



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 AM UTC

PDB ID : 4LUH / pdb_00004luh
Title : Complex of ovine serum albumin with 3,5-diiodosalicylic acid
Authors : Bujacz, A.; Talaj, J.A.; Pietrzyk, A.J.; Bujacz, G.
Deposited on : 2013-07-25
Resolution : 2.20 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

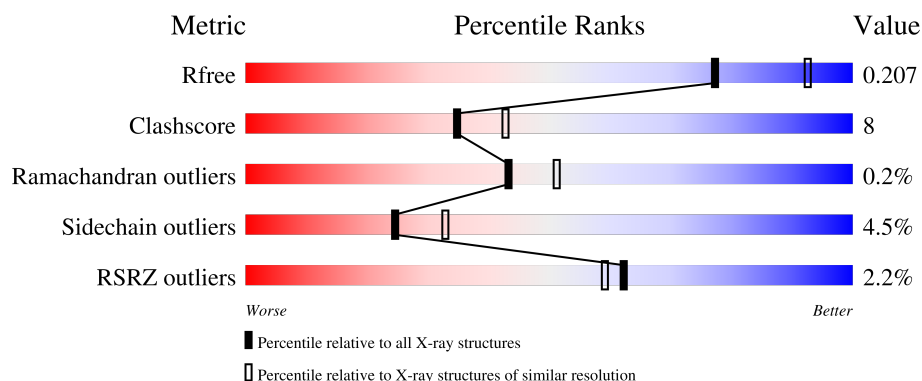
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

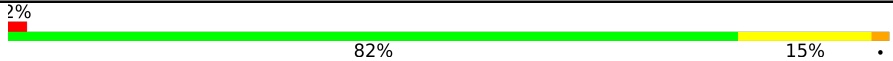
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	583	

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	DIU	A	601	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DIU	A	602	-	-	X	-
4	MLI	A	606	-	X	-	-

2 Entry composition [i](#)

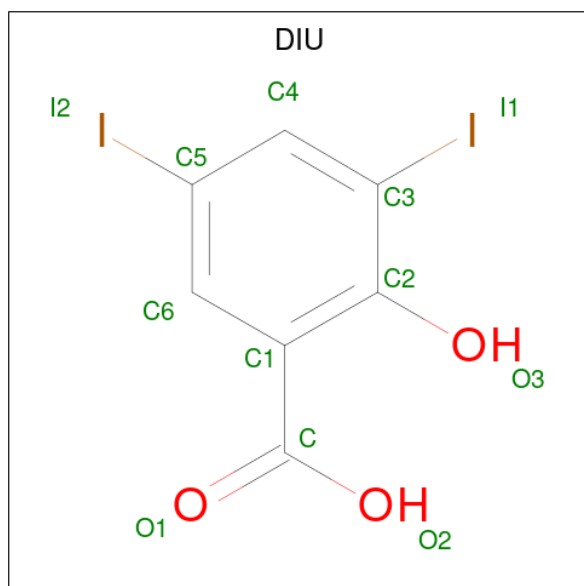
There are 9 unique types of molecules in this entry. The entry contains 4991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	1	0
			4652	2938	782	893	39			

- Molecule 2 is 2-HYDROXY-3,5-DIODO-BENZOIC ACID (CCD ID: DIU) (formula: $C_7H_4I_2O_3$).



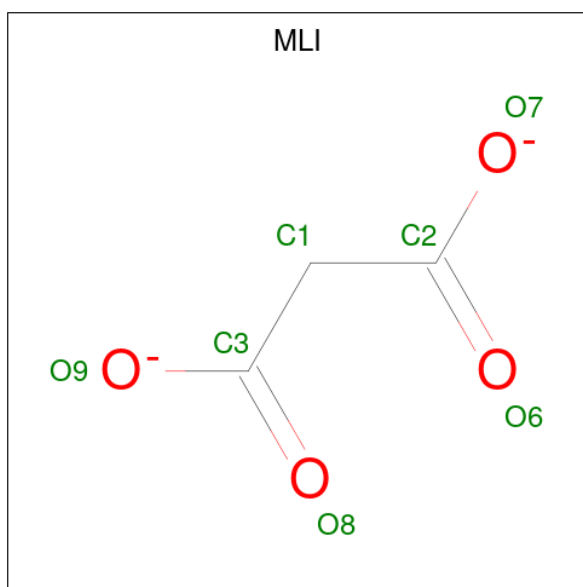
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	A	1	Total	C	I	O	0	0
			12	7	2	3		

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



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

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2^-$).



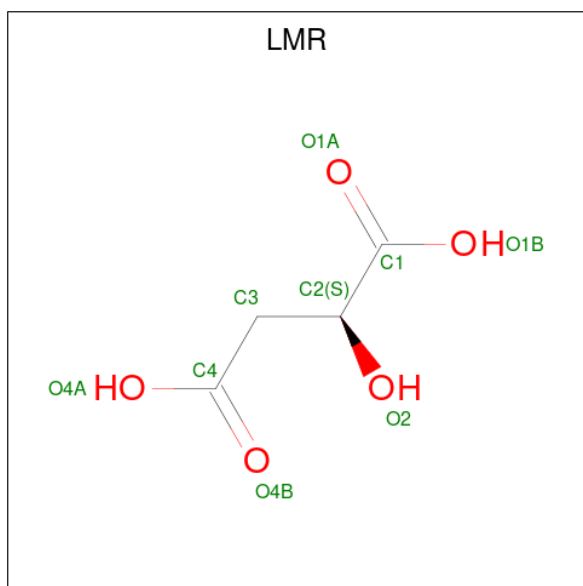
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

