



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:23 PM UTC

PDB ID : 9EZJ / pdb_00009ezj
Title : Apo human TDO in complex with a bound inhibitor (Cpd-4)
Authors : Wicki, M.; Mac Sweeney, A.
Deposited on : 2024-04-12
Resolution : 2.61 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

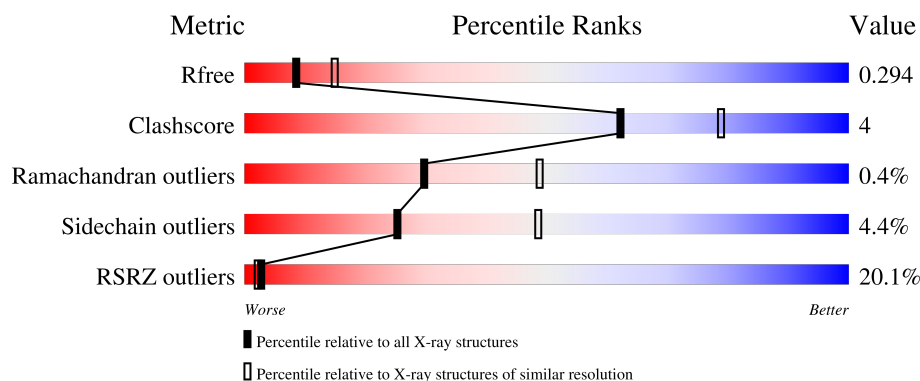
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	403	14% 67% 10% 22%
1	B	403	14% 69% 9% 21%
1	C	403	21% 69% 8% 22%
1	D	403	14% 67% 9% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10283 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	1	0
			2523	1640	428	445	10			
1	B	319	Total	C	N	O	S	0	1	0
			2539	1648	429	451	11			
1	C	315	Total	C	N	O	S	0	1	0
			2506	1627	424	445	10			
1	D	312	Total	C	N	O	S	0	0	0
			2487	1616	423	439	9			

There are 60 discrepancies between the modelled and reference sequences:

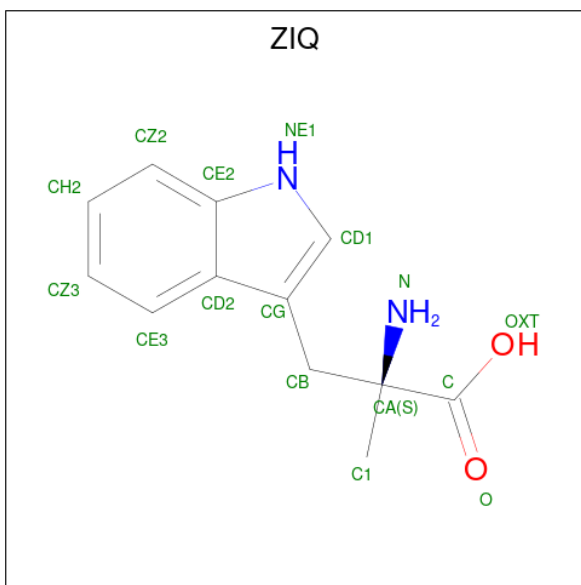
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P48775
A	5	ARG	-	expression tag	UNP P48775
A	6	GLY	-	expression tag	UNP P48775
A	7	SER	-	expression tag	UNP P48775
A	8	HIS	-	expression tag	UNP P48775
A	9	HIS	-	expression tag	UNP P48775
A	10	HIS	-	expression tag	UNP P48775
A	11	HIS	-	expression tag	UNP P48775
A	12	HIS	-	expression tag	UNP P48775
A	13	HIS	-	expression tag	UNP P48775
A	14	GLY	-	expression tag	UNP P48775
A	15	ILE	-	expression tag	UNP P48775
A	16	ASP	-	expression tag	UNP P48775
A	17	HIS	-	expression tag	UNP P48775
A	18	MET	-	expression tag	UNP P48775
B	4	MET	-	initiating methionine	UNP P48775
B	5	ARG	-	expression tag	UNP P48775
B	6	GLY	-	expression tag	UNP P48775
B	7	SER	-	expression tag	UNP P48775
B	8	HIS	-	expression tag	UNP P48775
B	9	HIS	-	expression tag	UNP P48775

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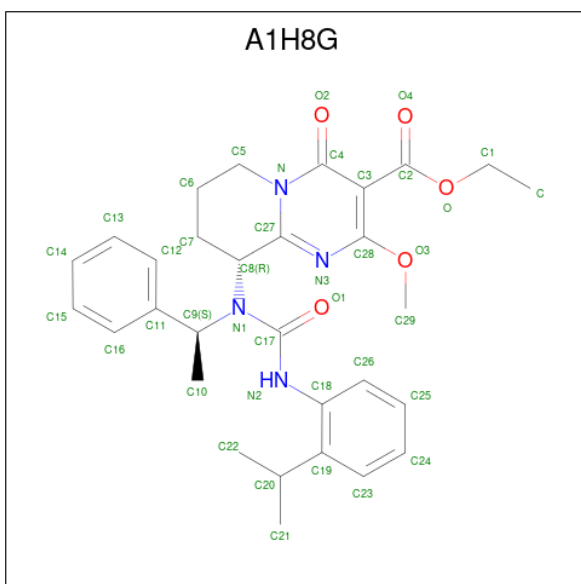
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP P48775
B	11	HIS	-	expression tag	UNP P48775
B	12	HIS	-	expression tag	UNP P48775
B	13	HIS	-	expression tag	UNP P48775
B	14	GLY	-	expression tag	UNP P48775
B	15	ILE	-	expression tag	UNP P48775
B	16	ASP	-	expression tag	UNP P48775
B	17	HIS	-	expression tag	UNP P48775
B	18	MET	-	expression tag	UNP P48775
C	4	MET	-	initiating methionine	UNP P48775
C	5	ARG	-	expression tag	UNP P48775
C	6	GLY	-	expression tag	UNP P48775
C	7	SER	-	expression tag	UNP P48775
C	8	HIS	-	expression tag	UNP P48775
C	9	HIS	-	expression tag	UNP P48775
C	10	HIS	-	expression tag	UNP P48775
C	11	HIS	-	expression tag	UNP P48775
C	12	HIS	-	expression tag	UNP P48775
C	13	HIS	-	expression tag	UNP P48775
C	14	GLY	-	expression tag	UNP P48775
C	15	ILE	-	expression tag	UNP P48775
C	16	ASP	-	expression tag	UNP P48775
C	17	HIS	-	expression tag	UNP P48775
C	18	MET	-	expression tag	UNP P48775
D	4	MET	-	initiating methionine	UNP P48775
D	5	ARG	-	expression tag	UNP P48775
D	6	GLY	-	expression tag	UNP P48775
D	7	SER	-	expression tag	UNP P48775
D	8	HIS	-	expression tag	UNP P48775
D	9	HIS	-	expression tag	UNP P48775
D	10	HIS	-	expression tag	UNP P48775
D	11	HIS	-	expression tag	UNP P48775
D	12	HIS	-	expression tag	UNP P48775
D	13	HIS	-	expression tag	UNP P48775
D	14	GLY	-	expression tag	UNP P48775
D	15	ILE	-	expression tag	UNP P48775
D	16	ASP	-	expression tag	UNP P48775
D	17	HIS	-	expression tag	UNP P48775
D	18	MET	-	expression tag	UNP P48775

- Molecule 2 is alpha-methyl-L-tryptophan (CCD ID: ZIQ) (formula: C₁₂H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	12	2	2		
2	B	1	Total	C	N	O	0	0
			16	12	2	2		
2	C	1	Total	C	N	O	0	0
			16	12	2	2		
2	D	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 3 is ethyl (9 {R})-2-methoxy-4-oxidanilidene-9-[[1 {S}]-1-phenylethyl]-[(2-prop an-2-ylphenyl)carbamoyl]amino]-6,7,8,9-tetrahydropyrido[1,2-a]pyrimidine-3-carboxylate (CCD ID: A1H8G) (formula: C₃₀H₃₆N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			39	30	4	5		
3	B	1	Total	C	N	O	0	0
			39	30	4	5		
3	C	1	Total	C	N	O	0	0
			39	30	4	5		
3	D	1	Total	C	N	O	0	0
			39	30	4	5		

