2	D	601	73I	O04-S01-O03	2.04	120.53	119.22

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	73I	C22-N01-S01-C11
2	A	601[A]	73I	C22-N01-S01-O04
2	A	601[A]	73I	C19-N01-S01-O04
2	A	601[B]	73I	F01-C01-C19-N01

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Mol	Chain	Res	Type	Atoms
2	A	601[B]	73I	C26-C11-S01-O03
2	A	601[B]	73I	C26-C11-S01-O04
2	A	601[B]	73I	C22-N01-S01-C11
2	A	601[B]	73I	C22-N01-S01-O04
2	A	601[B]	73I	C19-N01-S01-O04
2	A	601[B]	73I	C01-C19-N01-C22
2	A	601[B]	73I	C01-C19-N01-S01
2	B	601	73I	C26-C11-S01-O03
2	B	601	73I	C26-C11-S01-O04
2	B	601	73I	C19-N01-S01-O03
2	B	601	73I	C19-N01-S01-O04
2	C	601	73I	F01-C01-C19-N01
2	C	601	73I	F02-C01-C19-N01
2	C	601	73I	F03-C01-C19-N01
2	C	601	73I	C19-N01-S01-O03
2	D	601	73I	C26-C11-S01-O03
2	D	601	73I	C26-C11-S01-O04
2	D	601	73I	C19-N01-S01-O04
2	D	601	73I	C01-C19-N01-C22
2	D	601	73I	C01-C19-N01-S01
2	A	601[B]	73I	C07-C22-N01-S01
2	A	601[B]	73I	C03-C11-S01-O03
2	B	601	73I	C19-N01-S01-C11
2	C	601	73I	C07-C22-N01-S01
2	B	601	73I	C05-C15-C23-C14
2	B	601	73I	C03-C11-S01-O03
2	B	601	73I	C03-C11-S01-O04
2	D	601	73I	C03-C11-S01-O03
2	B	601	73I	C06-C15-C23-C14
2	D	601	73I	C06-C15-C23-C14
2	D	601	73I	C05-C15-C23-C14
2	A	601[A]	73I	C26-C11-S01-O04
2	A	601[B]	73I	C23-C14-C21-C10
2	A	601[A]	73I	C23-C14-C21-C10
2	A	601[A]	73I	C03-C11-S01-O03
2	A	601[B]	73I	C03-C11-S01-O04
2	D	601	73I	C03-C11-S01-O04
2	C	601	73I	C19-N01-S01-C11
2	A	601[A]	73I	C23-C14-C21-C25
2	A	601[B]	73I	C23-C14-C21-C25
2	C	601	73I	C19-N01-S01-O04
2	A	601[A]	73I	C03-C11-S01-O04

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Mol	Chain	Res	Type	Atoms
2	A	601[A]	73I	C19-N01-S01-C11
2	A	601[B]	73I	C19-N01-S01-C11
2	D	601	73I	C19-N01-S01-C11
2	A	601[B]	73I	C26-C14-C21-C10
2	C	601	73I	C18-C22-N01-S01
2	A	601[B]	73I	C26-C14-C21-C25

There are no ring outliers.

