



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:25 AM UTC

PDB ID : 6EOR / pdb_00006eor
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

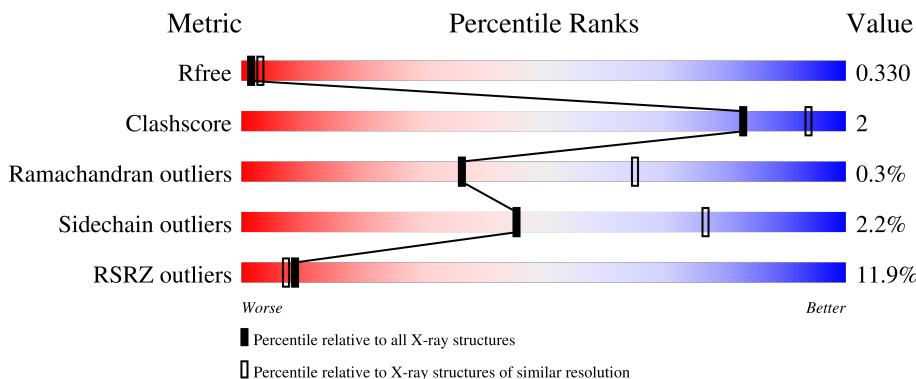
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	
1	B	869	
1	C	869	
1	D	869	

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

There are 24 discrepancies between the modelled and reference sequences:

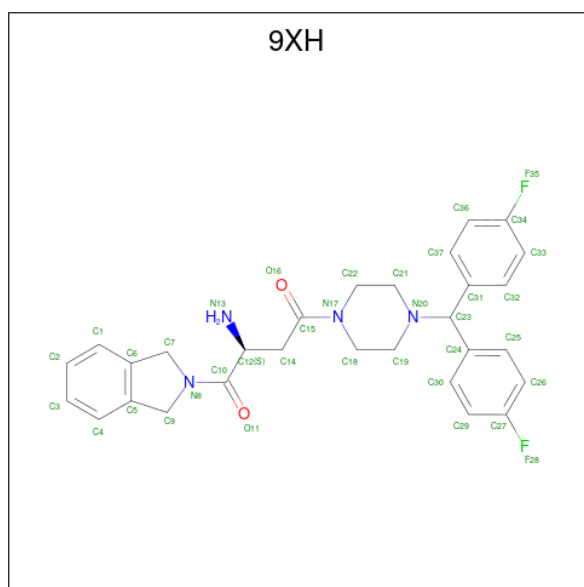
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	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 (CCD ID: 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		