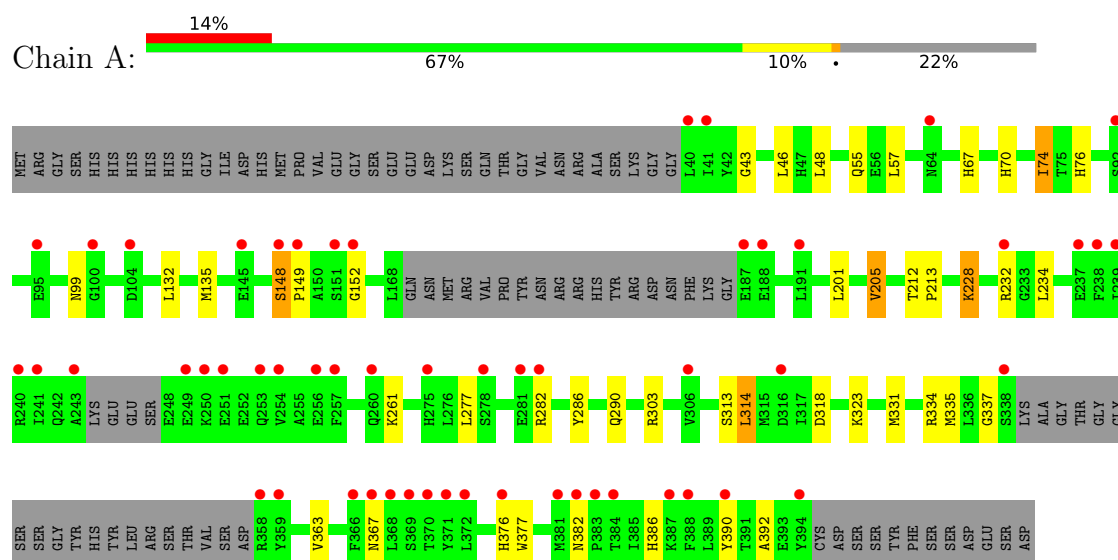
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

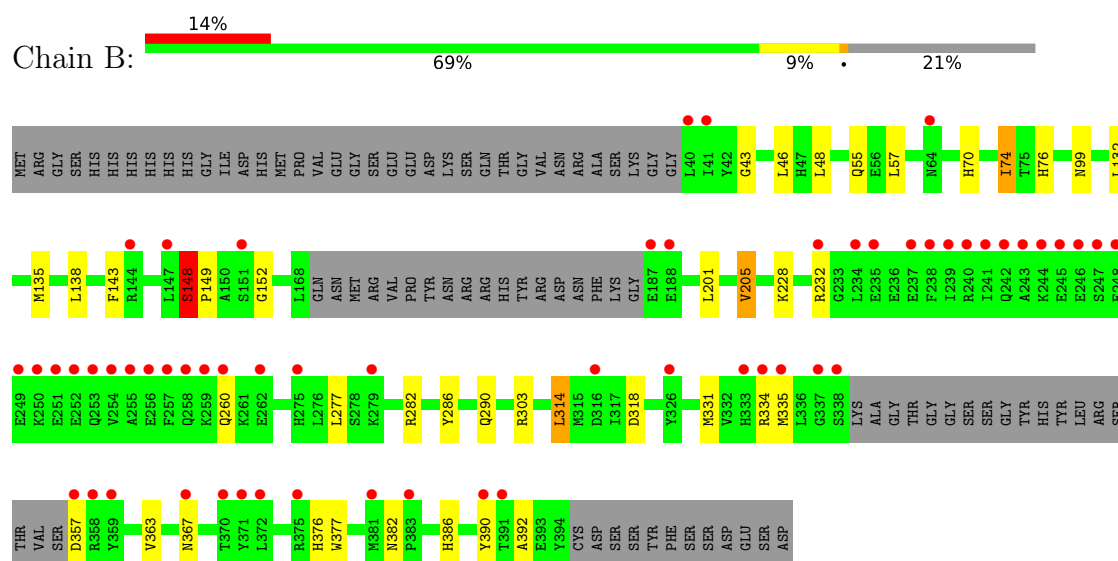
3 Residue-property plots [i](#)

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.

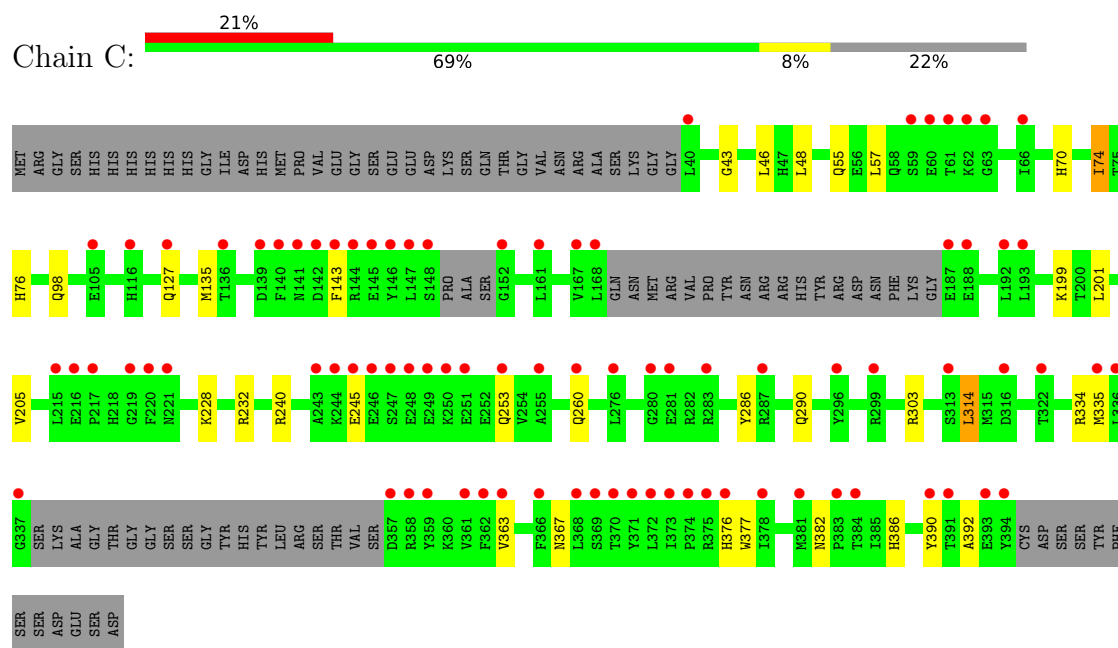
• Molecule 1: Tryptophan 2,3-dioxygenase



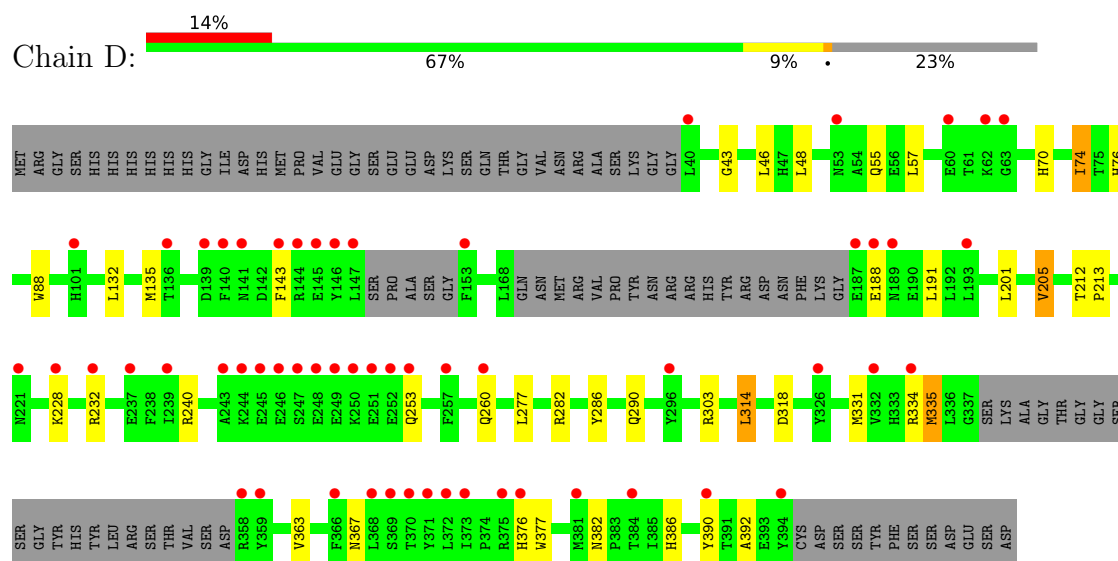
• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.79Å 156.16Å 90.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.33 – 2.61 45.33 – 2.61	Depositor EDS
% Data completeness (in resolution range)	74.7 (45.33-2.61) 74.6 (45.33-2.61)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.298 , 0.330 0.292 , 0.294	Depositor DCC
R_{free} test set	2199 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10283	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6072e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1H8G, ZIQ