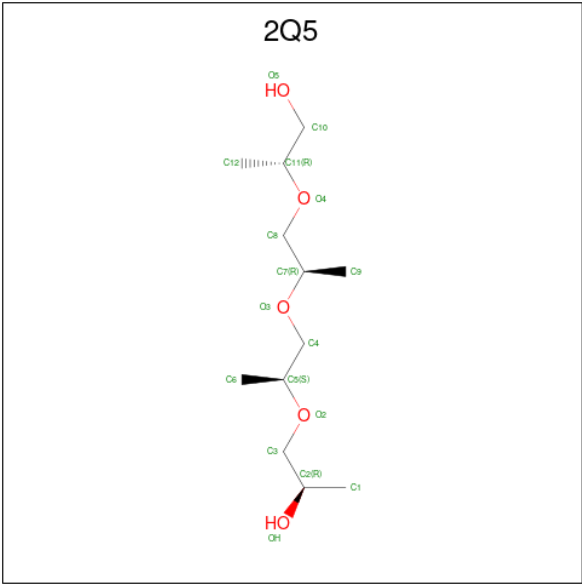
- Molecule 7 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	4	5		
7	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 8 is (2R)-2-{[(2R)-2-{[(2S)-2-{[(2R)-2-hydroxypropyl]oxy}propyl]oxy}propyl]oxy}

propan-1-ol (CCD ID: 2Q5) (formula: C₁₂H₂₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	12	5		
8	A	1	Total	C	O	0	0
			17	12	5		

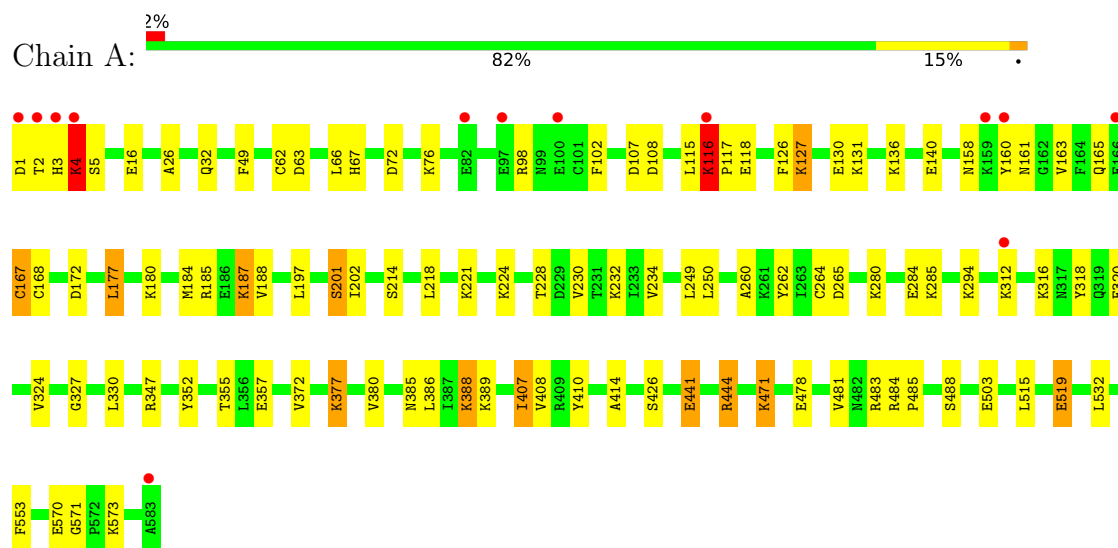
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	210	Total	O	0	0
			210	210		

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: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.53Å 118.53Å 120.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.22 – 2.20 47.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.22-2.20) 100.0 (47.22-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.171 , 0.209 0.168 , 0.207	Depositor DCC
R_{free} test set	1502 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4991	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: LMR, FMT, DIU, ACT, 2Q5, MLI, SIN

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	1.22	6/4753 (0.1%)	1.30	25/6417 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	SER	CA-C	-5.76	1.45	1.52
1	A	172	ASP	CA-C	5.51	1.59	1.53
1	A	441	GLU	N-CA	-5.44	1.39	1.46
1	A	294	LYS	C-O	-5.21	1.17	1.23
1	A	471	LYS	C-O	-5.16	1.17	1.24
1	A	265	ASP	C-O	-5.05	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	N-CA-C	-10.22	100.56	113.23
1	A	201	SER	CB-CA-C	-7.31	99.11	110.81
1	A	108	ASP	CA-C-N	-6.95	114.74	123.15
1	A	108	ASP	C-N-CA	-6.95	114.74	123.15
1	A	177	LEU	N-CA-C	6.70	118.67	111.36
1	A	161	ASN	N-CA-C	-6.67	103.48	111.69
1	A	4	LYS	CA-C-N	-6.51	111.85	122.26
1	A	4	LYS	C-N-CA	-6.51	111.85	122.26
1	A	327	GLY	N-CA-C	-6.29	105.19	112.73
1	A	158	ASN	N-CA-C	5.95	117.76	111.28
1	A	202	ILE	N-CA-C	-5.93	104.96	110.53
1	A	230	VAL	N-CA-C	-5.75	104.76	110.62
1	A	414	ALA	CA-C-N	-5.62	114.02	119.87
1	A	414	ALA	C-N-CA	-5.62	114.02	119.87
1	A	410	TYR	CA-CB-CG	-5.61	103.80	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LYS	CA-C-N	5.59	126.83	119.84
1	A	116	LYS	C-N-CA	5.59	126.83	119.84
1	A	380	VAL	N-CA-C	-5.52	105.73	111.58
1	A	320	GLU	N-CA-C	5.45	117.22	111.28
1	A	118	GLU	CA-C-N	5.38	126.56	119.84
1	A	118	GLU	C-N-CA	5.38	126.56	119.84
1	A	167	CYS	N-CA-C	5.29	117.73	111.33
1	A	49	PHE	N-CA-C	-5.25	105.64	111.36
1	A	16	GLU	N-CA-C	5.13	117.27	111.11
1	A	352	TYR	N-CA-C	-5.03	105.88	111.36

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	4652	0	4555	68	0
2	A	24	0	6	8	0
3	A	24	0	12	2	0
4	A	14	0	4	0	0
5	A	12	0	9	0	0
6	A	3	0	1	0	0
7	A	18	0	8	0	0
8	A	34	0	52	5	0
9	A	210	0	0	12	0
All	All	4991	0	4647	71	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 8.

