



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:46 PM EDT

PDB ID : 6EOR
Title : DPP9 - 1G244
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

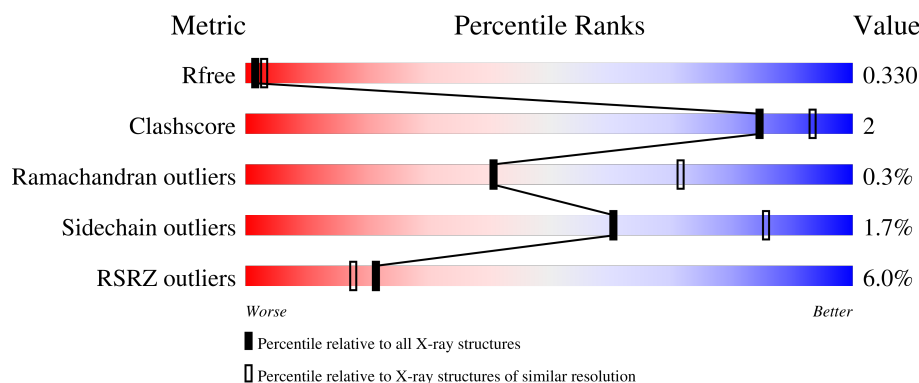
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	869	<div> <div>6%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	B	869	<div> <div>6%</div> <div>85%</div> <div>7%</div> <div>7%</div> </div>
1	C	869	<div> <div>5%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	D	869	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>

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	9XH	D	901	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26627 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 Dipeptidyl peptidase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6563	4226	1123	1186	28			
1	B	805	Total	C	N	O	S	0	0	0
			6540	4213	1115	1184	28			
1	C	808	Total	C	N	O	S	0	0	0
			6560	4222	1118	1192	28			
1	D	812	Total	C	N	O	S	0	0	0
			6585	4236	1122	1199	28			

There are 24 discrepancies between the modelled and reference sequences:

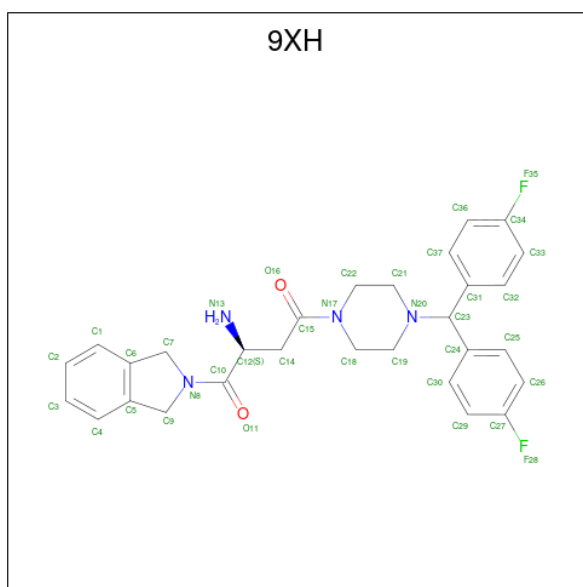
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is (2 {S})-2-azanyl-4-[4-[bis(4-fluorophenyl)methyl]piperazin-1-yl]-1-(1,3-dihydroisoindol-2-yl)butane-1,4-dione (three-letter code: 9XH) (formula: C₂₉H₃₀F₂N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	29	2	4	2		
2	B	1	Total	C	F	N	O	0	0
			37	29	2	4	2		
2	C	1	Total	C	F	N	O	0	0
			37	29	2	4	2		
2	D	1	Total	C	F	N	O	0	0
			37	29	2	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	58	Total	O	0	0
			58	58		
3	C	53	Total	O	0	0
			53	53		

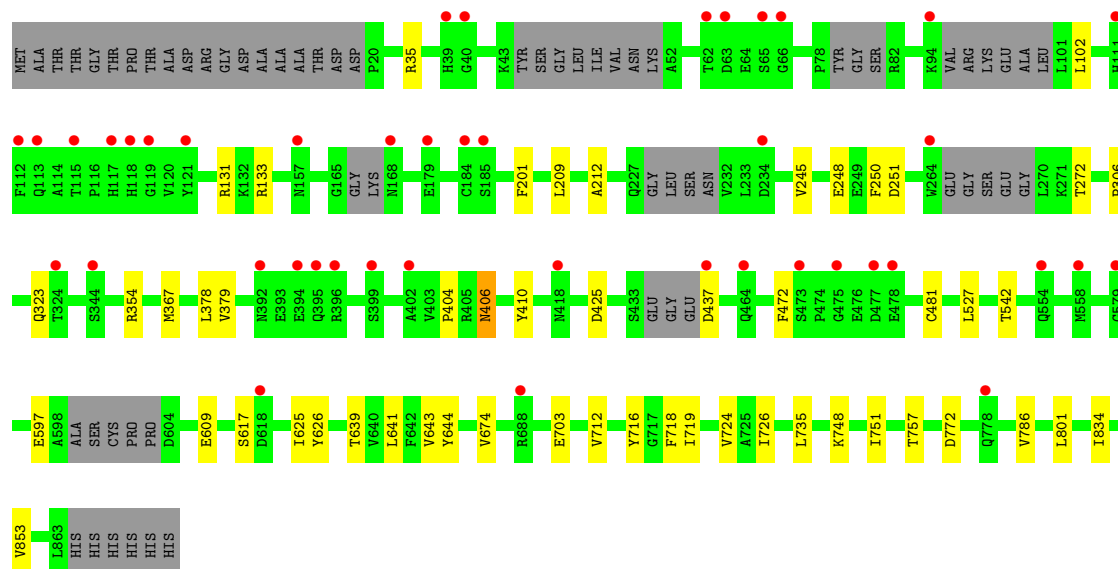
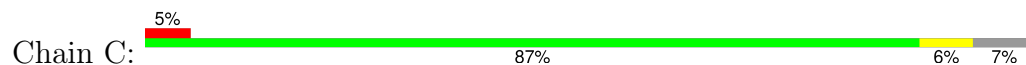
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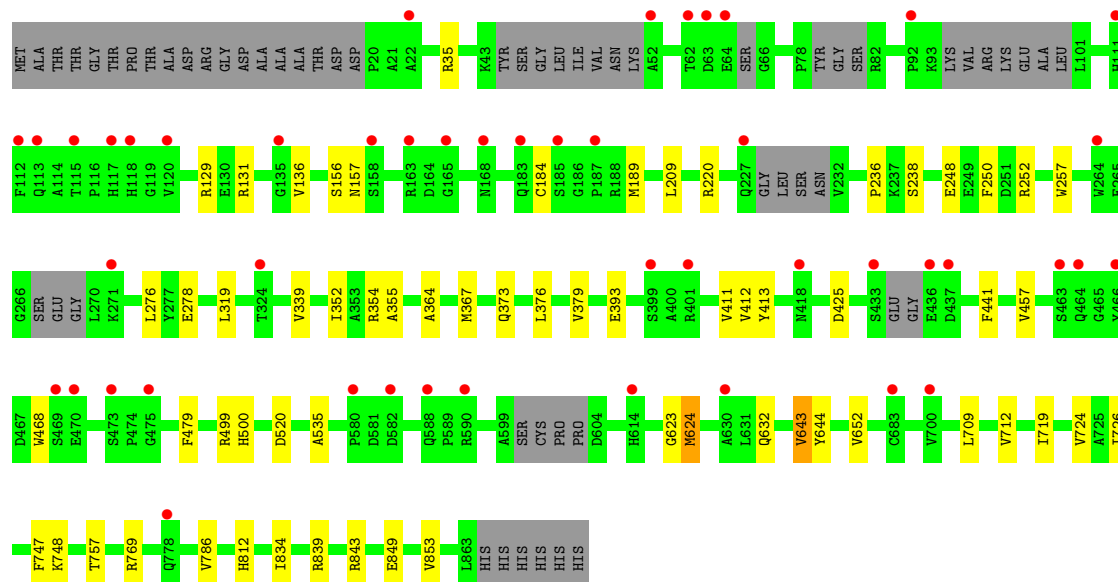
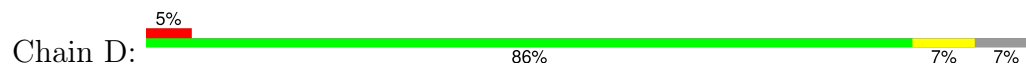
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	59	Total	O	0	0
			59	59		