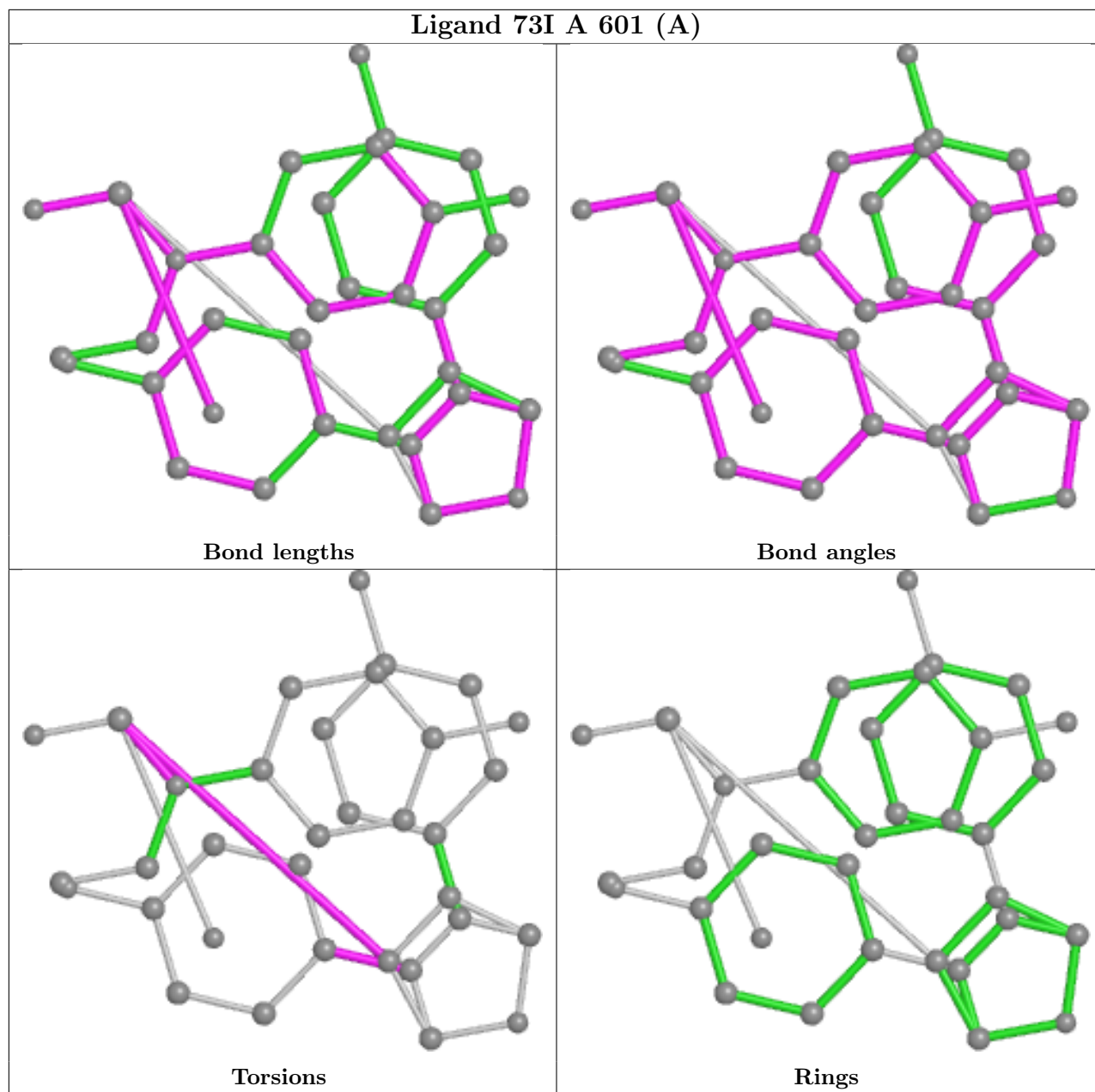3 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	73I	1	0
2	A	601[B]	73I	40	0
2	A	601[A]	73I	15	0

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

Ligand 73I C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand 73I A 601 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 73I B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand 73I A 601 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 73I D 601