All (71) 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:4:LYS:HD2	1:A:63:ASP:O	1.46	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD21	1:A:250:LEU:CD1	1.83	1.08
1:A:66:LEU:HD21	1:A:250:LEU:HD12	1.35	1.07
1:A:386:LEU:HD23	9:A:853:HOH:O	1.64	0.98
1:A:32:GLN:HE22	1:A:107:ASP:H	1.21	0.87
1:A:4:LYS:CD	1:A:63:ASP:O	2.24	0.85
1:A:386:LEU:CD2	9:A:853:HOH:O	2.23	0.83
1:A:66:LEU:CD2	1:A:250:LEU:HD12	2.12	0.77
1:A:388:LYS:NZ	1:A:444:ARG:HH22	1.84	0.76
1:A:160:TYR:CE2	1:A:184:MET:HG3	2.24	0.73
1:A:377:LYS:HA	9:A:803:HOH:O	1.88	0.73
1:A:1:ASP:O	1:A:4:LYS:N	2.23	0.70
1:A:1:ASP:O	1:A:4:LYS:HB2	1.97	0.65
1:A:131:LYS:HE2	8:A:614:2Q5:H20	1.79	0.63
1:A:66:LEU:HD21	1:A:250:LEU:HD13	1.76	0.63
1:A:187:LYS:HE3	9:A:851:HOH:O	2.00	0.61
1:A:218:LEU:HD11	2:A:601:DIU:I1	2.71	0.60
1:A:388:LYS:HZ1	1:A:444:ARG:HH22	1.48	0.60
1:A:484:ARG:HD2	1:A:484:ARG:C	2.27	0.59
1:A:127:LYS:HE3	1:A:168:CYS:O	2.02	0.59
1:A:330:LEU:HD22	8:A:615:2Q5:H16	1.87	0.57
1:A:72:ASP:O	1:A:76:LYS:HG3	2.05	0.57
1:A:2:THR:C	1:A:4:LYS:H	2.14	0.56
1:A:136:LYS:HE2	1:A:140:GLU:OE1	2.05	0.55
8:A:615:2Q5:H7	9:A:895:HOH:O	2.06	0.54
1:A:197:LEU:HD21	2:A:602:DIU:H4	1.89	0.54
1:A:126:PHE:CE1	1:A:130:GLU:HG2	2.43	0.54
1:A:32:GLN:NE2	1:A:107:ASP:H	2.01	0.54
1:A:160:TYR:CD2	1:A:184:MET:HG3	2.44	0.52
1:A:115:LEU:HB2	9:A:909:HOH:O	2.10	0.52
1:A:160:TYR:O	1:A:163:VAL:HB	2.10	0.51
1:A:232:LYS:HE3	1:A:262:TYR:CZ	2.44	0.51
1:A:185:ARG:NH1	3:A:605:SIN:O2	2.44	0.51
1:A:117:PRO:HA	9:A:903:HOH:O	2.10	0.50
1:A:197:LEU:CD2	2:A:602:DIU:H4	2.41	0.50
1:A:347:ARG:HD2	9:A:838:HOH:O	2.10	0.50
1:A:471:LYS:NZ	9:A:845:HOH:O	2.44	0.49
1:A:488:SER:O	9:A:772:HOH:O	2.20	0.49
1:A:67[B]:HIS:HB2	9:A:817:HOH:O	2.12	0.49
1:A:388:LYS:HZ3	1:A:444:ARG:HH22	1.56	0.48
1:A:570:GLU:OE2	1:A:573:LYS:HE2	2.13	0.48
8:A:615:2Q5:H17	8:A:615:2Q5:H20	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG11	3:A:605:SIN:H32	1.94	0.48
1:A:408:VAL:HG22	1:A:532:LEU:HD11	1.95	0.47
1:A:4:LYS:CE	1:A:63:ASP:O	2.62	0.47
1:A:98:ARG:HG2	1:A:102:PHE:CE2	2.51	0.46
1:A:484:ARG:HB3	1:A:485:PRO:HD3	1.98	0.45
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.80	0.45
1:A:324:VAL:HA	8:A:615:2Q5:C1	2.47	0.45
1:A:407:ILE:HG13	1:A:426:SER:CB	2.46	0.45
1:A:515:LEU:HD13	1:A:519:GLU:HB3	1.98	0.45
1:A:264:CYS:SG	1:A:285:LYS:HD2	2.57	0.45
1:A:66:LEU:CD2	1:A:250:LEU:CD1	2.74	0.45
1:A:280:LYS:HD3	1:A:284:GLU:HG2	1.98	0.44
1:A:66:LEU:HD23	9:A:702:HOH:O	2.17	0.44
1:A:318:TYR:OH	1:A:357:GLU:OE2	2.34	0.44
1:A:232:LYS:HE3	1:A:262:TYR:CE1	2.53	0.43
1:A:570:GLU:OE2	1:A:573:LYS:CE	2.66	0.43
1:A:2:THR:C	1:A:4:LYS:N	2.73	0.43
1:A:201:SER:OG	2:A:602:DIU:I2	3.01	0.43
1:A:260:ALA:HB2	2:A:601:DIU:I2	2.88	0.43
1:A:197:LEU:HD23	2:A:602:DIU:C4	2.48	0.43
2:A:602:DIU:O2	2:A:602:DIU:O3	2.37	0.42
1:A:197:LEU:CD2	2:A:602:DIU:C4	2.98	0.42
1:A:5:SER:HA	1:A:62:CYS:O	2.21	0.41
1:A:26:ALA:HB2	1:A:249:LEU:HD12	2.01	0.41
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.69	0.41
1:A:355:THR:HG21	1:A:372:VAL:HG23	2.02	0.41
1:A:167:CYS:HB3	1:A:177:LEU:HG	2.02	0.40
1:A:214:SER:HB2	1:A:234:VAL:HG13	2.02	0.40
1:A:553:PHE:CZ	1:A:571:GLY:HA2	2.56	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	582/583 (100%)	564 (97%)	17 (3%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS

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	517/516 (100%)	494 (96%)	23 (4%)	25	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	116	LYS
1	A	127	LYS
1	A	165	GLN
1	A	180	LYS
1	A	187	LYS
1	A	221	LYS
1	A	224	LYS
1	A	228	THR
1	A	312	LYS
1	A	316	LYS
1	A	377	LYS
1	A	385	ASN
1	A	388	LYS
1	A	389	LYS
1	A	407	ILE
1	A	441	GLU
1	A	444	ARG
1	A	478	GLU
1	A	481	VAL