• Molecule 1: Dipeptidyl peptidase 9



• Molecule 1: Dipeptidyl peptidase 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.36Å 117.21Å 163.40Å 90.00° 105.57° 90.00°	Depositor
Resolution (Å)	43.52 – 2.90 43.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.52-2.90) 99.0 (43.52-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.265 , 0.332 0.268 , 0.330	Depositor DCC
R_{free} test set	4755 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26627	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 58.33 % 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 2.0761e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9XH

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	0.44	0/6759	0.64	0/9165
1	B	0.44	0/6733	0.65	0/9128
1	C	0.45	0/6754	0.66	0/9159
1	D	0.45	0/6779	0.66	0/9192
All	All	0.45	0/27025	0.65	0/36644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6563	0	6348	35	0
1	B	6540	0	6340	27	0
1	C	6560	0	6347	27	0
1	D	6585	0	6365	29	0
2	A	37	0	0	4	0
2	B	37	0	0	1	0
2	C	37	0	0	4	0
2	D	37	0	0	0	0
3	A	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	58	0	0	0	0
3	C	53	0	0	0	0
3	D	59	0	0	1	0
All	All	26627	0	25400	117	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 2.

All (117) 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)
2:C:901:9XH:C37	2:C:901:9XH:C25	2.50	0.86
1:D:252:ARG:NH1	1:D:352:ILE:O	2.22	0.73
1:C:644:TYR:O	1:C:735:LEU:HD12	1.90	0.72
1:D:712:VAL:HG12	1:D:719:ILE:HG13	1.71	0.70
1:D:354:ARG:NH2	1:D:425:ASP:OD1	2.27	0.68
1:B:249:GLU:OE1	2:B:901:9XH:N13	2.29	0.65
1:A:379:VAL:HG12	1:A:411:VAL:HG22	1.79	0.64
1:A:834:ILE:HD11	1:B:834:ILE:HD11	1.80	0.63
1:A:248:GLU:OE2	2:A:901:9XH:N13	2.32	0.63
1:A:200:PHE:CZ	1:A:324:THR:HG21	2.36	0.60
1:C:643:VAL:HG12	1:C:644:TYR:N	2.17	0.59
1:C:625:ILE:HD12	1:C:712:VAL:HG13	1.84	0.58
1:A:252:ARG:NH1	1:A:352:ILE:O	2.37	0.57
1:D:339:VAL:HG11	1:D:468:TRP:HB3	1.87	0.57
1:C:712:VAL:HG12	1:C:719:ILE:HG13	1.86	0.57
1:B:641:LEU:HD23	1:B:726:ILE:HG13	1.87	0.56
1:A:860:GLN:O	1:A:864:HIS:NE2	2.39	0.56
1:A:626:TYR:HB2	1:A:674:VAL:HB	1.87	0.55
1:C:626:TYR:HB2	1:C:674:VAL:HB	1.89	0.55
1:B:232:VAL:O	1:B:234:ASP:N	2.35	0.55
1:C:834:ILE:HD11	1:D:834:ILE:HD11	1.89	0.54
1:C:133:ARG:HG2	2:C:901:9XH:C30	2.38	0.54
1:C:272:THR:HG22	1:C:323:GLN:HG2	1.89	0.53
1:B:200:PHE:CZ	1:B:324:THR:HG21	2.43	0.53
1:D:413:TYR:CE1	1:D:457:VAL:HG21	2.43	0.53
1:A:257:TRP:CZ2	1:A:355:ALA:HB3	2.44	0.53
2:C:901:9XH:C30	2:C:901:9XH:C19	2.87	0.53
1:B:712:VAL:HG12	1:B:719:ILE:HG13	1.90	0.52
1:C:133:ARG:HG2	2:C:901:9XH:C29	2.39	0.52
1:C:131:ARG:NE	1:C:248:GLU:HG2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:VAL:HG12	1:D:644:TYR:N	2.25	0.52
1:D:624:MET:HE2	1:D:652:VAL:HG22	1.92	0.52
1:A:615:THR:HG21	1:A:680:ARG:NH1	2.26	0.51
1:D:252:ARG:NH2	1:D:278:GLU:OE2	2.44	0.51
1:D:367:MET:HE3	1:D:376:LEU:HD11	1.92	0.51
1:D:757:THR:HA	1:D:786:VAL:HG22	1.93	0.50
1:A:243:THR:CG2	1:A:280:VAL:HG11	2.41	0.50
1:A:134:LEU:O	1:A:843:ARG:NH2	2.44	0.50
1:C:35:ARG:HG2	1:C:853:VAL:HG21	1.93	0.50
1:A:790:VAL:HG11	1:A:823:LEU:HA	1.94	0.49
1:A:712:VAL:HG12	1:A:719:ILE:HG13	1.95	0.49
1:B:426:ILE:HD12	1:B:498:ALA:HB2	1.95	0.49
1:A:395:GLN:HE22	1:C:404:PRO:CD	2.27	0.48
1:B:645:GLY:HA3	1:B:735:LEU:CD1	2.44	0.48
1:B:35:ARG:HG2	1:B:853:VAL:HG21	1.96	0.48
1:D:35:ARG:HG2	1:D:853:VAL:HG21	1.95	0.48
1:A:756:VAL:HG23	2:A:901:9XH:C3	2.44	0.48
1:C:367:MET:HG3	1:C:378:LEU:HD23	1.95	0.47
1:B:716:TYR:HB3	1:B:718:PHE:CE2	2.49	0.47
1:C:354:ARG:NH2	1:C:425:ASP:OD1	2.41	0.47
1:D:129:ARG:NH1	1:D:136:VAL:O	2.47	0.47
1:D:709:LEU:HD21	1:D:724:VAL:HG11	1.95	0.47
1:A:642:PHE:HB3	1:A:676:VAL:HG22	1.97	0.47
1:B:285:VAL:O	1:B:304:ARG:NH1	2.41	0.47
1:A:354:ARG:NH2	1:A:425:ASP:OD1	2.48	0.46
1:A:670:LEU:HD12	1:A:856:LEU:HD22	1.96	0.46
1:B:201:PHE:CZ	1:B:212:ALA:HB3	2.50	0.46
1:C:245:VAL:HG21	1:C:306:PRO:HG2	1.97	0.46
1:D:726:ILE:HB	1:D:747:PHE:CD1	2.50	0.46
1:C:639:THR:O	1:C:724:VAL:HA	2.15	0.46
1:C:410:TYR:HB3	1:C:481:CYS:SG	2.55	0.46
1:D:131:ARG:NE	1:D:248:GLU:HG2	2.30	0.46