Bond lengths

Bond angles

Torsions

Rings
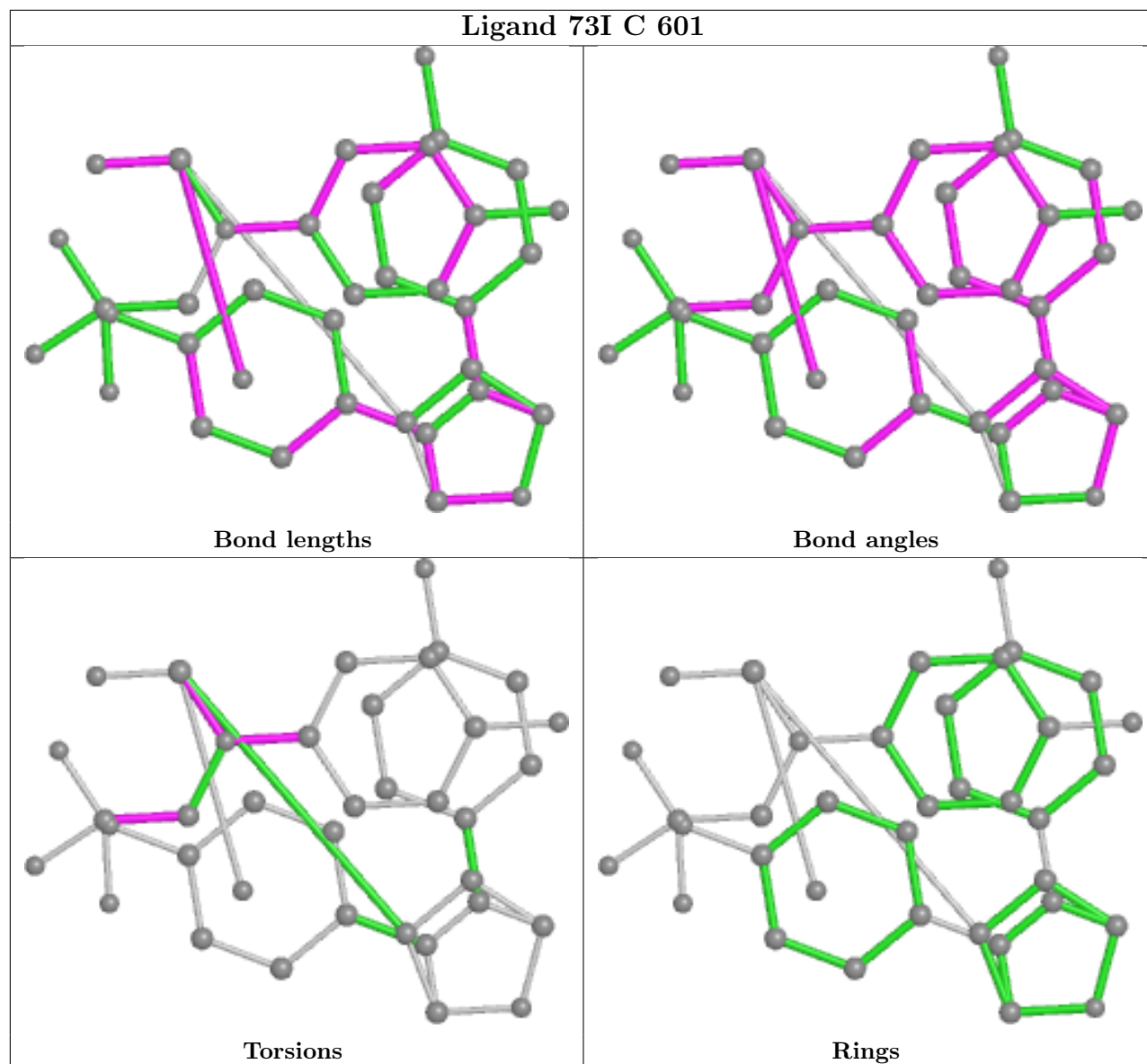