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Mol	Chain	Res	Type
1	A	483	ARG
1	A	503	GLU
1	A	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	59	HIS
1	A	165	GLN
1	A	366	HIS
1	A	378	HIS
1	A	482	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	DIU	A	601	-	12,12,12	1.68	3 (25%)	17,17,17	3.31	10 (58%)
8	2Q5	A	615	-	16,16,16	1.05	0	19,19,19	2.12	4 (21%)
6	FMT	A	611	-	2,2,2	0.72	0	1,1,1	0.87	0
4	MLI	A	607	-	6,6,6	1.30	1 (16%)	7,7,7	1.66	1 (14%)
5	ACT	A	608	-	3,3,3	1.69	1 (33%)	3,3,3	0.19	0
7	LMR	A	612	-	8,8,8	1.29	0	10,10,10	2.30	4 (40%)
7	LMR	A	613	-	8,8,8	1.39	1 (12%)	10,10,10	1.80	3 (30%)
3	SIN	A	604	-	7,7,7	0.97	0	8,8,8	1.49	1 (12%)
2	DIU	A	602	-	12,12,12	1.66	2 (16%)	17,17,17	1.57	4 (23%)
4	MLI	A	606	-	6,6,6	2.23	4 (66%)	7,7,7	1.65	2 (28%)
8	2Q5	A	614	-	16,16,16	1.10	0	19,19,19	1.64	4 (21%)
3	SIN	A	605	-	7,7,7	1.17	0	8,8,8	1.24	1 (12%)
5	ACT	A	610	-	3,3,3	0.96	0	3,3,3	1.04	0
5	ACT	A	609	-	3,3,3	1.30	0	3,3,3	0.52	0
3	SIN	A	603	-	7,7,7	1.40	0	8,8,8	1.46	1 (12%)

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	DIU	A	601	-	-	2/4/4/4	0/1/1/1
8	2Q5	A	615	-	-	7/17/17/17	-
4	MLI	A	607	-	-	2/4/4/4	-
7	LMR	A	612	-	-	6/8/8/8	-
7	LMR	A	613	-	-	0/8/8/8	-
3	SIN	A	604	-	-	4/5/5/5	-
2	DIU	A	602	-	-	1/4/4/4	0/1/1/1
4	MLI	A	606	-	-	2/4/4/4	-
8	2Q5	A	614	-	-	4/17/17/17	-
3	SIN	A	605	-	-	3/5/5/5	-
3	SIN	A	603	-	-	4/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	DIU	C3-I1	4.12	2.19	2.10
4	A	606	MLI	C1-C3	3.27	1.56	1.51
2	A	601	DIU	C6-C1	3.13	1.44	1.39
2	A	601	DIU	C1-C2	2.69	1.45	1.41
5	A	608	ACT	O-C	2.44	1.32	1.22
4	A	606	MLI	O7-C2	-2.43	1.22	1.30
2	A	601	DIU	C4-C3	-2.40	1.34	1.39
4	A	606	MLI	C1-C2	2.32	1.54	1.51
2	A	602	DIU	C5-I2	2.13	2.15	2.10
7	A	613	LMR	O1B-C1	-2.10	1.24	1.30
4	A	606	MLI	O6-C2	2.07	1.28	1.22
4	A	607	MLI	O8-C3	2.03	1.28	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	DIU	C3-C4-C5	6.73	125.69	119.42
8	A	615	2Q5	O5-C10-C11	-5.87	96.69	111.77
2	A	601	DIU	O3-C2-C1	5.73	131.32	121.11
2	A	601	DIU	O1-C-C1	-4.94	110.18	121.97
2	A	601	DIU	C6-C1-C2	4.89	125.09	119.39
7	A	612	LMR	C3-C2-C1	4.30	121.08	110.53
2	A	601	DIU	C1-C6-C5	-3.94	112.66	119.06
4	A	607	MLI	C3-C1-C2	-3.80	99.53	112.95
8	A	614	2Q5	C8-O4-C11	3.77	120.61	115.05
2	A	602	DIU	C3-C4-C5	3.51	122.69	119.42
8	A	614	2Q5	O4-C8-C7	3.36	119.00	110.82
8	A	615	2Q5	O4-C11-C12	3.31	122.22	110.22
7	A	613	LMR	C2-C3-C4	3.27	120.62	112.08
7	A	612	LMR	O1B-C1-O1A	-3.23	116.75	124.08
8	A	615	2Q5	C3-O2-C5	3.22	119.80	115.05
2	A	601	DIU	C1-C2-C3	-3.16	115.23	118.95
2	A	601	DIU	O2-C-O1	3.01	129.82	123.35
7	A	612	LMR	O2-C2-C3	-3.00	102.74	109.96
7	A	613	LMR	O1B-C1-C2	2.88	118.83	112.74
8	A	614	2Q5	O4-C11-C10	2.84	116.21	108.64
7	A	612	LMR	O1B-C1-C2	2.79	118.64	112.74
2	A	601	DIU	C2-C1-C	2.73	122.91	119.86
3	A	603	SIN	O2-C1-C2	2.71	122.56	114.00
2	A	601	DIU	O3-C2-C3	-2.65	113.45	120.30
3	A	605	SIN	C3-C2-C1	-2.60	106.78	113.67
2	A	602	DIU	C6-C1-C2	2.52	122.34	119.39
7	A	613	LMR	O2-C2-C1	-2.50	104.01	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	DIU	O3-C2-C1	-2.46	116.72	121.11
4	A	606	MLI	O9-C3-O8	-2.44	117.06	123.33
8	A	614	2Q5	C4-O3-C7	2.27	118.39	115.05
4	A	606	MLI	C3-C1-C2	2.25	120.89	112.95
8	A	615	2Q5	OH-C2-C1	-2.22	99.92	109.45
3	A	604	SIN	C3-C2-C1	-2.13	108.03	113.67
2	A	601	DIU	C6-C1-C	-2.10	111.99	117.89
2	A	602	DIU	C4-C3-C2	-2.02	117.51	121.33