1:A:291:PRO:HA	1:A:300:THR:HG22	1.98	0.45
1:B:645:GLY:HA3	1:B:735:LEU:HD12	1.99	0.45
1:B:209:LEU:HD11	1:B:275:ILE:HG21	1.99	0.45
1:C:625:ILE:HD12	1:C:712:VAL:CG1	2.46	0.45
1:A:380:LEU:HD11	1:A:439:LEU:HD22	1.99	0.45
1:A:133:ARG:HG2	2:A:901:9XH:C25	2.46	0.45
1:C:751:ILE:HG23	1:C:801:LEU:HD23	1.98	0.45
1:C:250:PHE:O	1:C:354:ARG:NH1	2.45	0.45
1:D:412:VAL:CG1	1:D:441:PHE:CE1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:GLN:OE1	1:D:769:ARG:HD3	2.17	0.44
1:C:527:LEU:HB3	1:C:542:THR:HG23	1.99	0.44
1:A:133:ARG:HG2	2:A:901:9XH:C26	2.48	0.44
1:C:716:TYR:HB3	1:C:718:PHE:CE2	2.52	0.44
1:A:205:ASN:HB3	1:A:210:TRP:CD1	2.52	0.43
1:B:751:ILE:HG23	1:B:801:LEU:HD23	1.99	0.43
1:C:641:LEU:HD23	1:C:726:ILE:HG13	2.00	0.43
1:A:457:VAL:HG22	1:A:486:GLU:HG3	2.00	0.43
1:A:426:ILE:HD12	1:A:498:ALA:HB2	2.01	0.43
1:C:406:ASN:HD22	1:C:406:ASN:N	2.15	0.43
1:D:643:VAL:HG12	1:D:644:TYR:H	1.81	0.43
1:B:643:VAL:HG12	1:B:644:TYR:N	2.34	0.43
1:A:757:THR:HA	1:A:786:VAL:HG22	2.00	0.43
1:A:232:VAL:HG13	1:A:233:LEU:H	1.83	0.43
1:B:243:THR:CG2	1:B:280:VAL:HG11	2.49	0.43
1:A:644:TYR:CE2	1:A:649:VAL:HG21	2.54	0.43
1:D:250:PHE:O	1:D:354:ARG:NH1	2.47	0.43
1:A:225:CYS:O	1:A:237:LYS:HB2	2.19	0.42
1:A:754:ALA:HA	1:A:804:HIS:CD2	2.55	0.42
1:B:849:GLU:O	1:B:853:VAL:HG23	2.19	0.42
1:D:156:SER:OG	1:D:157:ASN:N	2.52	0.42
1:D:379:VAL:HG12	1:D:411:VAL:HG22	2.01	0.42
1:D:623:GLY:HA2	1:D:652:VAL:HG21	2.01	0.42
1:B:71:ARG:NH1	1:B:164:ASP:OD2	2.52	0.42
1:A:201:PHE:CZ	1:A:212:ALA:HB3	2.55	0.42
1:B:412:VAL:CG1	1:B:441:PHE:CE1	3.03	0.41
1:A:758:VAL:HG12	1:A:760:MET:HB2	2.02	0.41
1:A:412:VAL:CG1	1:A:441:PHE:CE1	3.03	0.41
1:B:754:ALA:HA	1:B:804:HIS:CD2	2.56	0.41
1:D:499:ARG:O	1:D:500:HIS:HB2	2.20	0.41
1:B:626:TYR:HB2	1:B:674:VAL:HB	2.02	0.41
1:A:708:GLY:O	1:A:712:VAL:HG23	2.20	0.41
1:B:245:VAL:HG21	1:B:306:PRO:HG2	2.02	0.41
1:C:643:VAL:CG1	1:C:644:TYR:N	2.82	0.41
1:D:276:LEU:HD22	1:D:364:ALA:HB1	2.03	0.41
1:C:201:PHE:CZ	1:C:212:ALA:HB3	2.56	0.41
1:D:812:HIS:HB3	3:D:1036:HOH:O	2.20	0.41
1:B:154:GLN:HE22	1:B:189:MET:CE	2.34	0.41
1:D:411:VAL:HG23	1:D:479:PHE:HB2	2.02	0.41
1:B:497:LEU:HD12	1:B:516:GLN:CG	2.51	0.40
1:B:804:HIS:CD2	1:B:816:THR:OG1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:THR:HA	1:C:786:VAL:HG22	2.03	0.40
1:D:849:GLU:O	1:D:853:VAL:HG23	2.21	0.40
1:B:738:MET:SD	1:B:786:VAL:HG12	2.61	0.40
1:D:257:TRP:CE2	1:D:355:ALA:HB3	2.57	0.40
1:A:814:PHE:O	1:A:818:PHE:N	2.48	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	790/869 (91%)	744 (94%)	44 (6%)	2 (0%)	41	71
1	B	785/869 (90%)	739 (94%)	43 (6%)	3 (0%)	34	66
1	C	790/869 (91%)	737 (93%)	53 (7%)	0	100	100
1	D	794/869 (91%)	746 (94%)	45 (6%)	3 (0%)	34	66
All	All	3159/3476 (91%)	2966 (94%)	185 (6%)	8 (0%)	41	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	HIS
1	A	118	HIS
1	B	233	LEU
1	D	236	PRO
1	D	535	ALA
1	D	839	ARG
1	B	112	PHE
1	A	232	VAL

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	712/759 (94%)	703 (99%)	9 (1%)	69	90
1	B	712/759 (94%)	699 (98%)	13 (2%)	59	85
1	C	714/759 (94%)	701 (98%)	13 (2%)	59	85
1	D	715/759 (94%)	702 (98%)	13 (2%)	59	85
All	All	2853/3036 (94%)	2805 (98%)	48 (2%)	60	86

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	150	LEU
1	A	172	VAL
1	A	209	LEU
1	A	226	HIS
1	A	248	GLU
1	A	343	SER
1	A	581	ASP
1	A	738	MET
1	B	42	ARG
1	B	150	LEU
1	B	156	SER
1	B	209	LEU
1	B	254	THR
1	B	298	ARG
1	B	433	SER
1	B	502	SER
1	B	581	ASP
1	B	662	LEU
1	B	714	GLU
1	B	809	GLU
1	B	847	SER
1	C	102	LEU
1	C	209	LEU

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Mol	Chain	Res	Type
1	C	251	ASP
1	C	379	VAL
1	C	406	ASN
1	C	437	ASP
1	C	472	PHE
1	C	597	GLU
1	C	609	GLU
1	C	617	SER
1	C	703	GLU
1	C	748	LYS
1	C	772	ASP
1	D	184	CYS
1	D	189	MET
1	D	209	LEU
1	D	220	ARG
1	D	238	SER
1	D	319	LEU
1	D	393	GLU
1	D	520	ASP
1	D	624	MET
1	D	632	GLN
1	D	643	VAL
1	D	748	LYS
1	D	843	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	247	GLN
1	A	392	ASN
1	A	395	GLN
1	A	507	ASN
1	A	548	HIS
1	A	555	ASN
1	A	705	GLN
1	A	778	GLN
1	A	798	ASN
1	A	804	HIS
1	A	833	GLN
1	A	860	GLN
1	B	154	GLN