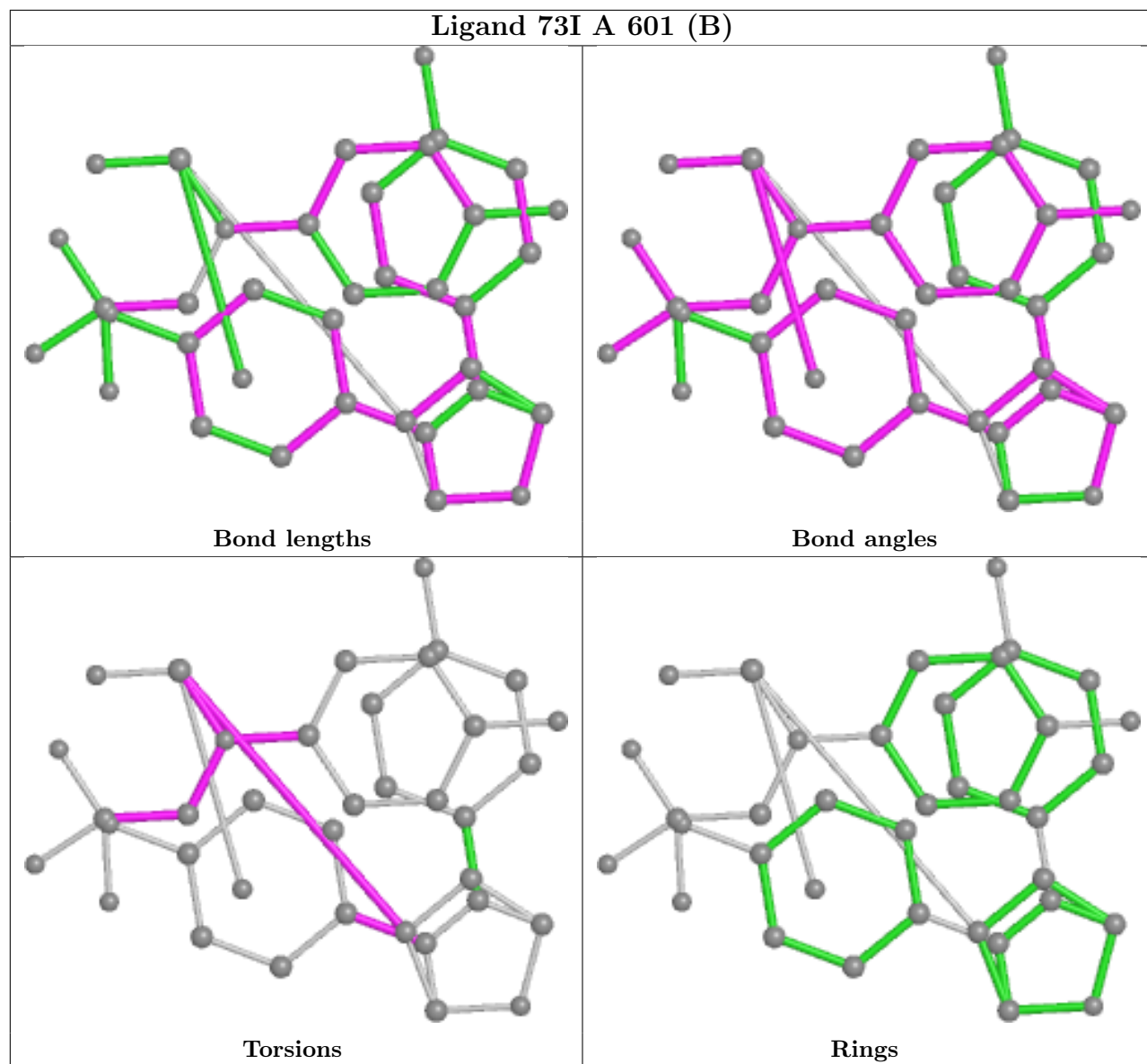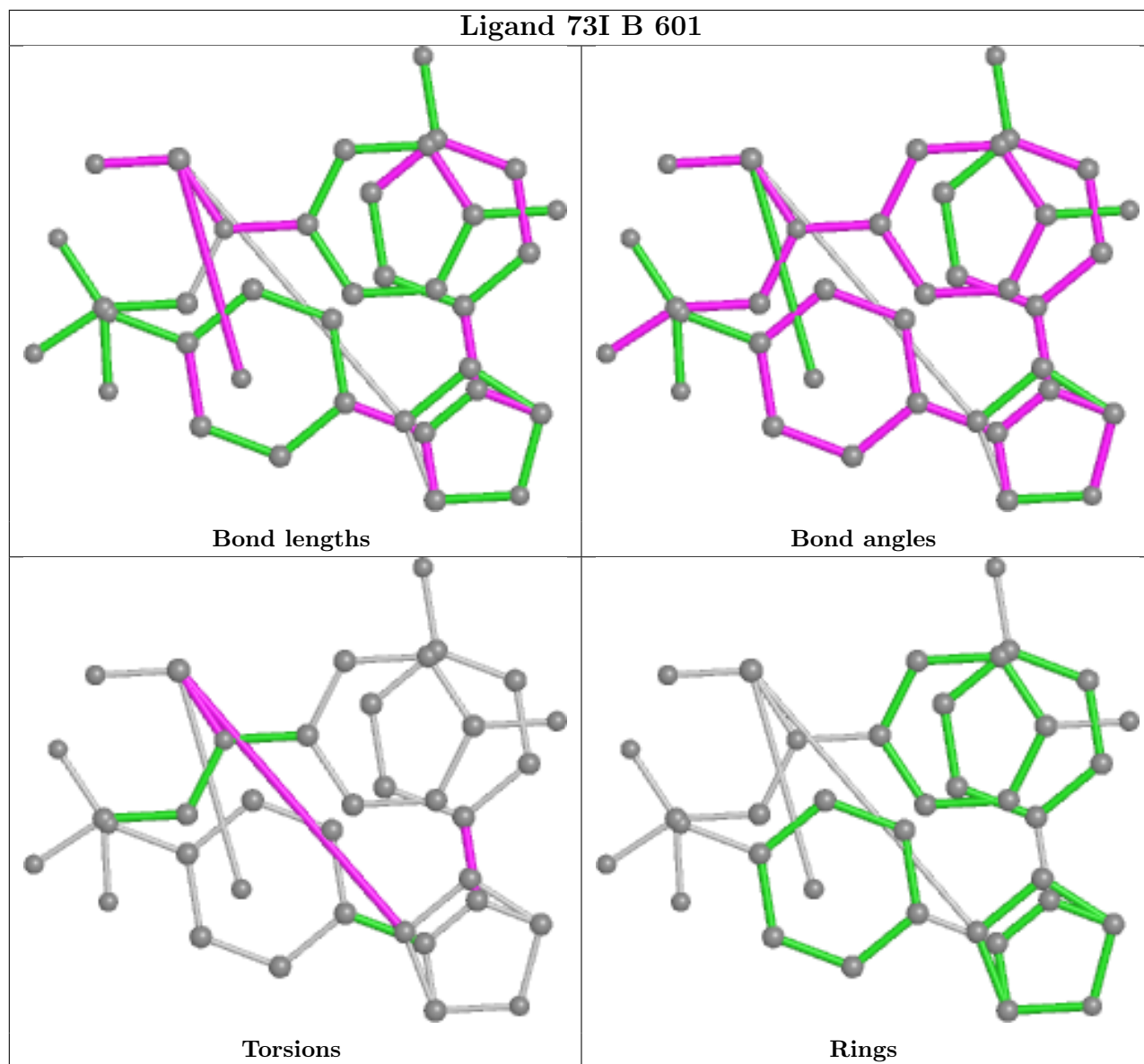