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	0.68	0/2581	1.07	3/3494 (0.1%)
1	B	0.68	1/2597 (0.0%)	1.08	2/3518 (0.1%)
1	C	0.67	0/2561	1.07	1/3467 (0.0%)
1	D	0.66	0/2542	1.08	1/3441 (0.0%)
All	All	0.67	1/10281 (0.0%)	1.08	7/13920 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	SER	CA-C	5.11	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	143	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	99	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	143	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	99	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	313	SER	CA-C-N	5.10	127.11	120.28
1	A	313	SER	C-N-CA	5.10	127.11	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2523	0	2393	25	0
1	B	2539	0	2379	21	0
1	C	2506	0	2351	21	0
1	D	2487	0	2345	23	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
3	C	39	0	0	0	0
3	D	39	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	10283	0	9468	80	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 (80) 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:334:ARG:HE	1:A:335[A]:MET:HE3	1.22	1.02
1:B:334:ARG:HE	1:B:335[A]:MET:HE3	1.23	1.01
1:C:334:ARG:HE	1:C:335[A]:MET:HE3	1.25	0.99
1:D:334:ARG:HE	1:D:335:MET:HE3	1.52	0.75
1:C:334:ARG:NE	1:C:335[A]:MET:HE3	2.04	0.70
1:A:334:ARG:NE	1:A:335[A]:MET:HE3	2.03	0.70
1:B:76:HIS:HB3	1:C:46:LEU:HD11	1.75	0.69
1:B:334:ARG:NE	1:B:335[A]:MET:HE3	2.03	0.67
1:A:76:HIS:HB3	1:D:46:LEU:HD11	1.79	0.62
1:A:376:HIS:CD2	1:A:377:TRP:CD1	2.95	0.55
1:A:148:SER:HB2	1:A:149:PRO:CD	2.38	0.53
1:B:376:HIS:CD2	1:B:377:TRP:CD1	2.97	0.53
1:C:70:HIS:CE1	1:C:74:ILE:HD13	2.44	0.53
1:C:376:HIS:CD2	1:C:377:TRP:CD1	2.97	0.53
1:D:376:HIS:CD2	1:D:377:TRP:HD1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:HIS:CD2	1:A:377:TRP:HD1	2.27	0.52
1:D:240:ARG:HH22	1:D:253:GLN:NE2	2.06	0.52
1:C:240:ARG:HH22	1:C:253:GLN:NE2	2.06	0.52
1:C:376:HIS:CD2	1:C:377:TRP:HD1	2.27	0.52
1:A:46:LEU:HD11	1:D:76:HIS:HB3	1.91	0.51
1:B:376:HIS:CD2	1:B:377:TRP:HD1	2.28	0.51
1:B:70:HIS:CE1	1:B:74:ILE:HD13	2.46	0.51
1:D:376:HIS:CD2	1:D:377:TRP:CD1	2.99	0.50
1:C:70:HIS:CE1	1:C:74:ILE:CD1	2.95	0.50
1:A:70:HIS:CE1	1:A:74:ILE:HD13	2.47	0.50
1:A:390:TYR:HB2	1:C:392:ALA:HB3	1.93	0.50
1:B:46:LEU:HD11	1:C:76:HIS:HB3	1.94	0.50
1:B:390:TYR:HB2	1:D:392:ALA:HB3	1.94	0.49
1:D:70:HIS:CE1	1:D:74:ILE:HD13	2.47	0.49
1:D:55:GLN:HG2	1:D:74:ILE:HD11	1.94	0.48
1:C:382:ASN:H	1:C:386:HIS:HD2	1.60	0.48
1:A:228:LYS:NZ	1:A:232:ARG:CG	2.77	0.48
1:B:382:ASN:H	1:B:386:HIS:HD2	1.59	0.47
1:B:55:GLN:HG2	1:B:74:ILE:HD11	1.96	0.47
1:A:67:HIS:CE1	1:D:88:TRP:CD1	3.02	0.47
1:A:382:ASN:H	1:A:386:HIS:HD2	1.62	0.47
1:D:382:ASN:H	1:D:386:HIS:HD2	1.62	0.47
1:A:67:HIS:CE1	1:D:88:TRP:NE1	2.83	0.47
1:A:286:TYR:O	1:A:290:GLN:HG3	2.15	0.47
1:B:286:TYR:O	1:B:290:GLN:HG3	2.15	0.47
1:D:70:HIS:CE1	1:D:74:ILE:CD1	2.98	0.47
1:A:392:ALA:HB3	1:C:390:TYR:HB2	1.96	0.47
1:A:135:MET:O	1:A:334:ARG:NH1	2.49	0.46
1:B:70:HIS:CE1	1:B:74:ILE:CD1	2.99	0.46
1:C:228:LYS:NZ	1:C:232:ARG:CG	2.79	0.46
1:B:135:MET:O	1:B:334:ARG:NH1	2.49	0.45
1:B:228:LYS:NZ	1:B:232:ARG:CG	2.80	0.45
1:D:228:LYS:NZ	1:D:232:ARG:CG	2.80	0.45
1:A:234:LEU:HD13	1:A:261:LYS:HG3	1.97	0.45
1:C:55:GLN:HG2	1:C:74:ILE:HD11	1.97	0.45
1:A:70:HIS:CE1	1:A:74:ILE:CD1	2.98	0.45
1:D:43:GLY:HA2	1:D:48:LEU:HD12	1.98	0.45
1:C:205:VAL:HG21	1:C:314:LEU:HD21	1.99	0.45
1:A:132:LEU:HD13	1:A:331:MET:HE2	1.98	0.45
1:A:205:VAL:HG21	1:A:314:LEU:HD21	1.97	0.45
1:C:43:GLY:HA2	1:C:48:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD13	1:B:331:MET:HE2	2.00	0.44
1:C:286:TYR:O	1:C:290:GLN:HG3	2.17	0.43
1:D:135:MET:O	1:D:334:ARG:NH1	2.51	0.43
1:B:392:ALA:HB3	1:D:390:TYR:HB2	2.01	0.43
1:C:70:HIS:ND1	1:C:74:ILE:HD13	2.34	0.43
1:C:98:GLN:HE21	1:C:199:LYS:HD2	1.83	0.42
1:A:277:LEU:HG	1:A:282:ARG:HB2	2.00	0.42
1:D:286:TYR:O	1:D:290:GLN:HG3	2.19	0.42
1:B:43:GLY:HA2	1:B:48:LEU:HD12	2.02	0.42
1:D:205:VAL:HG21	1:D:314:LEU:HD21	2.01	0.42
1:C:135:MET:O	1:C:334:ARG:NH1	2.53	0.41
1:C:240:ARG:HH22	1:C:253:GLN:HE21	1.69	0.41
1:A:212:THR:HA	1:A:213:PRO:HD3	1.99	0.41
1:B:277:LEU:HG	1:B:282:ARG:HB2	2.03	0.41
1:B:132:LEU:HB3	1:B:331:MET:HE2	2.03	0.41
1:A:43:GLY:HA2	1:A:48:LEU:HD12	2.02	0.41
1:D:277:LEU:HG	1:D:282:ARG:HB2	2.01	0.41
1:A:55:GLN:HG2	1:A:74:ILE:HD11	2.02	0.41
1:D:212:THR:HA	1:D:213:PRO:HD3	1.97	0.41
1:A:148:SER:HB2	1:A:149:PRO:HD2	2.03	0.40
1:B:205:VAL:HG21	1:B:314:LEU:HD21	2.02	0.40
1:B:148:SER:CB	1:B:149:PRO:CD	2.99	0.40
1:D:132:LEU:HB3	1:D:331:MET:HE2	2.03	0.40
1:D:188:GLU:HA	1:D:191:LEU:HD12	2.04	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	307/403 (76%)	298 (97%)	6 (2%)	3 (1%)	12 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	314/403 (78%)	305 (97%)	7 (2%)	2 (1%)	21	39
1	C	308/403 (76%)	301 (98%)	7 (2%)	0	100	100
1	D	304/403 (75%)	296 (97%)	8 (3%)	0	100	100
All	All	1233/1612 (76%)	1200 (97%)	28 (2%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	B	148	SER
1	A	152	GLY
1	B	152	GLY
1	A	337	GLY