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	2Q5	C9-C7-O3-C4
8	A	615	2Q5	C6-C5-O2-C3
8	A	615	2Q5	O3-C4-C5-C6
8	A	615	2Q5	C9-C7-O3-C4
8	A	615	2Q5	O3-C7-C8-O4
8	A	615	2Q5	C9-C7-C8-O4
8	A	615	2Q5	C12-C11-O4-C8
3	A	605	SIN	C1-C2-C3-C4
4	A	607	MLI	C2-C1-C3-O9
4	A	606	MLI	C2-C1-C3-O9
7	A	612	LMR	O1A-C1-C2-C3
7	A	612	LMR	O1B-C1-C2-C3
8	A	614	2Q5	O3-C4-C5-C6
2	A	601	DIU	O2-C-C1-C2
8	A	614	2Q5	O3-C4-C5-O2
4	A	607	MLI	C2-C1-C3-O8
8	A	614	2Q5	C12-C11-O4-C8
8	A	615	2Q5	C1-C2-C3-O2
2	A	601	DIU	O1-C-C1-C2
4	A	606	MLI	C2-C1-C3-O8
3	A	604	SIN	C2-C3-C4-O3
2	A	602	DIU	O1-C-C1-C2
3	A	604	SIN	C2-C3-C4-O4
7	A	612	LMR	O1B-C1-C2-O2
3	A	603	SIN	O2-C1-C2-C3
3	A	605	SIN	O1-C1-C2-C3
3	A	603	SIN	O1-C1-C2-C3
3	A	604	SIN	O2-C1-C2-C3
3	A	604	SIN	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	605	SIN	O2-C1-C2-C3
7	A	612	LMR	O2-C2-C3-C4
7	A	612	LMR	C1-C2-C3-C4
7	A	612	LMR	O1A-C1-C2-O2
3	A	603	SIN	C2-C3-C4-O3
3	A	603	SIN	C2-C3-C4-O4

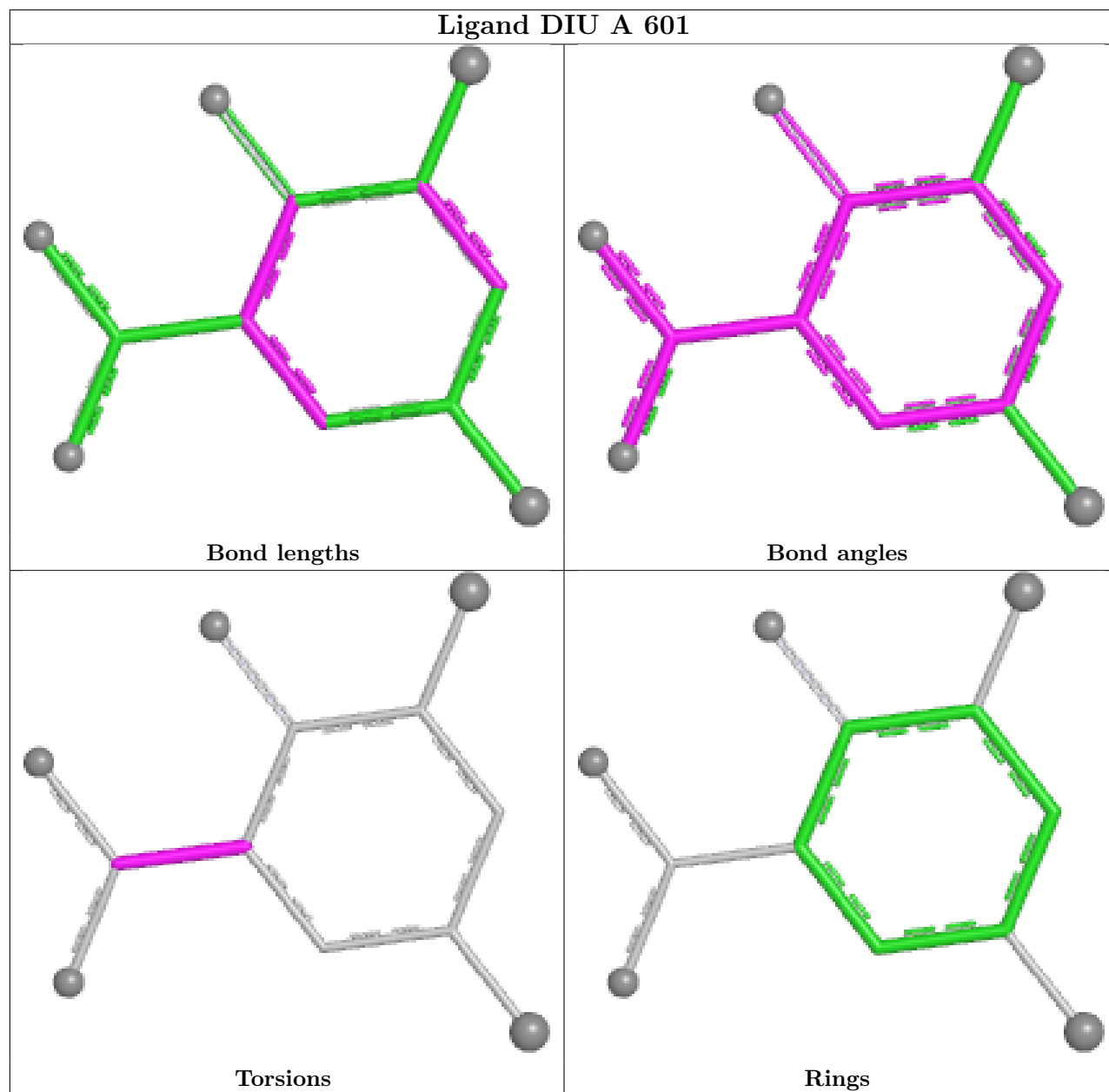
There are no ring outliers.