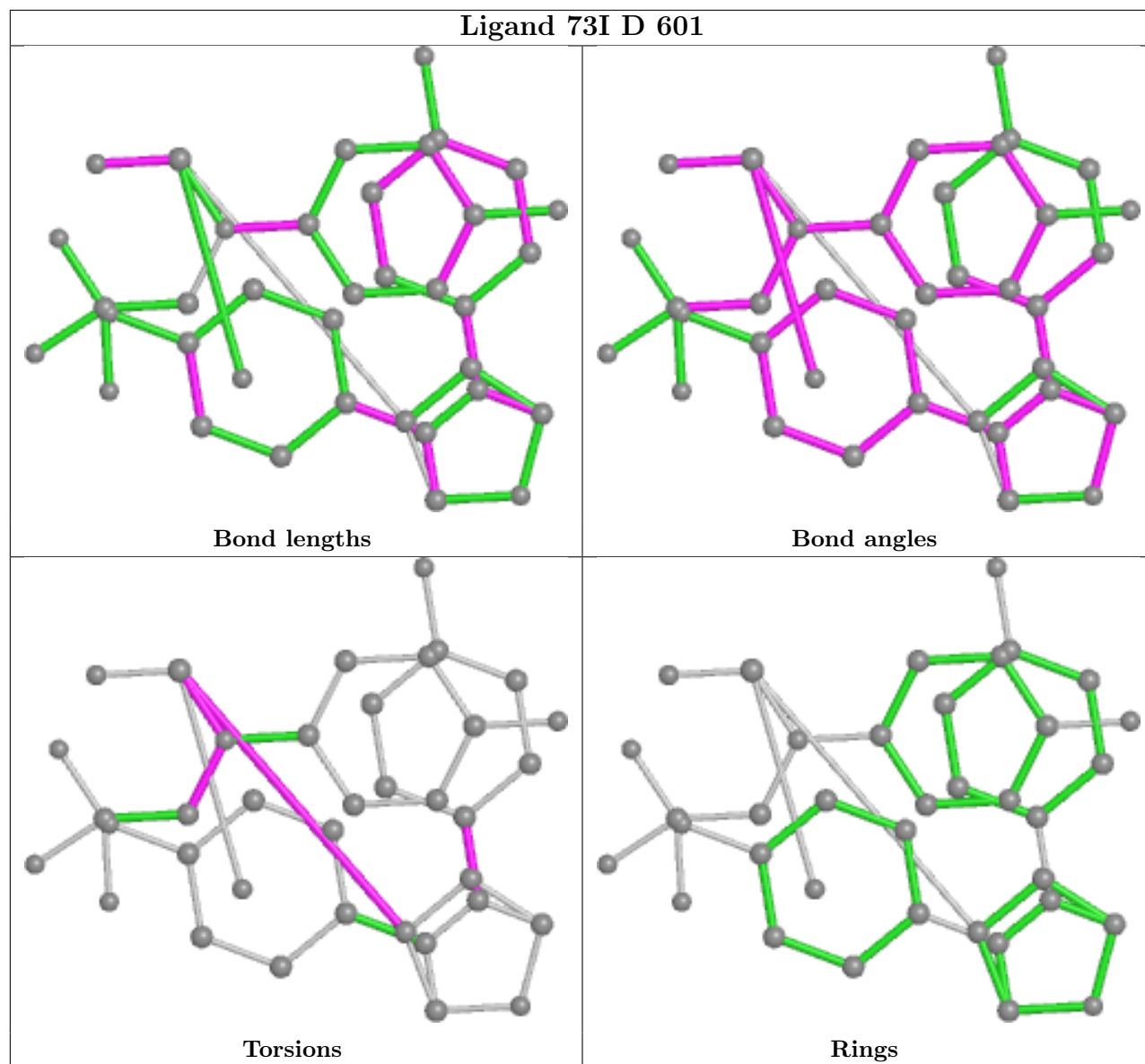
5.7 Other polymers (i)