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	253/368 (69%)	242 (96%)	11 (4%)	26	49
1	B	250/368 (68%)	238 (95%)	12 (5%)	23	45
1	C	247/368 (67%)	237 (96%)	10 (4%)	28	53
1	D	246/368 (67%)	235 (96%)	11 (4%)	24	48
All	All	996/1472 (68%)	952 (96%)	44 (4%)	25	48

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	74	ILE
1	A	201	LEU
1	A	205	VAL
1	A	228	LYS
1	A	303	ARG

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Mol	Chain	Res	Type
1	A	314	LEU
1	A	318	ASP
1	A	323	LYS
1	A	363	VAL
1	A	367	ASN
1	B	57	LEU
1	B	74	ILE
1	B	138	LEU
1	B	201	LEU
1	B	205	VAL
1	B	260	GLN
1	B	303	ARG
1	B	314	LEU
1	B	318	ASP
1	B	357	ASP
1	B	363	VAL
1	B	367	ASN
1	C	57	LEU
1	C	74	ILE
1	C	127	GLN
1	C	201	LEU
1	C	245	GLU
1	C	260	GLN
1	C	303	ARG
1	C	314	LEU
1	C	363	VAL
1	C	367	ASN
1	D	57	LEU
1	D	74	ILE
1	D	201	LEU
1	D	205	VAL
1	D	260	GLN
1	D	303	ARG
1	D	314	LEU
1	D	318	ASP
1	D	335	MET
1	D	363	VAL
1	D	367	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	128	GLN
1	A	260	GLN
1	A	309	GLN
1	A	386	HIS
1	B	64	ASN
1	B	127	GLN
1	B	128	GLN
1	B	260	GLN
1	B	309	GLN
1	B	386	HIS
1	C	64	ASN
1	C	98	GLN
1	C	128	GLN
1	C	253	GLN
1	C	260	GLN
1	C	309	GLN
1	C	386	HIS
1	D	64	ASN
1	D	128	GLN
1	D	253	GLN
1	D	260	GLN
1	D	309	GLN
1	D	327	ASN
1	D	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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$
3	A1H8G	A	502	-	41,42,42	0.53	1 (2%)	49,59,59	0.47	0
3	A1H8G	B	502	-	41,42,42	0.51	1 (2%)	49,59,59	0.46	0
3	A1H8G	C	502	-	41,42,42	0.48	1 (2%)	49,59,59	0.46	0
2	ZIQ	A	501	-	14,17,17	1.40	1 (7%)	20,25,25	1.50	4 (20%)
2	ZIQ	B	501	-	14,17,17	1.46	1 (7%)	20,25,25	1.46	3 (15%)
3	A1H8G	D	502	-	41,42,42	0.46	1 (2%)	49,59,59	0.45	0
2	ZIQ	C	501	-	14,17,17	1.37	2 (14%)	20,25,25	1.31	4 (20%)
2	ZIQ	D	501	-	14,17,17	1.48	2 (14%)	20,25,25	1.42	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H8G	A	502	-	-	3/30/43/43	0/4/4/4
3	A1H8G	B	502	-	-	3/30/43/43	0/4/4/4
3	A1H8G	C	502	-	-	3/30/43/43	0/4/4/4
2	ZIQ	A	501	-	-	4/11/11/11	0/2/2/2
2	ZIQ	B	501	-	-	4/11/11/11	0/2/2/2
3	A1H8G	D	502	-	-	3/30/43/43	0/4/4/4
2	ZIQ	C	501	-	-	4/11/11/11	0/2/2/2
2	ZIQ	D	501	-	-	4/11/11/11	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ZIQ	CD2-CG	-3.19	1.38	1.44
2	D	501	ZIQ	CD2-CG	-3.18	1.38	1.44
2	A	501	ZIQ	CD2-CG	-3.00	1.39	1.44
2	C	501	ZIQ	CD2-CG	-2.84	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1H8G	C27-N	2.73	1.42	1.38
3	B	502	A1H8G	C27-N	2.66	1.42	1.38
3	D	502	A1H8G	C27-N	2.37	1.41	1.38
2	D	501	ZIQ	CD2-CE2	-2.26	1.38	1.41
3	C	502	A1H8G	C27-N	2.14	1.41	1.38
2	C	501	ZIQ	CD2-CE2	-2.04	1.38	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ZIQ	CZ2-CE2-CD2	-3.74	118.57	122.19
2	B	501	ZIQ	CE3-CD2-CE2	3.28	122.24	118.84
2	B	501	ZIQ	CZ2-CE2-CD2	-3.23	119.06	122.19
2	D	501	ZIQ	CZ2-CE2-CD2	-3.16	119.13	122.19
2	D	501	ZIQ	CE3-CD2-CE2	3.14	122.10	118.84
2	A	501	ZIQ	CE3-CD2-CE2	2.99	121.94	118.84
2	B	501	ZIQ	CE3-CD2-CG	-2.93	129.48	133.85
2	C	501	ZIQ	CZ2-CE2-CD2	-2.84	119.44	122.19
2	A	501	ZIQ	CE3-CD2-CG	-2.76	129.74	133.85
2	D	501	ZIQ	CE3-CD2-CG	-2.72	129.80	133.85
2	C	501	ZIQ	CE3-CD2-CE2	2.67	121.61	118.84
2	C	501	ZIQ	CE3-CD2-CG	-2.63	129.94	133.85
2	D	501	ZIQ	O-C-CA	-2.27	118.70	122.78
2	C	501	ZIQ	O-C-CA	-2.18	118.87	122.78
2	A	501	ZIQ	O-C-CA	-2.04	119.11	122.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ZIQ	OXT-C-CA-C1
2	B	501	ZIQ	OXT-C-CA-C1
2	C	501	ZIQ	OXT-C-CA-C1
2	D	501	ZIQ	OXT-C-CA-C1
2	A	501	ZIQ	O-C-CA-C1
2	B	501	ZIQ	O-C-CA-C1
2	C	501	ZIQ	O-C-CA-C1
2	D	501	ZIQ	O-C-CA-C1
3	B	502	A1H8G	C26-C18-N2-C17
3	A	502	A1H8G	C26-C18-N2-C17
3	C	502	A1H8G	C26-C18-N2-C17
2	A	501	ZIQ	O-C-CA-CB

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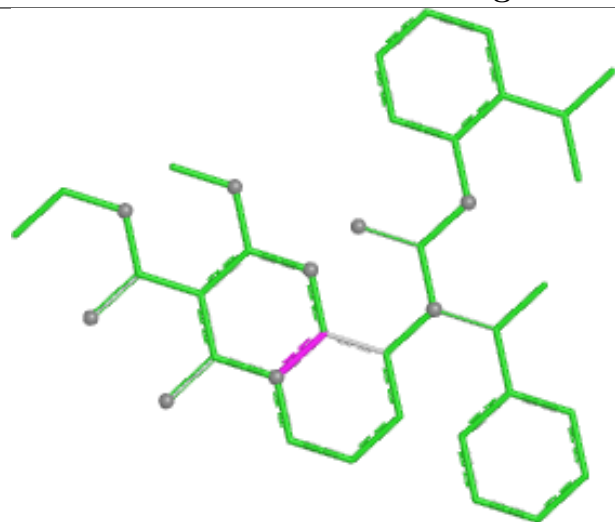
Mol	Chain	Res	Type	Atoms
2	A	501	ZIQ	OXT-C-CA-CB
2	B	501	ZIQ	O-C-CA-CB
2	B	501	ZIQ	OXT-C-CA-CB
2	C	501	ZIQ	O-C-CA-CB
2	C	501	ZIQ	OXT-C-CA-CB
2	D	501	ZIQ	O-C-CA-CB
2	D	501	ZIQ	OXT-C-CA-CB
3	D	502	A1H8G	C26-C18-N2-C17
3	B	502	A1H8G	C19-C18-N2-C17
3	A	502	A1H8G	C-C1-O-C2
3	A	502	A1H8G	C19-C18-N2-C17
3	C	502	A1H8G	C19-C18-N2-C17
3	D	502	A1H8G	C19-C18-N2-C17
3	B	502	A1H8G	C-C1-O-C2
3	C	502	A1H8G	C-C1-O-C2
3	D	502	A1H8G	C-C1-O-C2

There are no ring outliers.