5 monomers are involved in 15 short contacts:

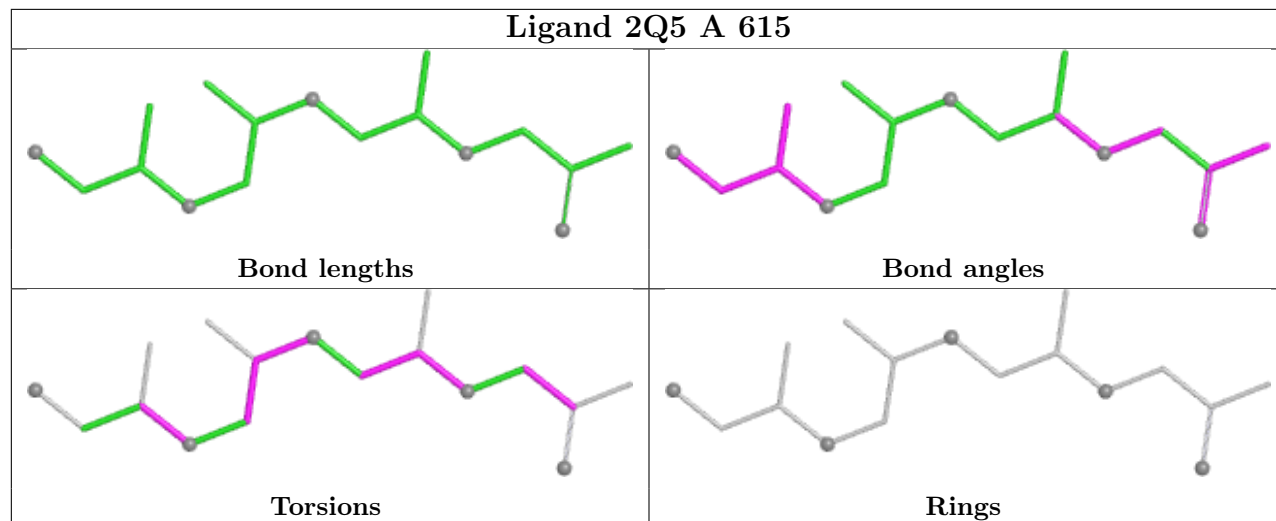
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DIU	2	0
8	A	615	2Q5	4	0
2	A	602	DIU	6	0
8	A	614	2Q5	1	0
3	A	605	SIN	2	0