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	242/257 (94%)	0.57	26 (10%)	6	5	12, 24, 57, 75	1 (0%)
1	B	227/257 (88%)	0.54	21 (9%)	8	8	13, 24, 63, 84	0
1	C	242/257 (94%)	0.64	24 (9%)	7	7	12, 25, 56, 92	0
1	D	237/257 (92%)	0.55	26 (10%)	5	5	13, 25, 63, 91	0
All	All	948/1028 (92%)	0.57	97 (10%)	6	6	12, 25, 60, 92	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PHE	8.8
1	B	305	SER	6.1
1	D	462	LEU	5.8
1	A	418	VAL	5.7
1	C	526	TYR	5.6
1	A	526	TYR	5.4
1	A	462	LEU	5.4
1	C	332	ASP	5.3
1	A	549	LEU	5.2
1	D	337	PHE	5.2
1	B	526	TYR	5.1
1	C	528	MET	5.1
1	D	464	SER	5.0
1	C	462	LEU	4.9
1	B	338	SER	4.9
1	A	420	GLY	4.9
1	B	461	PHE	4.9
1	C	533	VAL	4.9
1	A	461	PHE	4.7
1	C	463	SER	4.6
1	C	305	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	413	ASN	4.3
1	C	306	LEU	4.2
1	A	305	SER	4.2
1	C	419	GLU	4.2
1	A	385	GLU	4.1
1	D	306	LEU	4.1
1	B	340	ALA	4.1
1	B	524	HIS	4.1
1	D	532	ASN	4.0
1	D	420	GLY	3.7
1	C	413	ASN	3.7
1	D	421	MET	3.6
1	D	331	TYR	3.6
1	C	460	THR	3.5
1	D	545	ASP	3.5
1	C	420	GLY	3.5
1	B	527	SER	3.5
1	D	415	GLY	3.5
1	A	463	SER	3.5
1	A	552	PRO	3.4
1	D	524	HIS	3.4
1	C	461	PHE	3.4
1	B	528	MET	3.3
1	C	549	LEU	3.3
1	B	413	ASN	3.3
1	C	551	ALA	3.2
1	D	546	ALA	3.1
1	A	550	HIS	3.0
1	B	459	TYR	3.0
1	B	306	LEU	3.0