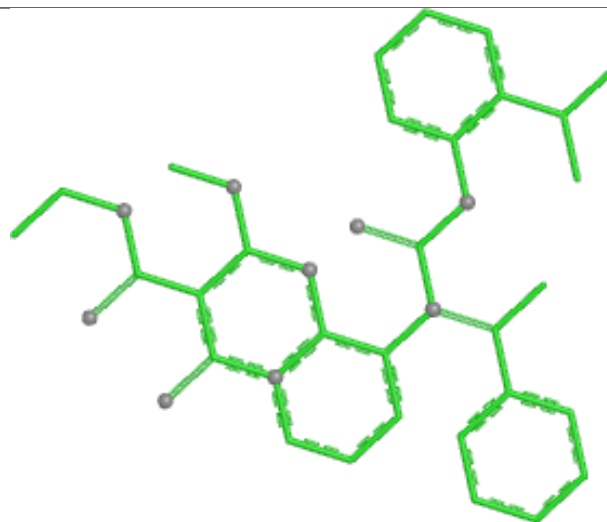
No monomer is involved in short contacts.

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.

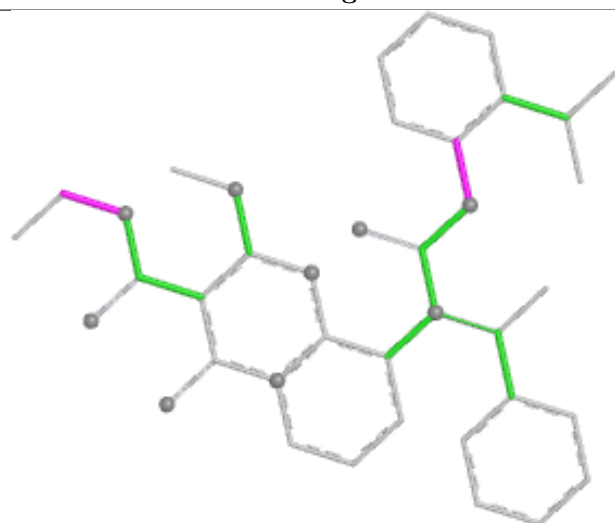
Ligand A1H8G A 502



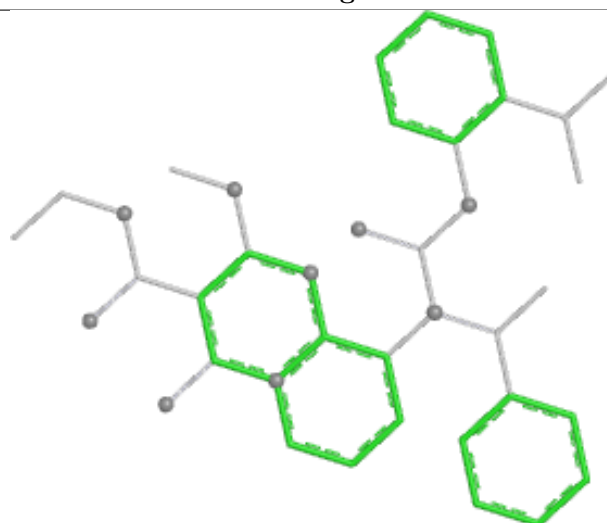
Bond lengths



Bond angles

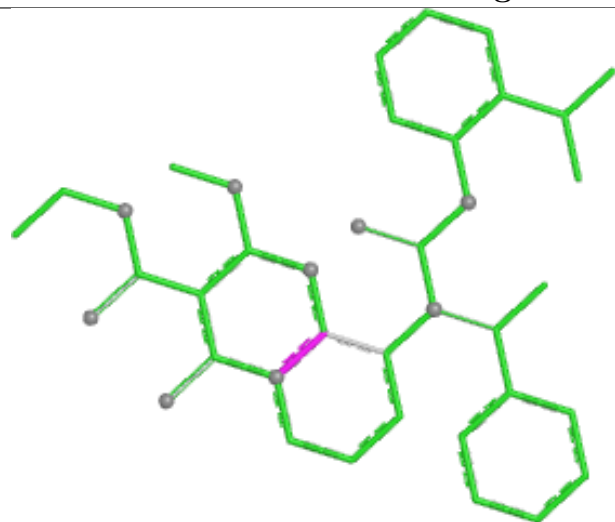


Torsions

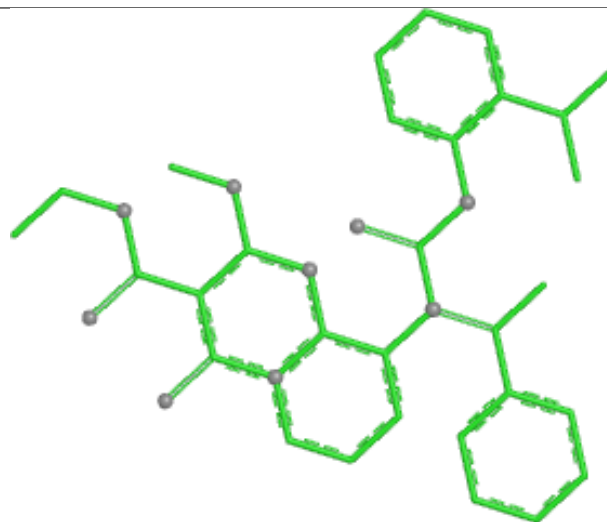


Rings

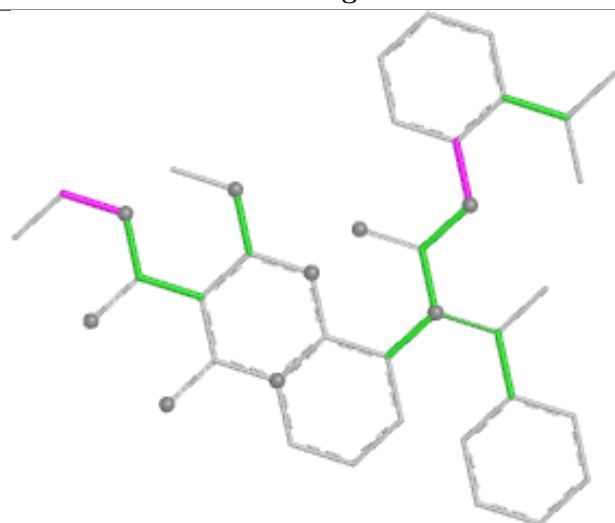
Ligand A1H8G B 502



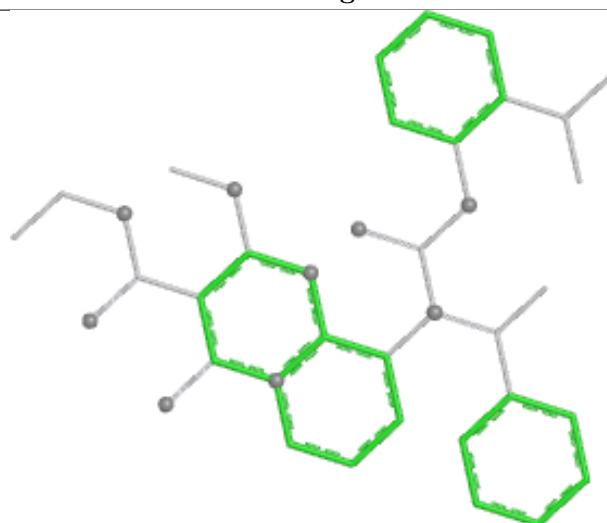
Bond lengths



Bond angles

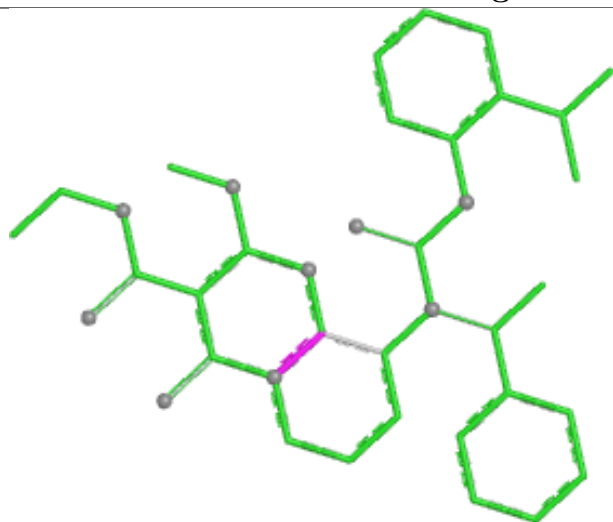


Torsions

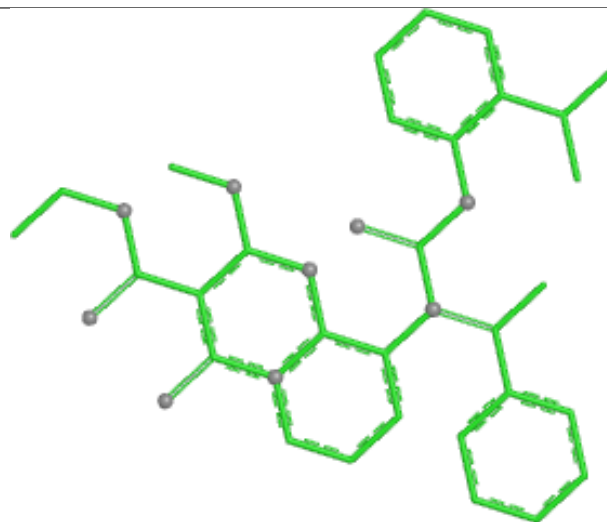


Rings

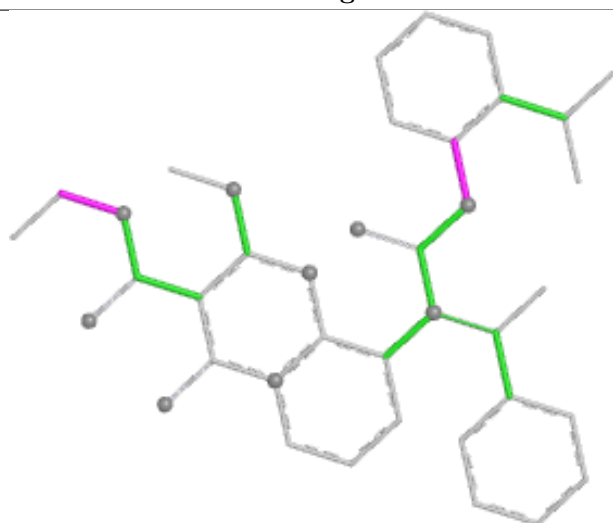
Ligand A1H8G C 502



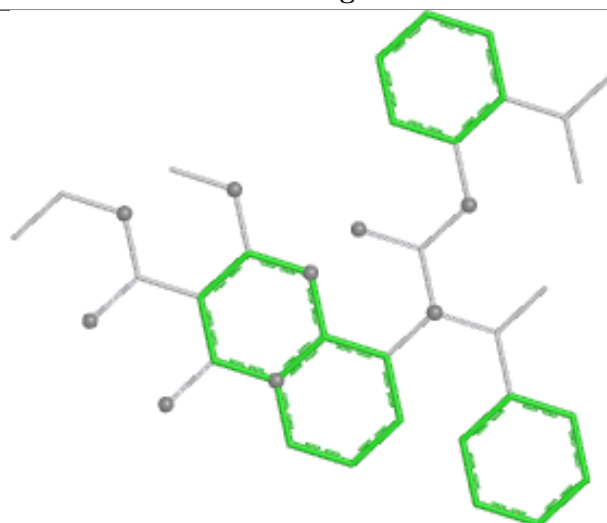
Bond lengths



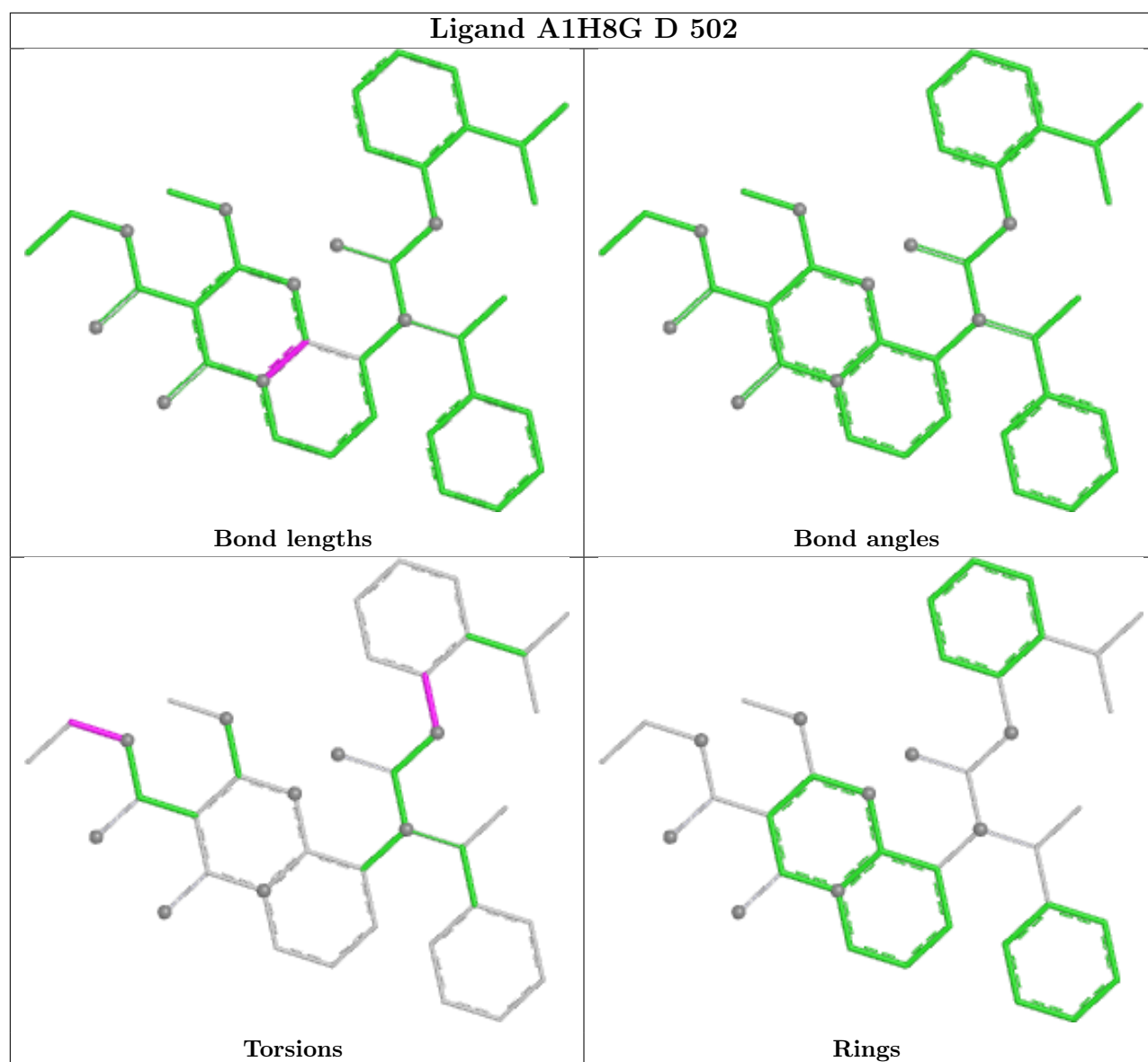
Bond angles



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	314/403 (77%)	1.00	55 (17%) 4 3	18, 33, 70, 88	1 (0%)
1	B	319/403 (79%)	0.91	57 (17%) 3 3	17, 34, 97, 115	1 (0%)
1	C	315/403 (78%)	1.42	84 (26%) 1 1	18, 39, 67, 81	1 (0%)
1	D	312/403 (77%)	1.00	57 (18%) 3 3	16, 38, 62, 77	0
All	All	1260/1612 (78%)	1.08	253 (20%) 3 2	16, 36, 70, 115	3 (0%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	TYR	6.6
1	C	369	SER	5.5
1	B	246	GLU	5.4
1	B	240	ARG	5.4
1	C	357	ASP	5.2
1	C	384	THR	5.2
1	B	241	ILE	4.9
1	B	151	SER	4.8
1	A	187	GLU	4.7
1	C	359	TYR	4.7
1	C	296	TYR	4.6
1	A	41	ILE	4.6
1	C	148	SER	4.6
1	B	245	GLU	4.6
1	C	146	TYR	4.6
1	A	359	TYR	4.5
1	B	359	TYR	4.5
1	D	368	LEU	4.4
1	B	64	ASN	4.3
1	A	390	TYR	4.3
1	C	250	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	147	LEU	4.2
1	B	243	ALA	4.2
1	B	358	ARG	4.1
1	B	244	LYS	4.0
1	A	40	LEU	4.0
1	A	251	GLU	4.0
1	C	247	SER	4.0
1	C	358	ARG	4.0
1	B	239	ILE	3.9
1	C	62	LYS	3.9
1	B	249	GLU	3.9
1	B	333	HIS	3.9
1	C	143	PHE	3.9
1	C	378	ILE	3.8
1	C	361	VAL	3.8
1	D	237	GLU	3.8
1	B	338	SER	3.8
1	B	40	LEU	3.8
1	D	62	LYS	3.8