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

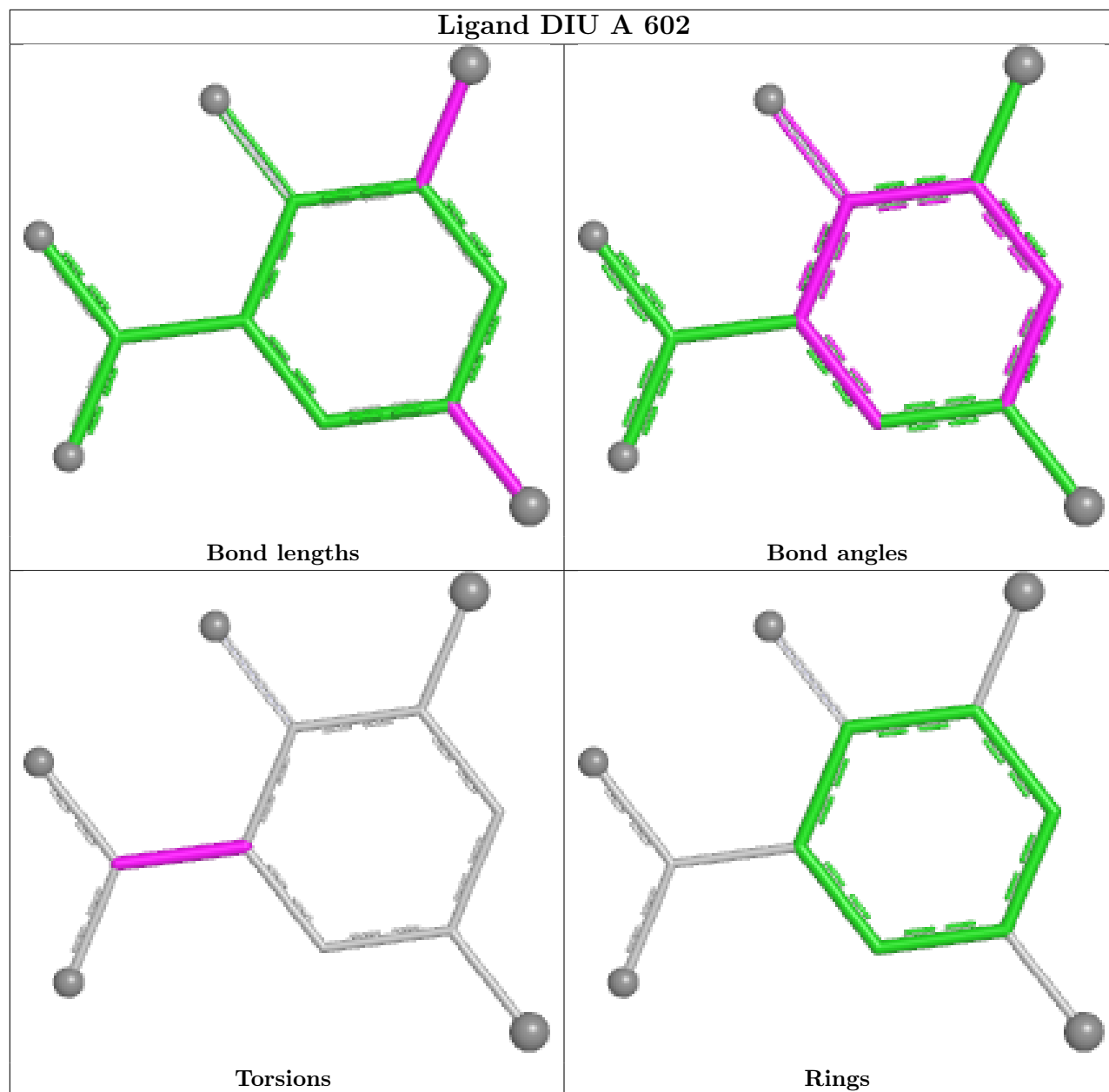
Ligand DIU A 601



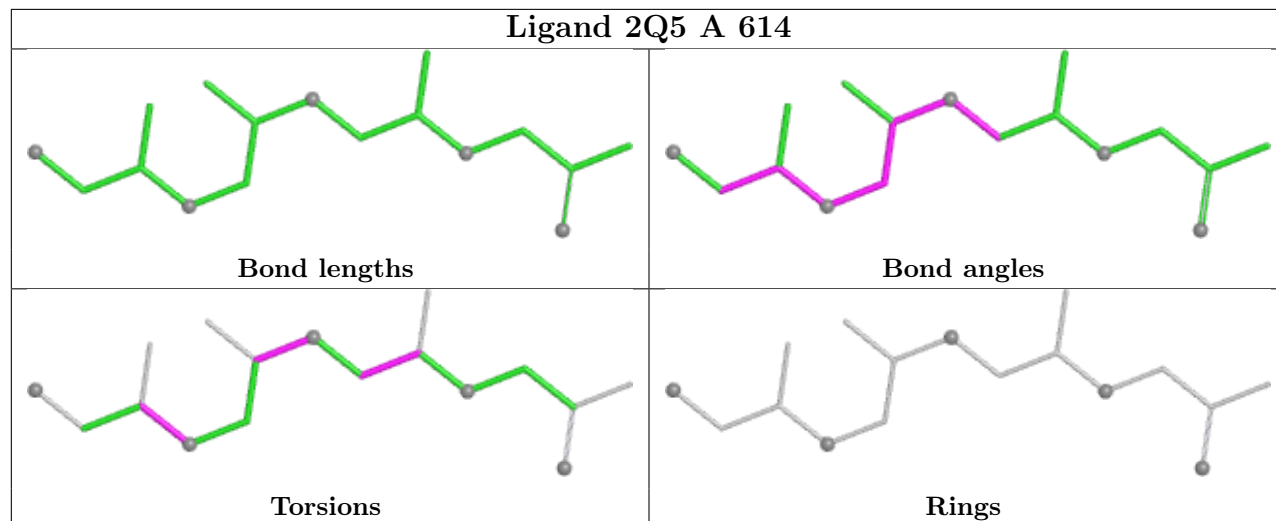
Ligand 2Q5 A 615



Ligand DIU A 602



Ligand 2Q5 A 614



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	583/583 (100%)	-0.22	13 (2%) 62 59	25, 40, 68, 111	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	8.0
1	A	3	HIS	5.9
1	A	4	LYS	5.0
1	A	1	ASP	3.7
1	A	160	TYR	3.2
1	A	82	GLU	2.8
1	A	116	LYS	2.7
1	A	583	ALA	2.5
1	A	312	LYS	2.2
1	A	159	LYS	2.2
1	A	97	GLU	2.1
1	A	166	GLU	2.1
1	A	100	GLU	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

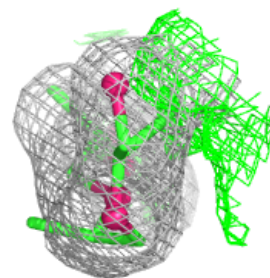
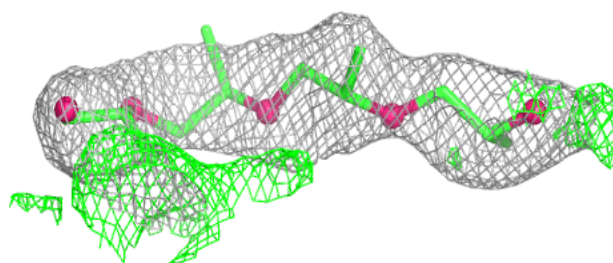
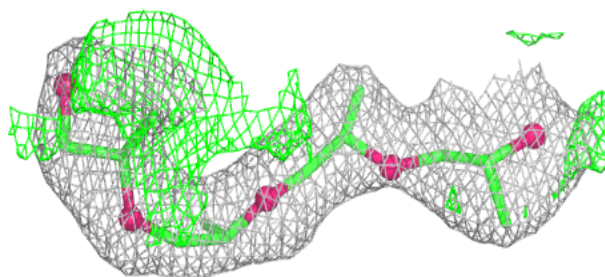
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	608	4/4	0.82	0.20	41,42,49,55	0
7	LMR	A	612	9/9	0.85	0.18	69,75,90,98	0
4	MLI	A	607	7/7	0.86	0.16	54,73,85,88	0
8	2Q5	A	615	17/17	0.88	0.18	51,67,81,81	0
2	DIU	A	602	12/12	0.89	0.25	74,84,96,97	0
3	SIN	A	605	8/8	0.89	0.15	54,79,91,91	0
7	LMR	A	613	9/9	0.92	0.12	62,70,79,82	0
3	SIN	A	603	8/8	0.92	0.14	56,61,75,84	0
8	2Q5	A	614	17/17	0.93	0.16	58,69,80,83	0
3	SIN	A	604	8/8	0.94	0.14	70,82,84,85	0
4	MLI	A	606	7/7	0.94	0.09	43,49,52,55	0
2	DIU	A	601	12/12	0.95	0.15	49,63,70,98	0
5	ACT	A	609	4/4	0.95	0.13	45,46,52,55	0
5	ACT	A	610	4/4	0.95	0.11	48,52,55,55	0
6	FMT	A	611	3/3	0.95	0.14	52,52,54,67	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.