1	D	340	ALA	2.9
1	D	525	LEU	2.8
1	C	527	SER	2.8
1	A	421	MET	2.7
1	B	414	GLN	2.7
1	D	527	SER	2.7
1	A	533	VAL	2.6
1	D	459	TYR	2.6
1	A	524	HIS	2.6
1	A	415	GLY	2.6
1	C	345	LEU	2.6
1	C	550	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	305	SER	2.6
1	A	460	THR	2.5
1	D	338	SER	2.5
1	B	460	THR	2.5
1	A	332	ASP	2.5
1	D	501	HIS	2.5
1	B	467	LYS	2.4
1	D	412	ARG	2.4
1	A	437	MET	2.4
1	C	525	LEU	2.4
1	D	416	LYS	2.4
1	B	525	LEU	2.4
1	A	306	LEU	2.4
1	D	526	TYR	2.4
1	C	418	VAL	2.3
1	B	321	ASP	2.3
1	C	523	GLU	2.3
1	D	414	GLN	2.3
1	A	304	ASN	2.3
1	B	331	TYR	2.3
1	B	537	TYR	2.2
1	A	413	ASN	2.2
1	C	411	ASP	2.1
1	B	421	MET	2.1
1	D	321	ASP	2.1
1	A	551	ALA	2.1
1	C	552	PRO	2.1
1	B	468	SER	2.1
1	A	419	GLU	2.1
1	C	331	TYR	2.1
1	D	461	PHE	2.1
1	A	345	LEU	2.0
1	A	525	LEU	2.0
1	A	411	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	YCM	C	417	10/11	0.74	0.17	43,51,69,81	0
1	YCM	D	417	6/11	0.75	0.13	68,76,82,91	0
1	YCM	A	417	6/11	0.81	0.17	46,51,55,73	0
1	YCM	A	381	10/11	0.91	0.15	13,20,50,61	0
1	YCM	C	381	10/11	0.91	0.13	13,23,44,50	0
1	YCM	B	381	10/11	0.96	0.11	15,19,65,70	0
1	YCM	D	381	10/11	0.97	0.09	15,19,56,70	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
2	73I	A	601[A]	34/37	0.86	0.56	19,35,93,95	34