1	D	369	SER	3.7
1	A	358	ARG	3.7
1	B	247	SER	3.7
1	D	187	GLU	3.7
1	B	391	THR	3.7
1	C	147	LEU	3.7
1	D	144	ARG	3.7
1	D	146	TYR	3.7
1	A	240	ARG	3.6
1	C	188	GLU	3.6
1	C	376	HIS	3.6
1	B	238	PHE	3.6
1	C	145	GLU	3.6
1	C	249	GLU	3.6
1	C	394	TYR	3.5
1	B	251	GLU	3.5
1	A	239	ILE	3.4
1	D	371	TYR	3.4
1	D	145	GLU	3.4
1	C	141	ASN	3.4
1	B	257	PHE	3.4
1	C	362	PHE	3.4
1	B	258	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	376	HIS	3.4
1	B	256	GLU	3.3
1	C	366	PHE	3.3
1	D	139	ASP	3.3
1	D	375	ARG	3.3
1	C	381	MET	3.3
1	D	193	LEU	3.3
1	A	253	GLN	3.3
1	D	141	ASN	3.3
1	D	334	ARG	3.3
1	A	383	PRO	3.3
1	D	358	ARG	3.2
1	A	243	ALA	3.2
1	D	244	LYS	3.2
1	D	245	GLU	3.2
1	C	116	HIS	3.2
1	C	144	ARG	3.2
1	D	188	GLU	3.2
1	C	63	GLY	3.2
1	A	238	PHE	3.2
1	C	66	ILE	3.2
1	A	388	PHE	3.2
1	B	371	TYR	3.2
1	A	151	SER	3.1
1	C	371	TYR	3.1
1	D	248	GLU	3.1
1	D	384	THR	3.1
1	C	220	PHE	3.1
1	A	394	TYR	3.1
1	C	368	LEU	3.1
1	A	278	SER	3.1
1	C	60	GLU	3.0
1	D	153	PHE	3.0
1	A	191	LEU	3.0
1	C	193	LEU	3.0
1	A	281	GLU	3.0
1	D	140	PHE	3.0
1	A	376	HIS	3.0
1	A	384	THR	3.0
1	D	136	THR	3.0
1	C	40	LEU	2.9
1	D	260	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	326	TYR	2.9
1	C	255	ALA	2.9
1	D	143	PHE	2.9
1	C	281	GLU	2.9
1	A	104	ASP	2.9
1	C	372	LEU	2.9
1	A	256	GLU	2.9
1	C	216	GLU	2.9
1	D	60	GLU	2.9
1	C	390	TYR	2.9
1	C	192	LEU	2.9
1	D	228	LYS	2.9
1	D	53	ASN	2.9
1	C	370	THR	2.9
1	C	374	PRO	2.8
1	D	381	MET	2.8
1	C	260	GLN	2.8
1	A	338	SER	2.8
1	C	221	ASN	2.8
1	B	253	GLN	2.8
1	D	40	LEU	2.8
1	D	372	LEU	2.8
1	B	252	GLU	2.8
1	A	371	TYR	2.8
1	A	387	LYS	2.7
1	B	381	MET	2.7
1	C	248	GLU	2.7
1	B	334	ARG	2.7
1	C	59	SER	2.7
1	C	187	GLU	2.7
1	C	316	ASP	2.7
1	B	242	GLN	2.7
1	D	373	ILE	2.7
1	A	366	PHE	2.7
1	C	363	VAL	2.7
1	C	276	LEU	2.7
1	C	251	GLU	2.7
1	D	247	SER	2.7
1	D	251	GLU	2.7
1	A	260	GLN	2.6
1	D	394	TYR	2.6
1	C	140	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	259	LYS	2.6