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Mol	Chain	Res	Type
1	B	507	ASN
1	B	548	HIS
1	B	562	HIS
1	B	705	GLN
1	B	798	ASN
1	B	804	HIS
1	B	833	GLN
1	B	860	GLN
1	C	70	HIS
1	C	247	GLN
1	C	406	ASN
1	C	507	ASN
1	C	548	HIS
1	C	650	GLN
1	C	684	GLN
1	C	705	GLN
1	C	798	ASN
1	C	804	HIS
1	C	831	GLN
1	C	833	GLN
1	C	860	GLN
1	D	154	GLN
1	D	161	HIS
1	D	247	GLN
1	D	334	GLN
1	D	340	GLN
1	D	548	HIS
1	D	650	GLN
1	D	684	GLN
1	D	705	GLN
1	D	798	ASN
1	D	804	HIS
1	D	833	GLN
1	D	860	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	9XH	B	901	-	41,41,41	1.04	2 (4%)	55,58,58	1.53	10 (18%)
2	9XH	A	901	-	41,41,41	0.94	3 (7%)	55,58,58	1.35	6 (10%)
2	9XH	D	901	-	41,41,41	1.12	2 (4%)	55,58,58	1.81	12 (21%)
2	9XH	C	901	-	41,41,41	0.91	1 (2%)	55,58,58	1.45	11 (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
2	9XH	B	901	-	-	5/28/46/46	0/5/5/5
2	9XH	A	901	-	-	5/28/46/46	0/5/5/5
2	9XH	D	901	-	-	10/28/46/46	0/5/5/5
2	9XH	C	901	-	-	13/28/46/46	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9XH	C6-C5	3.26	1.45	1.39
2	D	901	9XH	C6-C5	3.13	1.45	1.39
2	A	901	9XH	C31-C23	-2.75	1.48	1.52
2	A	901	9XH	C6-C5	2.65	1.44	1.39
2	C	901	9XH	C6-C5	2.63	1.44	1.39
2	A	901	9XH	C24-C23	-2.33	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	9XH	C23-N20	2.21	1.52	1.48
2	B	901	9XH	C24-C23	-2.03	1.49	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9XH	C31-C23-C24	-5.07	99.34	112.54
2	D	901	9XH	C24-C23-N20	4.98	118.77	111.50
2	D	901	9XH	C5-C9-N8	4.90	104.72	102.42
2	D	901	9XH	C31-C23-N20	-3.95	105.75	111.50
2	B	901	9XH	C21-N20-C23	3.71	119.06	111.64
2	D	901	9XH	C6-C7-N8	3.61	104.12	102.42
2	A	901	9XH	C29-C27-C26	-3.60	118.08	122.80
2	B	901	9XH	C24-C23-N20	3.47	116.57	111.50
2	C	901	9XH	C36-C37-C31	3.44	124.62	121.18
2	C	901	9XH	C19-C18-N17	-3.42	103.61	110.42
2	D	901	9XH	C19-N20-C23	3.42	118.48	111.64
2	B	901	9XH	C31-C23-C24	-3.16	104.33	112.54
2	C	901	9XH	C32-C33-C34	3.04	121.50	118.38
2	B	901	9XH	C6-C7-N8	2.94	103.80	102.42
2	B	901	9XH	C36-C34-C33	-2.93	118.96	122.80
2	C	901	9XH	C36-C34-C33	-2.91	118.99	122.80
2	D	901	9XH	C29-C27-C26	-2.87	119.03	122.80
2	A	901	9XH	C30-C29-C27	2.87	121.32	118.38
2	D	901	9XH	C36-C34-C33	-2.83	119.09	122.80
2	D	901	9XH	C30-C24-C23	2.78	126.47	120.67
2	D	901	9XH	C30-C29-C27	2.77	121.23	118.38
2	B	901	9XH	C5-C9-N8	2.77	103.72	102.42
2	C	901	9XH	F35-C34-C33	2.74	122.94	118.55
2	B	901	9XH	C22-N17-C18	2.64	118.06	112.68
2	C	901	9XH	O16-C15-C14	-2.45	117.49	122.07
2	C	901	9XH	C19-N20-C23	2.44	116.54	111.64
2	C	901	9XH	C25-C24-C23	2.37	125.61	120.67
2	A	901	9XH	C36-C34-C33	-2.30	119.79	122.80
2	C	901	9XH	C29-C27-C26	-2.28	119.82	122.80
2	D	901	9XH	C31-C23-C24	2.27	118.44	112.54
2	C	901	9XH	C25-C24-C30	-2.26	115.50	118.30
2	B	901	9XH	C29-C27-C26	-2.24	119.86	122.80
2	A	901	9XH	C25-C26-C27	2.19	120.63	118.38
2	D	901	9XH	C26-C25-C24	2.18	123.36	121.18
2	B	901	9XH	C37-C36-C34	2.12	120.55	118.38
2	B	901	9XH	C32-C33-C34	2.08	120.51	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9XH	C19-C18-N17	-2.07	106.30	110.42
2	D	901	9XH	C32-C33-C34	2.06	120.49	118.38
2	C	901	9XH	C26-C25-C24	2.04	123.22	121.18

There are no chirality outliers.

All (33) torsion outliers are listed below:

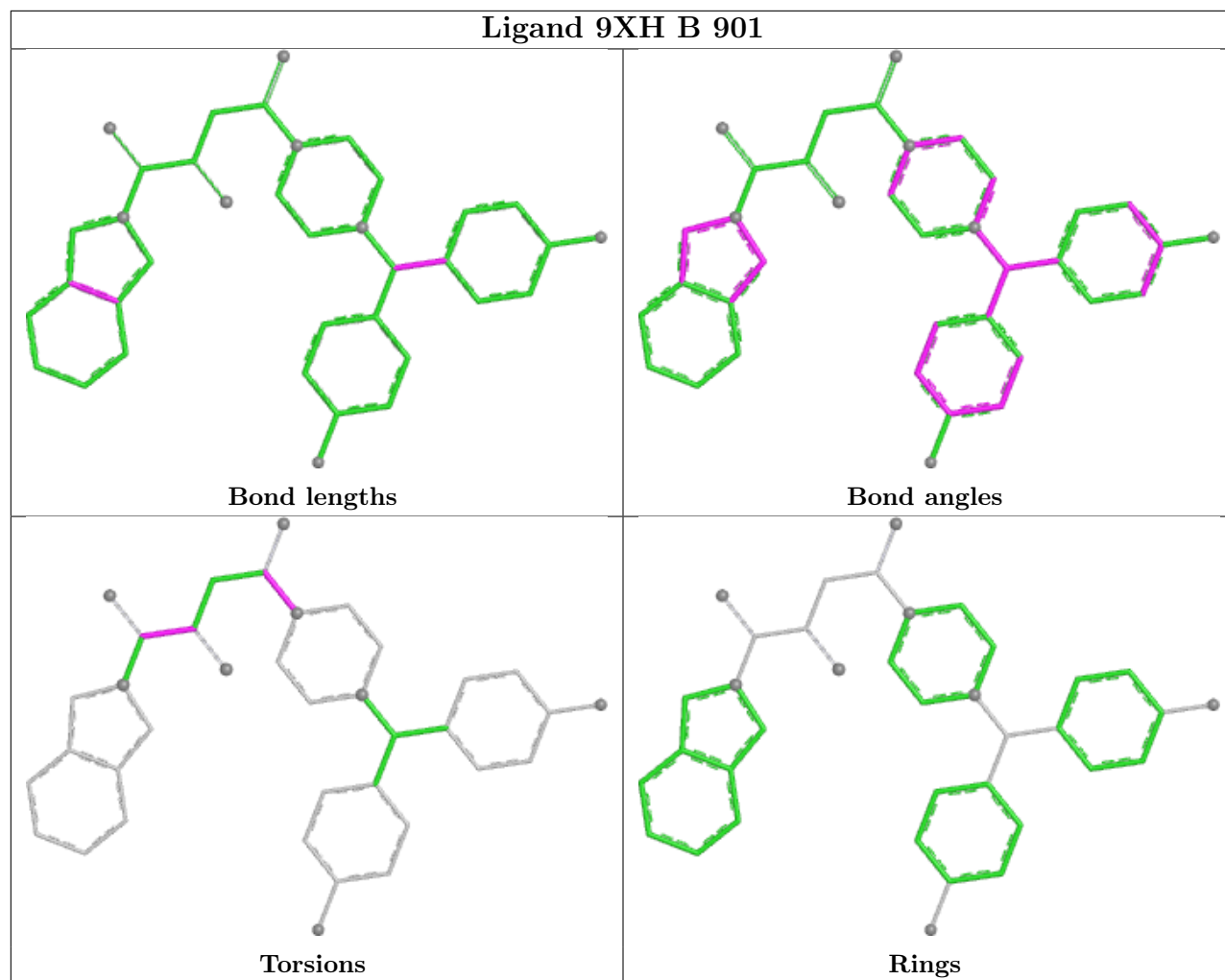
Mol	Chain	Res	Type	Atoms
2	A	901	9XH	C14-C15-N17-C18
2	A	901	9XH	C14-C15-N17-C22
2	A	901	9XH	O16-C15-N17-C18
2	A	901	9XH	O16-C15-N17-C22
2	B	901	9XH	O11-C10-C12-N13
2	B	901	9XH	C14-C15-N17-C18
2	B	901	9XH	C14-C15-N17-C22
2	B	901	9XH	O16-C15-N17-C18
2	B	901	9XH	O16-C15-N17-C22
2	C	901	9XH	C12-C10-N8-C7
2	C	901	9XH	O11-C10-N8-C7
2	C	901	9XH	C12-C10-N8-C9
2	C	901	9XH	O11-C10-N8-C9
2	D	901	9XH	C14-C15-N17-C22
2	D	901	9XH	O16-C15-N17-C22
2	D	901	9XH	C24-C23-N20-C21
2	D	901	9XH	C31-C23-N20-C19
2	D	901	9XH	C31-C23-N20-C21
2	C	901	9XH	C24-C23-N20-C19
2	C	901	9XH	C24-C23-N20-C21
2	C	901	9XH	C31-C23-N20-C21
2	D	901	9XH	C24-C23-N20-C19
2	D	901	9XH	O16-C15-N17-C18
2	C	901	9XH	C31-C23-N20-C19
2	C	901	9XH	C14-C15-N17-C22
2	D	901	9XH	C14-C15-N17-C18
2	C	901	9XH	O16-C15-N17-C18
2	C	901	9XH	O16-C15-N17-C22
2	C	901	9XH	C14-C15-N17-C18
2	D	901	9XH	C31-C23-C24-C25
2	D	901	9XH	C31-C23-C24-C30
2	A	901	9XH	O11-C10-N8-C7
2	C	901	9XH	C31-C23-C24-C25

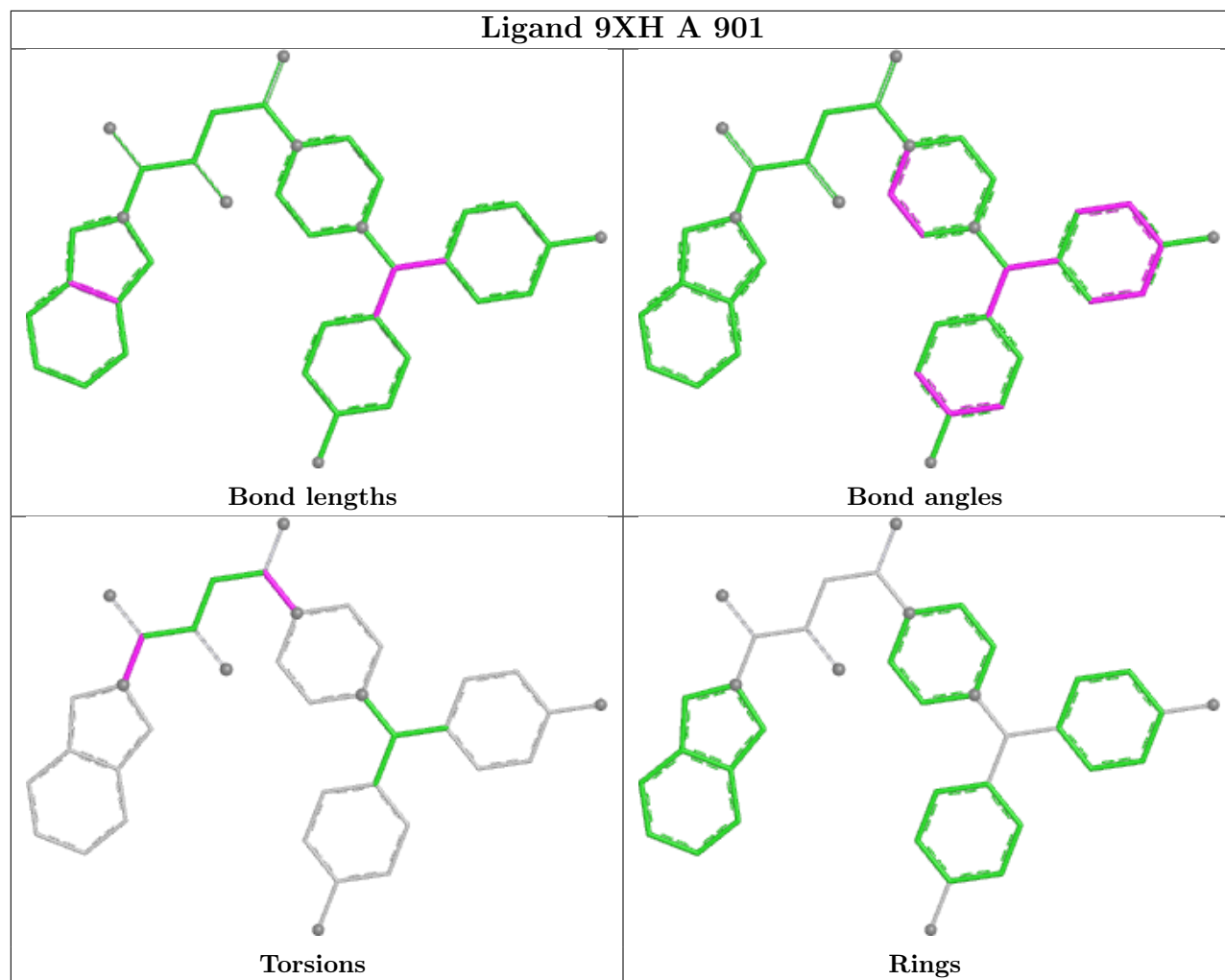
There are no ring outliers.