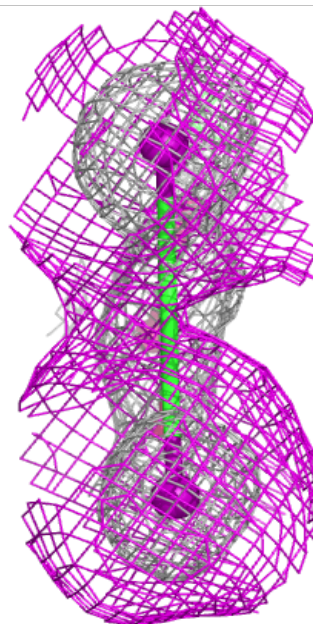
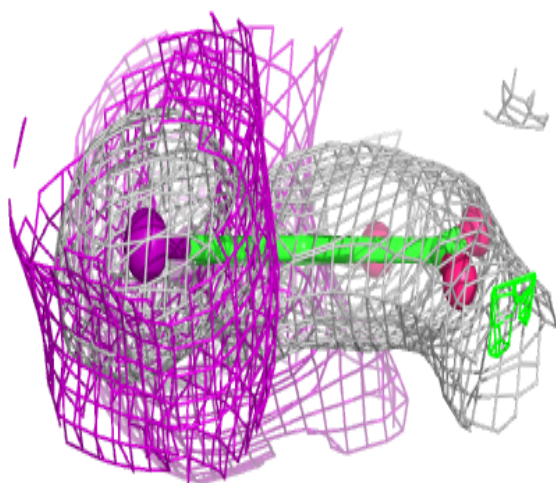
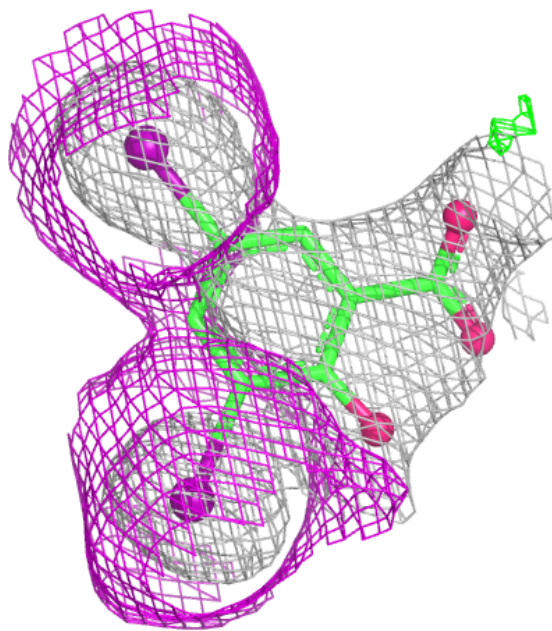
Electron density around 2Q5 A 615:

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



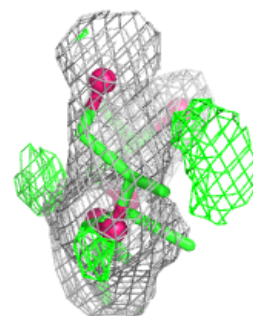
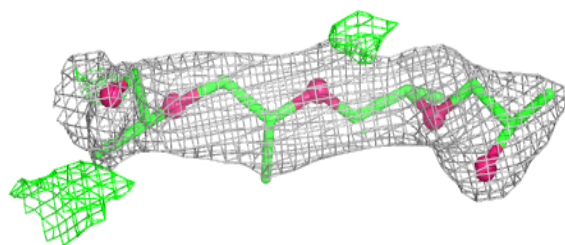
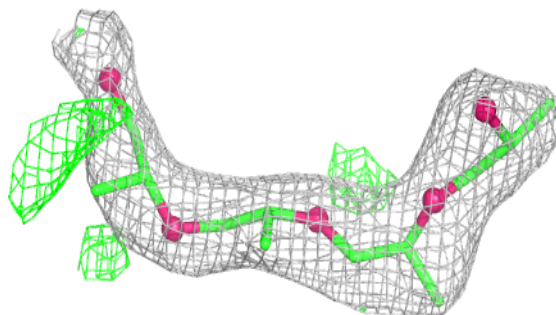
Electron density around DIU A 602:

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



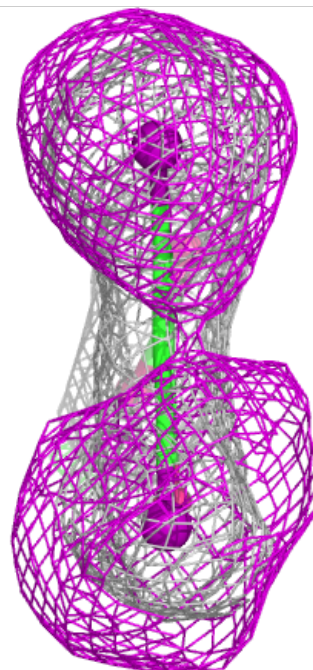
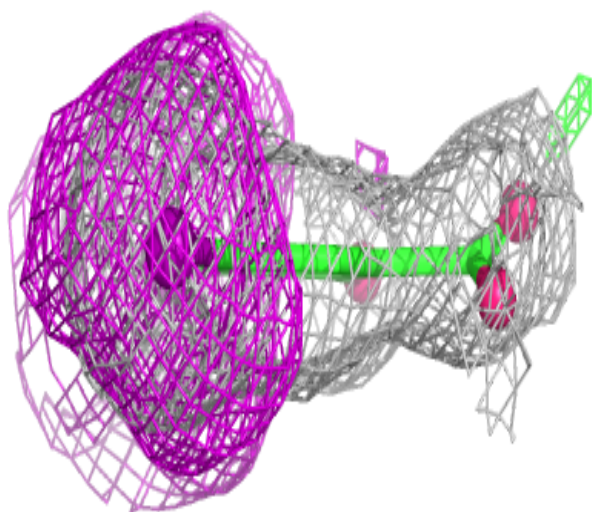
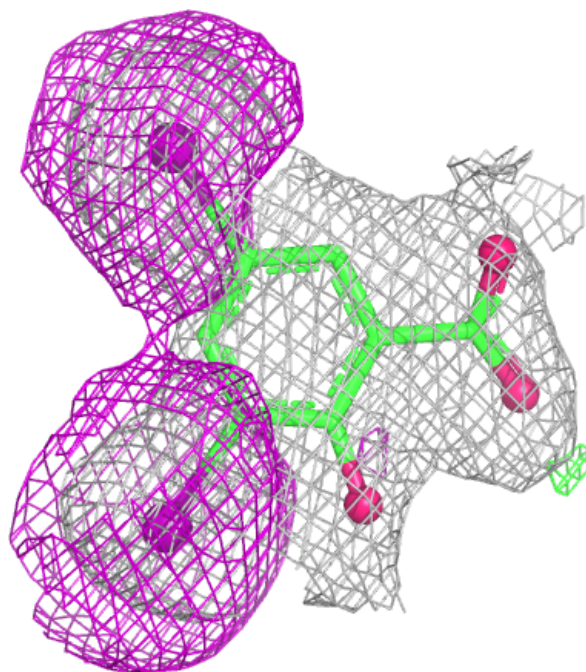
Electron density around 2Q5 A 614:

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



Electron density around DIU A 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.