1	B	260	GLN	2.6
1	C	217	PRO	2.6
1	D	243	ALA	2.6
1	C	335[A]	MET	2.6
1	A	368	LEU	2.6
1	D	250	LYS	2.6
1	B	248	GLU	2.6
1	C	167	VAL	2.6
1	A	64	ASN	2.6
1	D	366	PHE	2.6
1	D	296	TYR	2.5
1	B	262	GLU	2.5
1	A	316	ASP	2.5
1	B	390	TYR	2.5
1	B	254	VAL	2.5
1	A	250	LYS	2.5
1	D	326	TYR	2.5
1	A	370	THR	2.5
1	D	189	ASN	2.5
1	C	161	LEU	2.5
1	B	316	ASP	2.5
1	C	245	GLU	2.5
1	C	244	LYS	2.4
1	A	367	ASN	2.4
1	C	283	ARG	2.4
1	D	232	ARG	2.4
1	C	373	ILE	2.4
1	A	148	SER	2.4
1	C	219	GLY	2.4
1	C	375	ARG	2.4
1	C	393	GLU	2.4
1	D	249	GLU	2.4
1	C	322	THR	2.4
1	A	275	HIS	2.4
1	A	249	GLU	2.4
1	B	279	LYS	2.4
1	A	254	VAL	2.4
1	B	237	GLU	2.4
1	C	280	GLY	2.4
1	B	255	ALA	2.4
1	C	215	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	GLU	2.3
1	A	369	SER	2.3
1	B	357	ASP	2.3
1	A	100	GLY	2.3
1	D	253	GLN	2.3
1	B	275	HIS	2.3
1	B	235	GLU	2.3
1	D	252	GLU	2.3
1	C	127	GLN	2.3
1	A	372	LEU	2.3
1	C	243	ALA	2.3
1	B	335[A]	MET	2.3
1	C	136	THR	2.3
1	B	370	THR	2.2
1	C	246	GLU	2.2
1	A	149	PRO	2.2
1	B	383	PRO	2.2
1	C	383	PRO	2.2
1	B	337	GLY	2.2
1	D	63	GLY	2.2
1	A	241	ILE	2.2
1	B	375	ARG	2.2
1	B	234	LEU	2.2
1	D	370	THR	2.2
1	C	168	LEU	2.2
1	C	336	LEU	2.2
1	A	188	GLU	2.2
1	B	367	ASN	2.2
1	D	390	TYR	2.2
1	B	250	LYS	2.2
1	B	147	LEU	2.2
1	A	92	SER	2.2
1	A	237	GLU	2.1
1	A	232	ARG	2.1
1	A	282	ARG	2.1
1	C	287	ARG	2.1
1	C	391	THR	2.1
1	A	381	MET	2.1
1	B	41	ILE	2.1
1	C	142	ASP	2.1
1	C	313	SER	2.1
1	B	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	246	GLU	2.1
1	D	101	HIS	2.1
1	D	239	ILE	2.1
1	C	139	ASP	2.1
1	A	306	VAL	2.1
1	D	257	PHE	2.1
1	A	145	GLU	2.0
1	B	144	ARG	2.0
1	C	61	THR	2.0
1	B	372	LEU	2.0
1	C	253	GLN	2.0
1	A	152	GLY	2.0
1	C	152	GLY	2.0
1	A	95	GLU	2.0
1	A	257	PHE	2.0
1	C	299	ARG	2.0
1	C	105	GLU	2.0
1	A	382	ASN	2.0
1	C	337	GLY	2.0
1	D	221	ASN	2.0
1	B	232	ARG	2.0
1	D	332	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZIQ	A	501	16/16	0.86	0.13	30,31,34,34	0