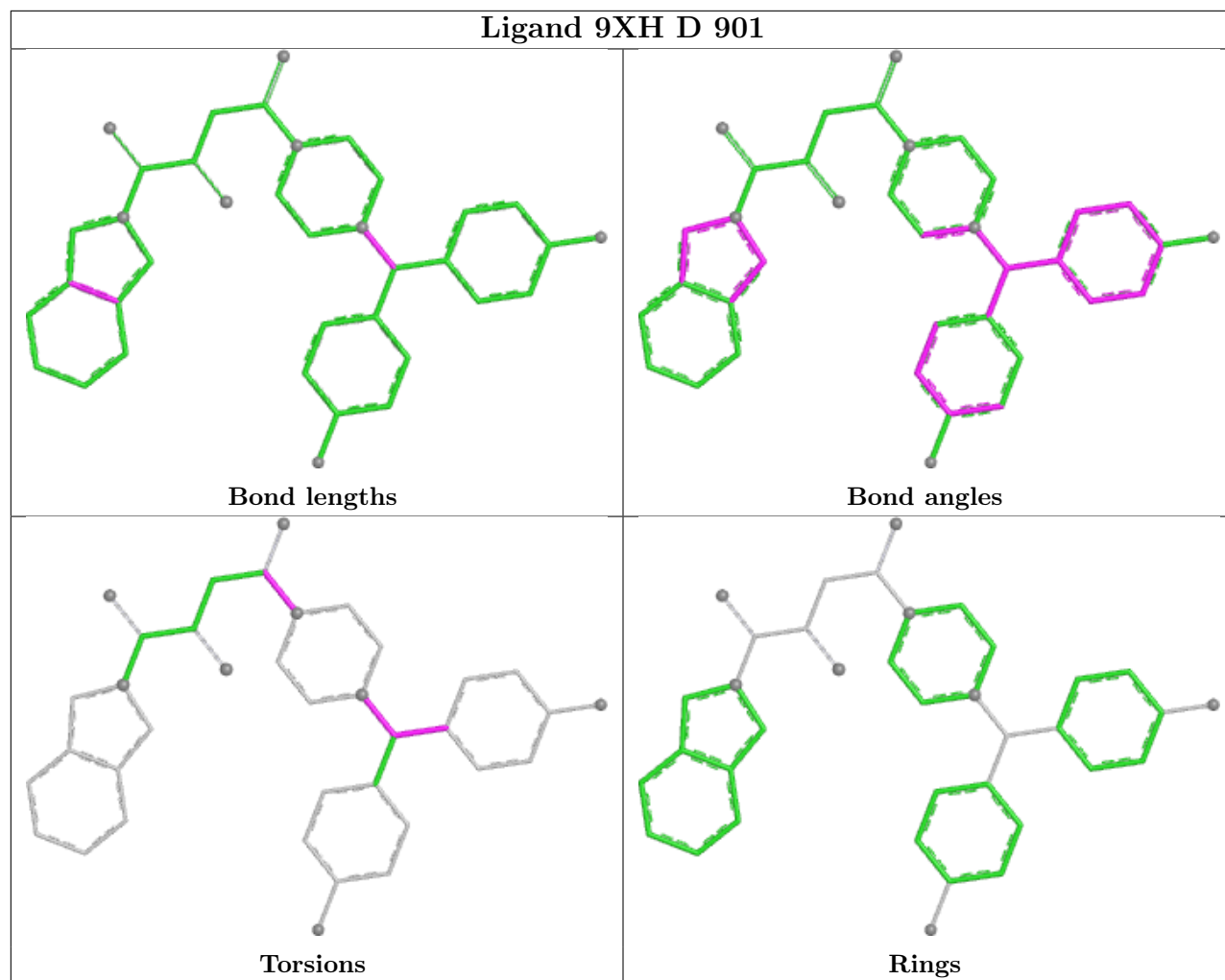
3 monomers are involved in 9 short contacts:

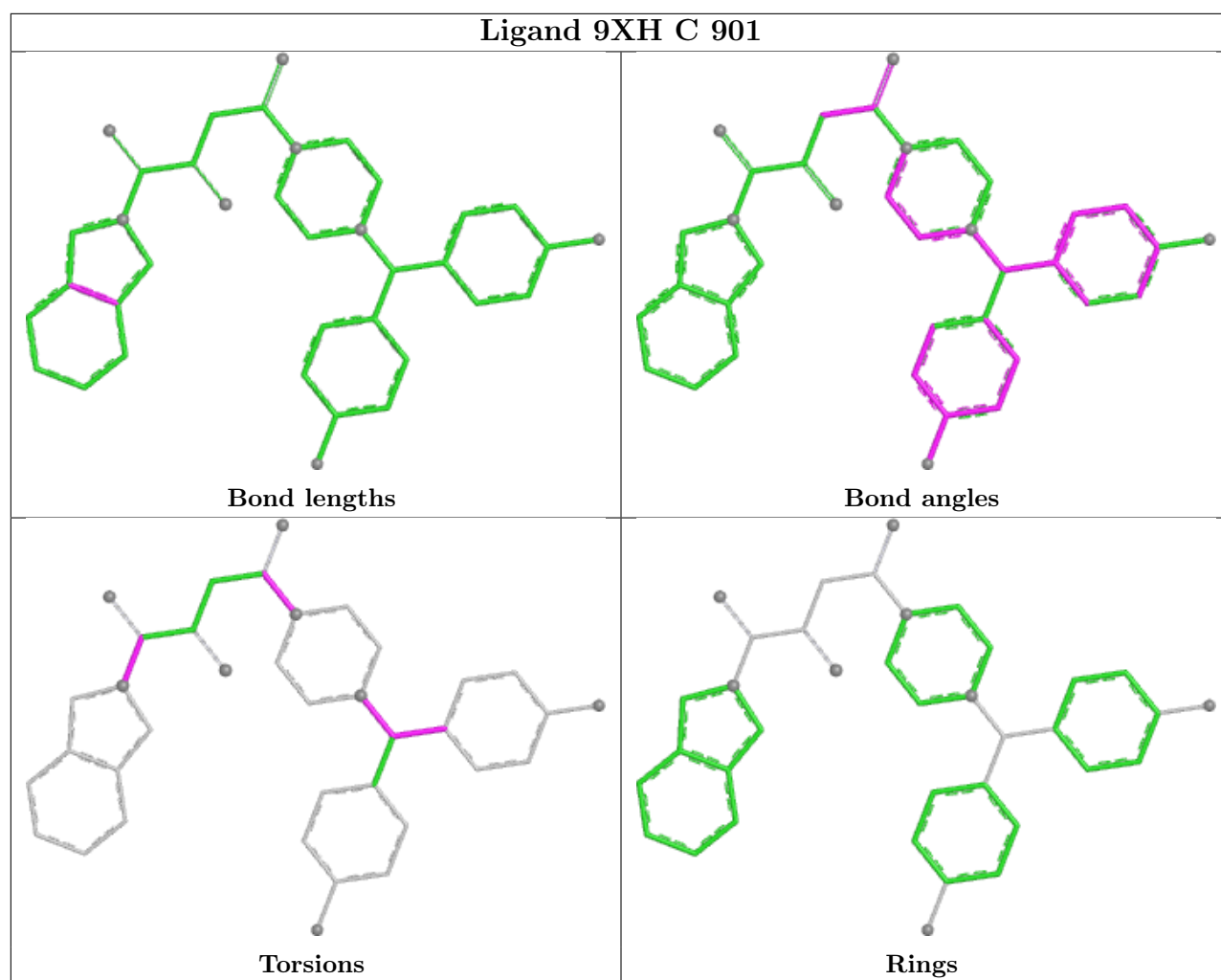
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	9XH	1	0
2	A	901	9XH	4	0
2	C	901	9XH	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	808/869 (92%)	0.36	50 (6%)	20 16	17, 38, 76, 100	0
1	B	805/869 (92%)	0.41	54 (6%)	17 13	17, 38, 70, 112	0
1	C	808/869 (92%)	0.29	43 (5%)	26 22	13, 33, 66, 84	0
1	D	812/869 (93%)	0.31	47 (5%)	23 19	14, 33, 67, 95	0
All	All	3233/3476 (93%)	0.34	194 (6%)	21 18	13, 36, 70, 112	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	HIS	9.1
1	B	118	HIS	7.5
1	B	117	HIS	7.3
1	B	111	HIS	6.7
1	C	475	GLY	6.5
1	D	118	HIS	6.1
1	A	113	GLN	5.4
1	C	118	HIS	5.3
1	B	327	GLN	5.1
1	B	113	GLN	5.0
1	A	185	SER	5.0
1	A	111	HIS	4.9
1	C	473	SER	4.9
1	A	469	SER	4.8
1	D	185	SER	4.5
1	C	65	SER	4.5
1	C	392	ASN	4.4
1	D	464	GLN	4.3
1	C	185	SER	4.2
1	B	115	THR	4.2
1	B	326	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	112	PHE	4.0
1	A	135	GLY	4.0
1	D	111	HIS	4.0
1	A	472	PHE	3.9
1	D	437	ASP	3.9
1	C	618	ASP	3.9
1	A	115	THR	3.8
1	A	392	ASN	3.8
1	A	158	SER	3.6
1	D	62	THR	3.6
1	A	264	TRP	3.6
1	B	178	LEU	3.5
1	B	391	GLU	3.5
1	A	326	SER	3.4
1	B	264	TRP	3.4
1	A	476	GLU	3.4
1	A	471	PRO	3.3
1	C	117	HIS	3.3
1	B	779	HIS	3.3
1	B	348	LYS	3.3
1	B	185	SER	3.3
1	B	433	SER	3.2
1	A	395	GLN	3.2
1	D	64	GLU	3.2
1	C	94	LYS	3.2
1	C	111	HIS	3.2
1	D	324	THR	3.2
1	C	112	PHE	3.2
1	B	110	ASP	3.2
1	D	399	SER	3.1
1	D	436	GLU	3.1
1	A	101	LEU	3.1
1	A	327	GLN	3.1
1	A	397	LEU	3.1
1	A	112	PHE	3.1
1	A	114	ALA	3.0
1	A	120	VAL	3.0
1	D	117	HIS	3.0
1	B	328	GLY	3.0
1	B	333	THR	3.0
1	B	158	SER	3.0
1	D	120	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	581	ASP	2.9
1	D	463	SER	2.9
1	B	588	GLN	2.9
1	B	137	PHE	2.9
1	C	66	GLY	2.9
1	C	344	SER	2.9
1	D	433	SER	2.9
1	D	113	GLN	2.8
1	D	264	TRP	2.8
1	A	172	VAL	2.8
1	B	184	CYS	2.8
1	B	147	GLU	2.8
1	C	464	GLN	2.8
1	A	157	ASN	2.8
1	A	169	GLY	2.8
1	B	119	GLY	2.7
1	C	184	CYS	2.7
1	B	392	ASN	2.7
1	A	463	SER	2.7
1	B	331	VAL	2.7
1	D	473	SER	2.7
1	B	227	GLN	2.7
1	C	115	THR	2.7
1	D	112	PHE	2.7
1	C	395	GLN	2.7
1	A	79	TYR	2.7
1	A	405	ARG	2.7
1	D	470	GLU	2.7
1	C	579	GLY	2.6
1	B	554	GLN	2.6
1	B	121	TYR	2.6
1	A	616	ARG	2.6
1	A	231	ASN	2.6
1	B	395	GLN	2.6
1	B	390	THR	2.6
1	D	469	SER	2.6
1	C	394	GLU	2.5
1	B	396	ARG	2.5
1	C	688	ARG	2.5
1	D	22	ALA	2.5
1	B	233	LEU	2.5
1	C	113	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	478	GLU	2.5
1	A	779	HIS	2.5
1	D	614	HIS	2.5
1	D	165	GLY	2.5
1	D	115	THR	2.5
1	D	187	PRO	2.5
1	A	683	CYS	2.5
1	B	114	ALA	2.5
1	D	778	GLN	2.5
1	B	778	GLN	2.5
1	D	466	TYR	2.5
1	A	116	PRO	2.4
1	A	237	LYS	2.4
1	A	324	THR	2.4
1	C	437	ASP	2.4
1	D	475	GLY	2.4
1	B	618	ASP	2.4
1	D	158	SER	2.4
1	B	394	GLU	2.4
1	C	179	GLU	2.4
1	B	578	SER	2.4
1	D	227	GLN	2.4
1	D	52	ALA	2.4
1	D	271	LYS	2.4
1	D	700	VAL	2.4
1	B	62	THR	2.4
1	C	63	ASP	2.4
1	B	776	ASN	2.4
1	B	500	HIS	2.4
1	D	580	PRO	2.4
1	B	619	VAL	2.3
1	A	431	PRO	2.3
1	A	325	ASP	2.3
1	A	473	SER	2.3
1	C	554	GLN	2.3
1	B	82	ARG	2.3
1	D	590	ARG	2.3
1	C	40	GLY	2.3
1	B	120	VAL	2.3
1	D	63	ASP	2.3
1	A	166	GLY	2.3
1	A	168	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	173	SER	2.3
1	D	163	ARG	2.3
1	C	402	ALA	2.3
1	B	64	GLU	2.3
1	A	155	ALA	2.3
1	B	582	ASP	2.2
1	C	62	THR	2.2
1	A	580	PRO	2.2
1	D	582	ASP	2.2
1	A	270	LEU	2.2
1	C	324	THR	2.2
1	D	92	PRO	2.2
1	C	121	TYR	2.2
1	A	167	LYS	2.2
1	C	39	HIS	2.2
1	B	157	ASN	2.2
1	A	480	LYS	2.2
1	A	65	SER	2.2
1	A	588	GLN	2.2
1	C	399	SER	2.2
1	A	121	TYR	2.2
1	D	135	GLY	2.1
1	B	437	ASP	2.1
1	C	264	TRP	2.1
1	D	418	ASN	2.1
1	B	332	SER	2.1
1	C	168	ASN	2.1
1	C	778	GLN	2.1
1	D	683	CYS	2.1
1	C	119	GLY	2.1
1	B	393	GLU	2.1
1	C	396	ARG	2.1
1	C	418	ASN	2.1
1	B	617	SER	2.1
1	D	183	GLN	2.1
1	D	401	ARG	2.1
1	A	795	ASN	2.1
1	C	157	ASN	2.1
1	D	588	GLN	2.0
1	C	234	ASP	2.0
1	C	477	ASP	2.0
1	B	43	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	329	LYS	2.0
1	D	630	ALA	2.0
1	C	558	MET	2.0
1	D	168	ASN	2.0
1	A	159	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