2	73I	A	601[B]	37/37	0.86	0.56	51,159,211,212	37
2	73I	B	601	37/37	0.88	0.12	22,35,56,59	0
2	73I	D	601	37/37	0.90	0.14	18,35,65,70	0
2	73I	C	601	37/37	0.93	0.11	15,25,61,72	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.
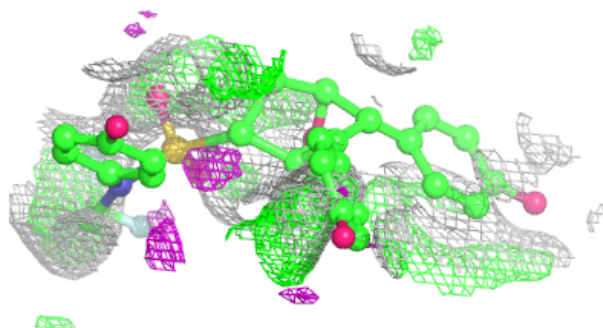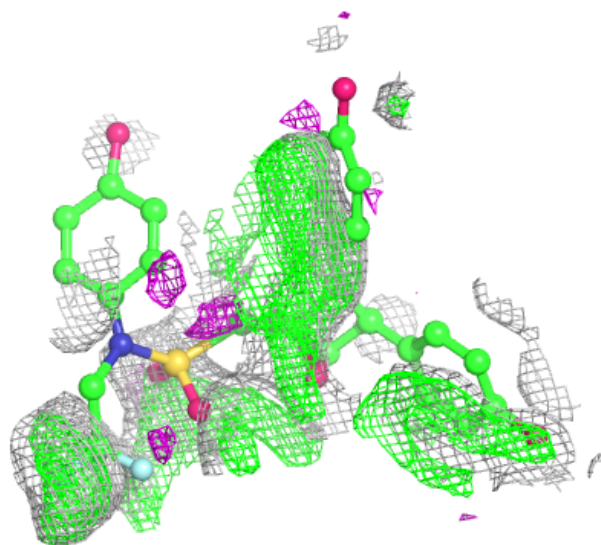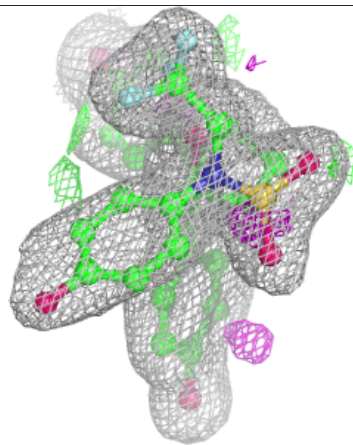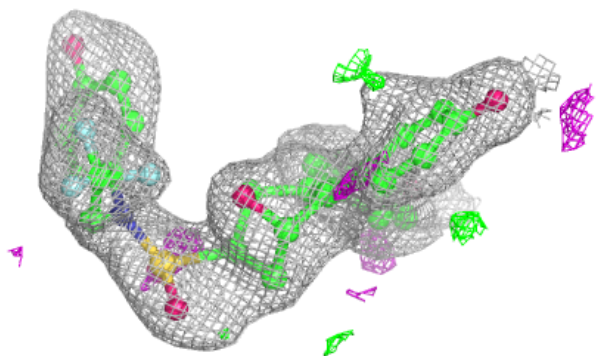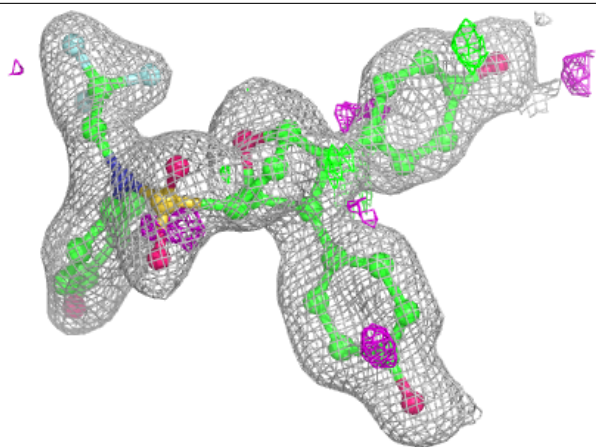
Electron density around 73I A 601 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
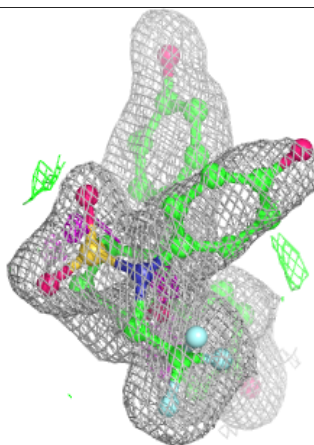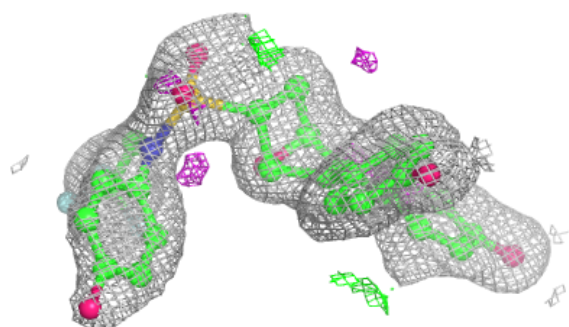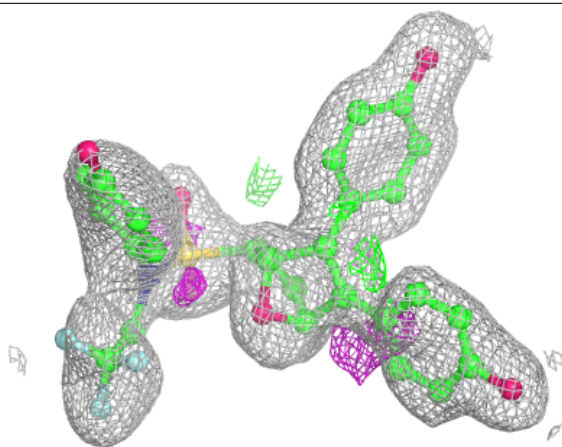mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
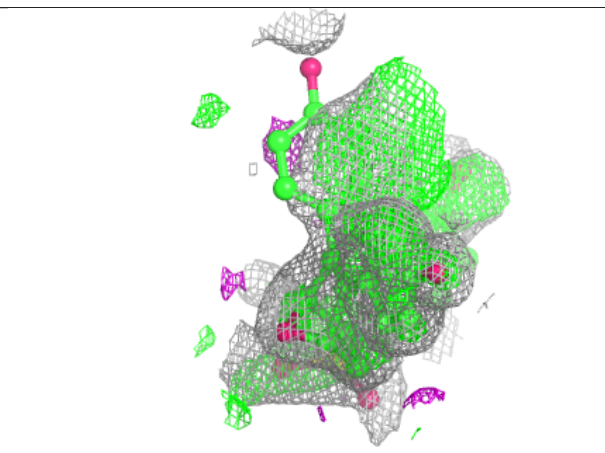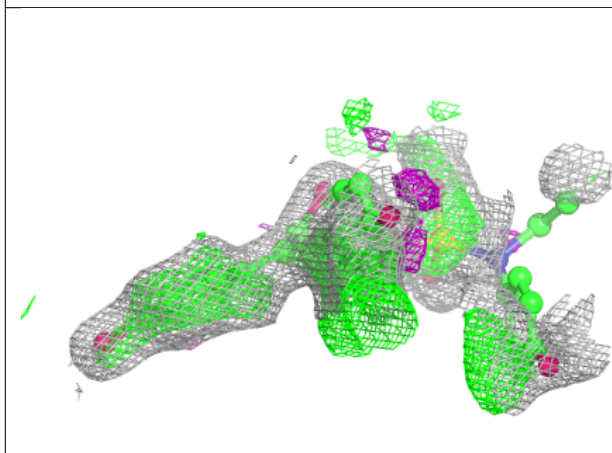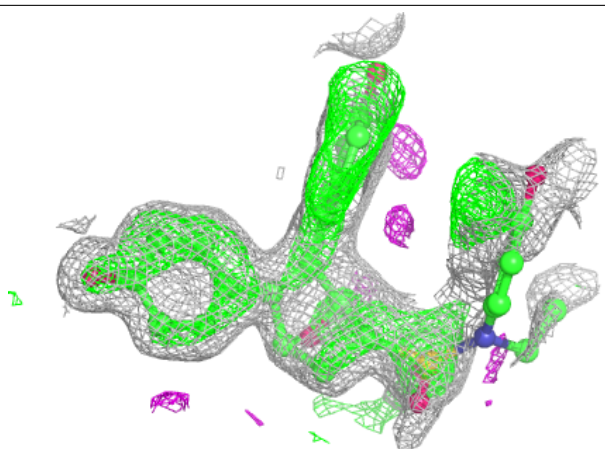
Electron density around 73I A 601 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
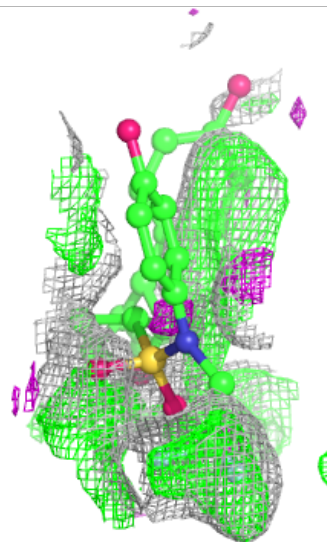
Electron density around 73I B 601:
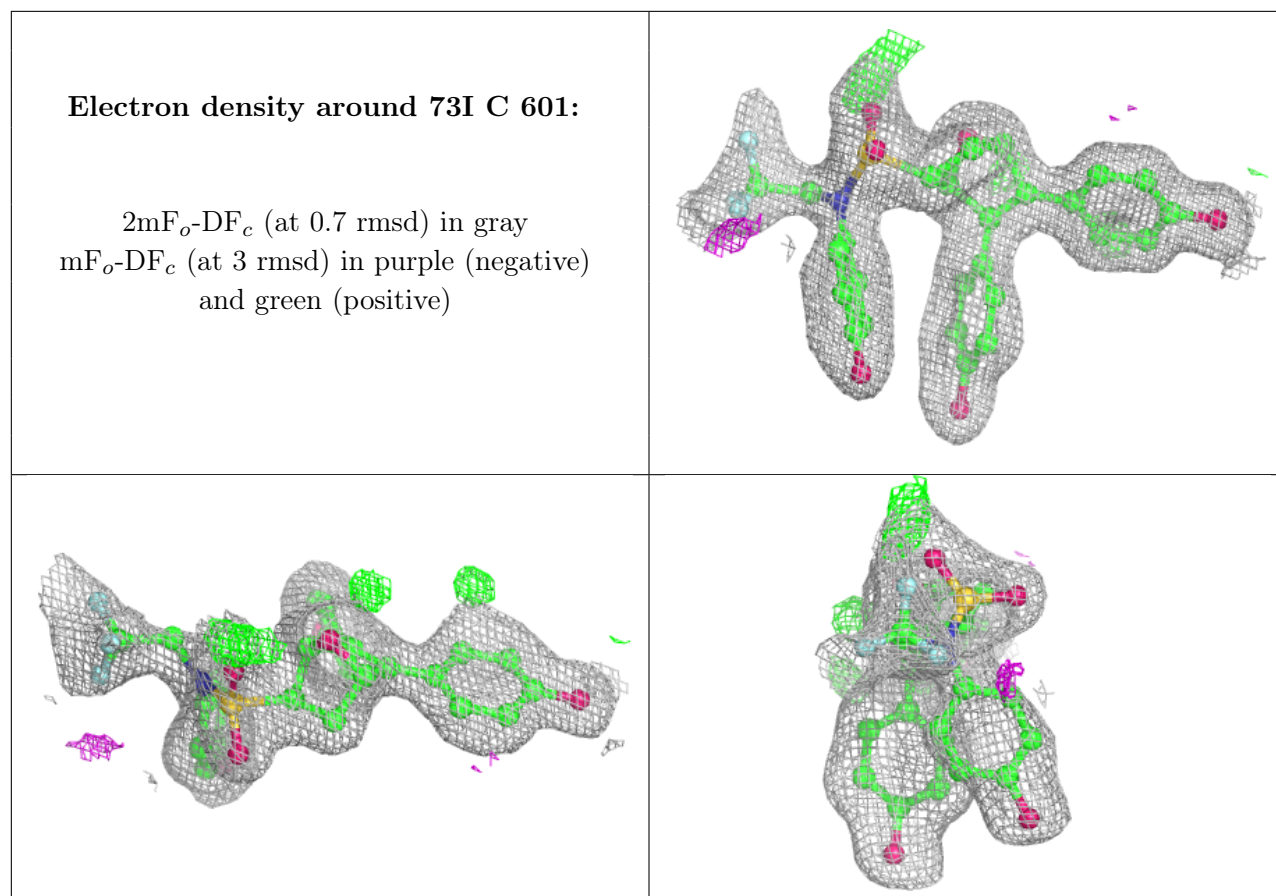
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 73I D 601:

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

Electron density around 73I C 601:

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.