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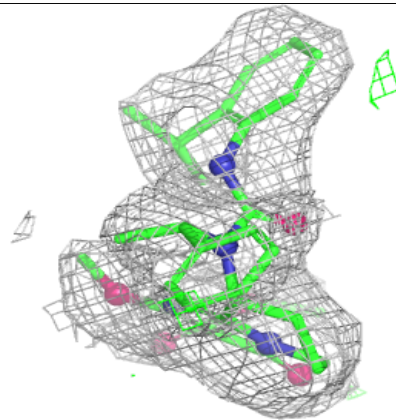
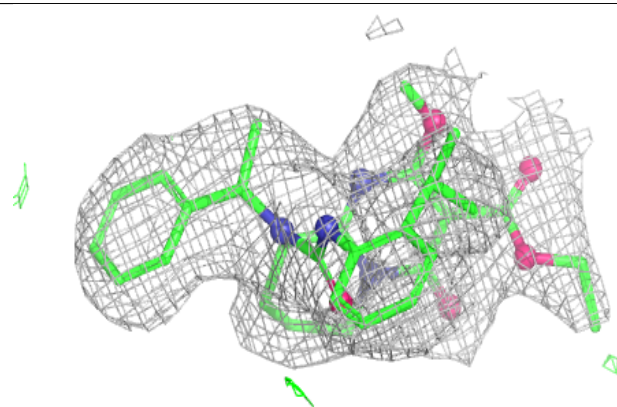
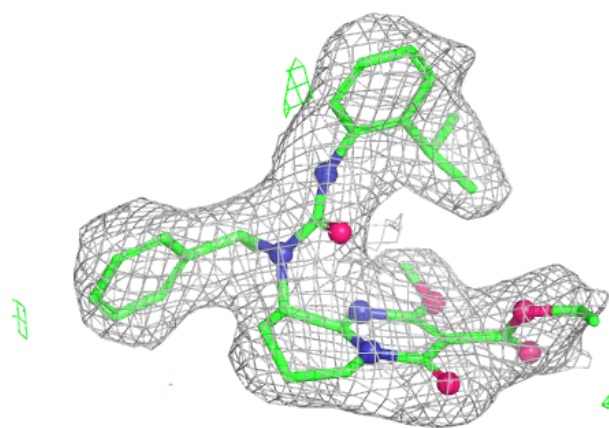
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1H8G	C	502	39/39	0.89	0.13	36,38,41,42	0
3	A1H8G	B	502	39/39	0.90	0.12	33,34,37,37	0
3	A1H8G	D	502	39/39	0.90	0.12	34,36,40,41	0
2	ZIQ	C	501	16/16	0.91	0.11	30,31,32,32	0
2	ZIQ	D	501	16/16	0.92	0.09	27,27,29,29	0
3	A1H8G	A	502	39/39	0.93	0.10	27,27,29,30	0
2	ZIQ	B	501	16/16	0.95	0.07	26,27,29,29	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.

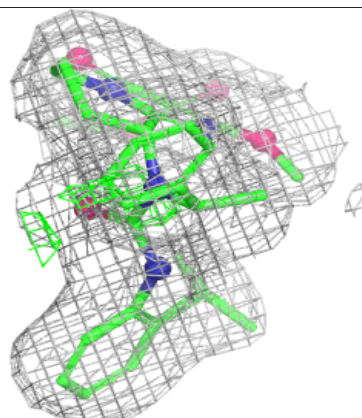
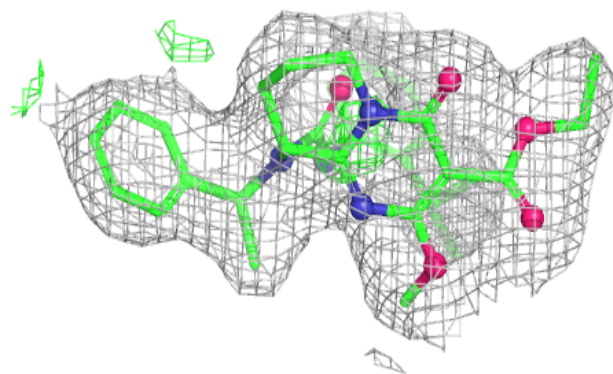
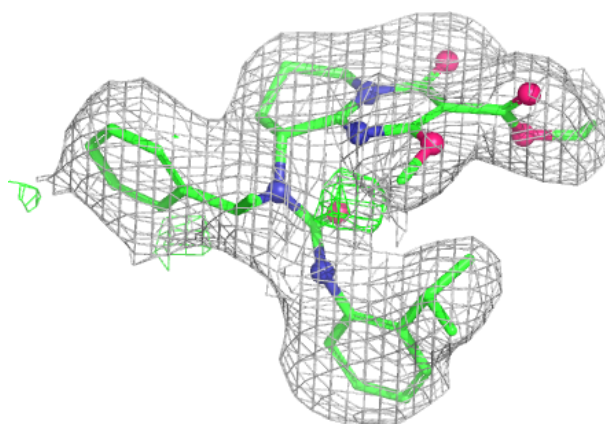
Electron density around A1H8G C 502:

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



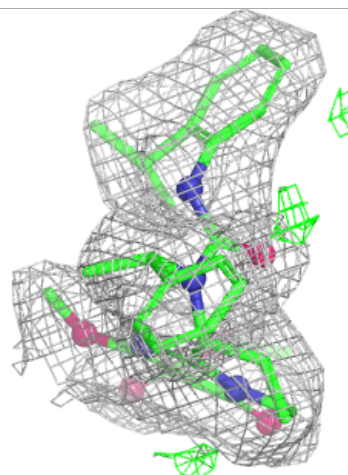
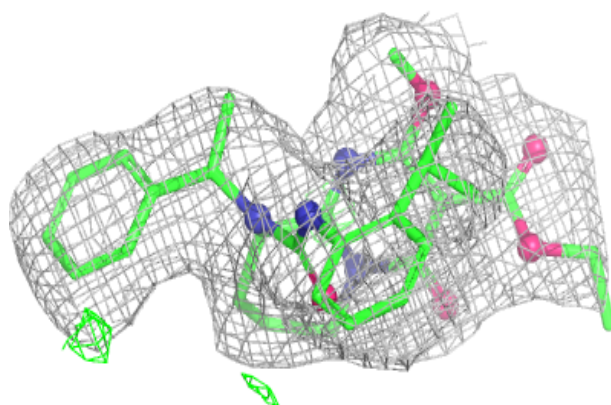
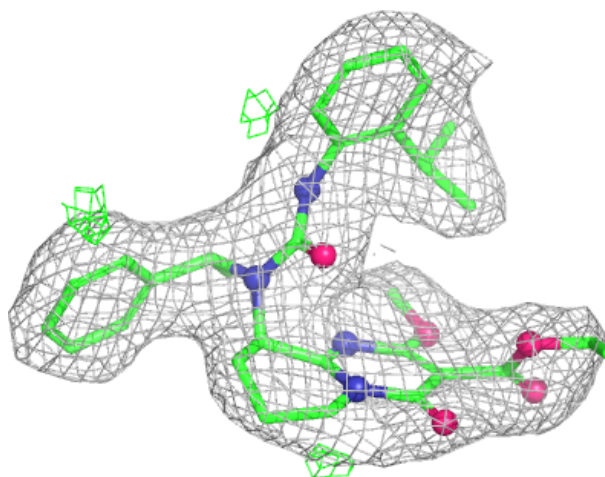
Electron density around A1H8G B 502:

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



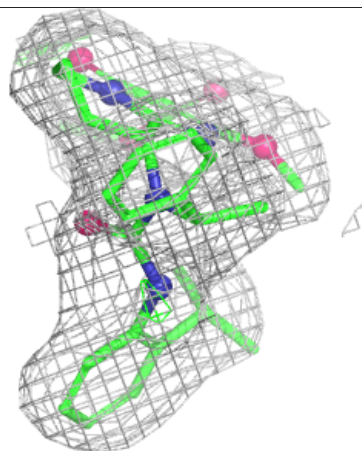
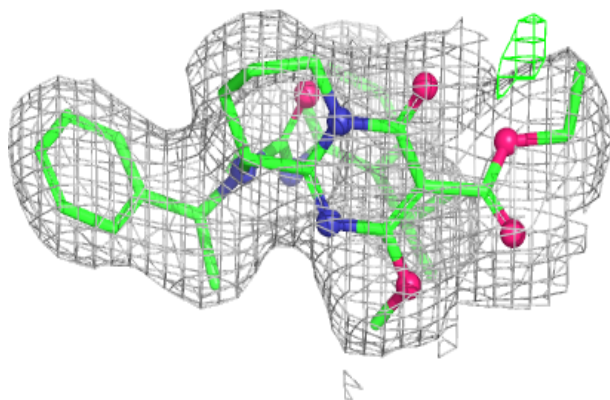
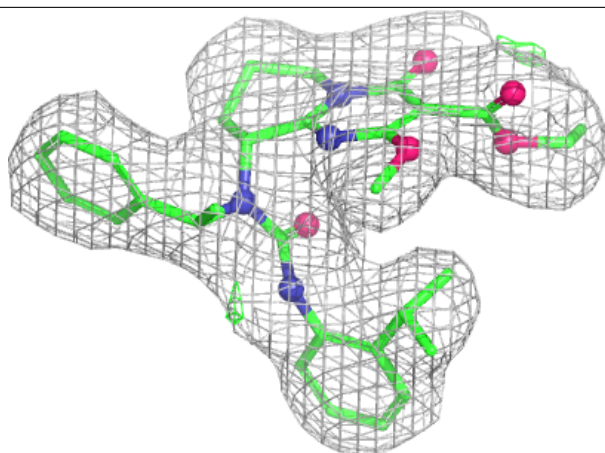
Electron density around A1H8G D 502:

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



Electron density around A1H8G A 502:

$2mF_o-DF_c$ (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.