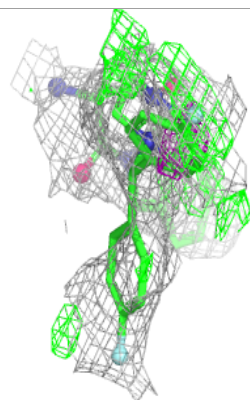
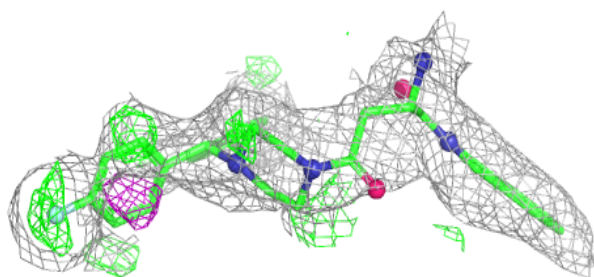
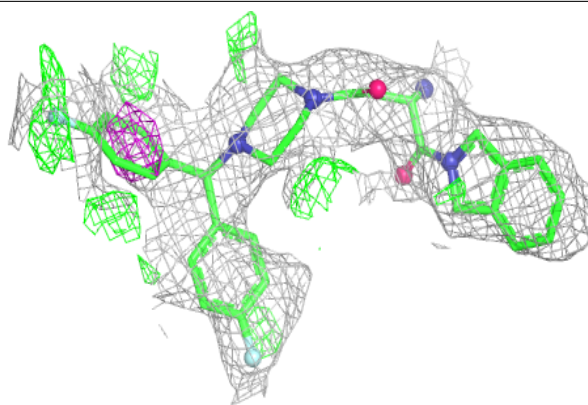
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9XH	D	901	37/37	0.73	0.42	44,65,80,82	0
2	9XH	C	901	37/37	0.84	0.40	37,65,83,87	0
2	9XH	B	901	37/37	0.84	0.44	48,68,98,102	0
2	9XH	A	901	37/37	0.86	0.30	40,79,93,93	0

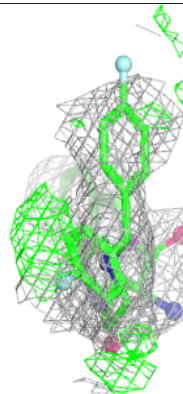
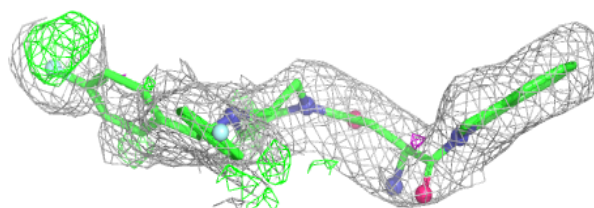
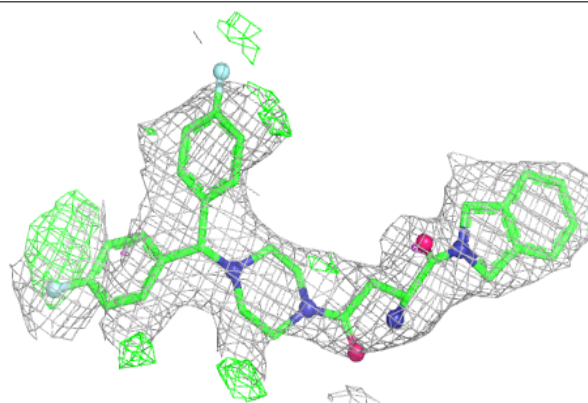
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9XH D 901:

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

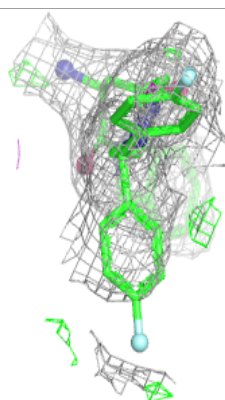
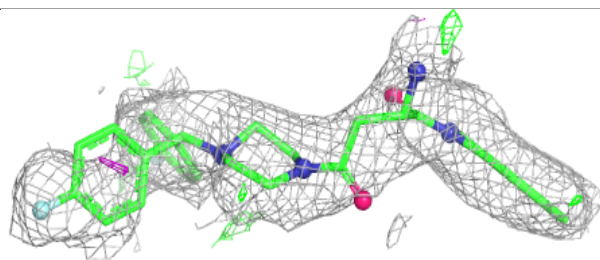
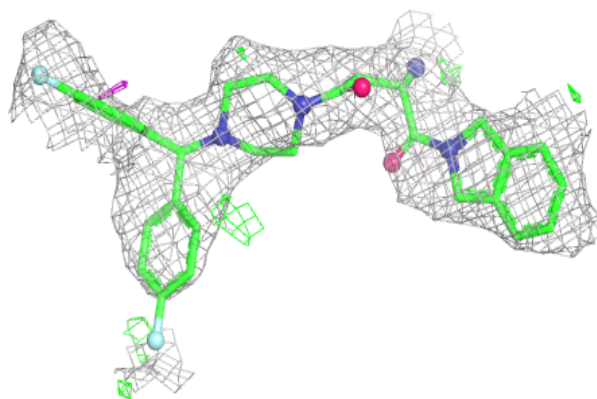
**Electron density around 9XH C 901:**

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

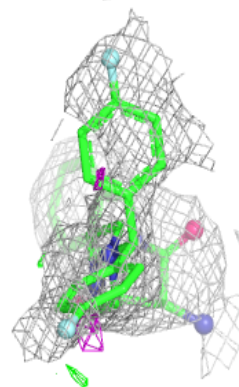
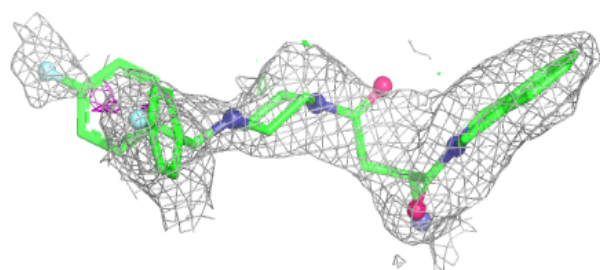
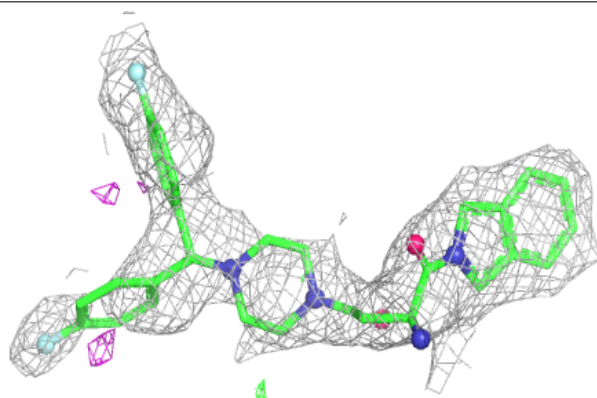


Electron density around 9XH B 901:

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

**Electron density around 9XH A 901:**

$2mF_o-DF_c$ (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.