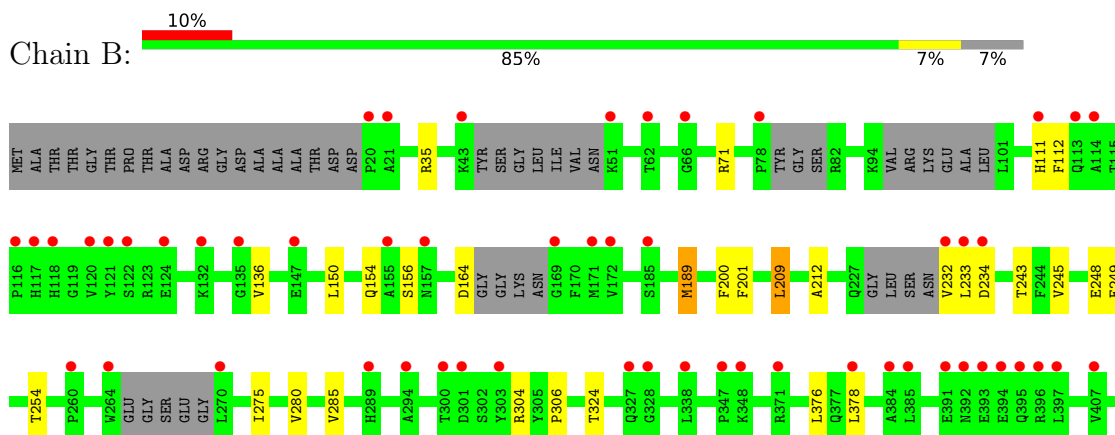
3 Residue-property plots

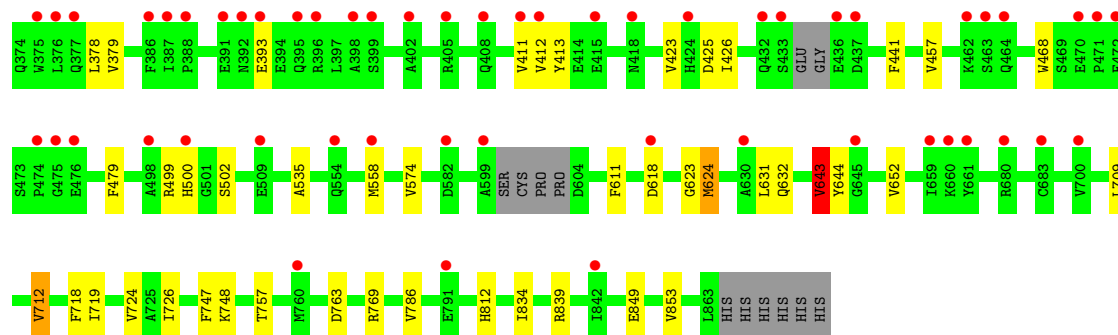
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 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)	Xtrriage
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	Xtrriage
Anisotropy	0.718	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.61	0/6759	0.83	3/9165 (0.0%)
1	B	0.61	0/6733	0.84	4/9128 (0.0%)
1	C	0.63	1/6754 (0.0%)	0.84	3/9159 (0.0%)
1	D	0.64	0/6779	0.84	5/9192 (0.1%)
All	All	0.62	1/27025 (0.0%)	0.84	15/36644 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	754	ALA	C-O	-5.06	1.21	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	PHE	N-CA-C	7.26	122.24	112.88
1	D	502	SER	N-CA-C	-7.07	100.54	110.50
1	B	495	GLU	N-CA-C	6.03	118.57	109.23
1	D	643	VAL	N-CA-C	5.61	118.21	108.90
1	B	658	GLY	N-CA-C	5.56	120.57	114.40
1	C	607	PRO	O-C-N	5.54	123.75	121.15
1	B	763	ASP	N-CA-C	5.48	117.15	110.41
1	C	495	GLU	N-CA-C	5.42	117.50	108.99
1	D	426	ILE	N-CA-C	5.37	115.93	108.84
1	A	763	ASP	N-CA-C	5.37	118.38	110.59
1	A	233	LEU	N-CA-C	-5.23	107.03	113.41
1	D	718	PHE	N-CA-C	5.21	120.29	112.94
1	B	426	ILE	N-CA-C	5.20	115.09	108.12
1	C	117	HIS	N-CA-C	5.07	117.21	111.02
1	D	763	ASP	N-CA-C	5.01	117.00	110.53

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	6563	0	6348	37	0
1	B	6540	0	6340	28	0
1	C	6560	0	6347	28	0
1	D	6585	0	6365	33	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
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	125	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 (125) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:367:MET:HE1	1:D:423:VAL:HG13	1.87	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
1:D:643:VAL:HG12	1:D:644:TYR:N	2.25	0.52
1:A:74:TYR:CE2	1:A:595:MET:HE1	2.46	0.51
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: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:B:697:MET:HE3	1:B:770:TYR:CB	2.41	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:D:91:ILE:HG21	1:D:558:MET:HE2	1.94	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:108:MET:HA	1:C:171:MET:HE1	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:611:PHE:CD1	1:A:611:PHE:C	2.95	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:D:624:MET:HE2	1:D:652:VAL:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:MET:HE3	1:D:574:VAL:HG12	1.99	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:D:611:PHE:CD1	1:D:611:PHE:C	2.97	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:D:154:GLN:HE22	1:D:189:MET:HE3	1.85	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
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%)	36	65
1	B	785/869 (90%)	739 (94%)	43 (6%)	3 (0%)	30	59
1	C	790/869 (91%)	737 (93%)	53 (7%)	0	100	100
1	D	794/869 (91%)	746 (94%)	45 (6%)	3 (0%)	30	59
All	All	3159/3476 (91%)	2966 (94%)	185 (6%)	8 (0%)	36	65

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	712/759 (94%)	702 (99%)	10 (1%)	59	85
1	B	712/759 (94%)	696 (98%)	16 (2%)	45	77
1	C	714/759 (94%)	697 (98%)	17 (2%)	43	75
1	D	715/759 (94%)	696 (97%)	19 (3%)	39	73
All	All	2853/3036 (94%)	2791 (98%)	62 (2%)	45	77

All (62) 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	378	LEU
1	A	707	GLU
1	A	738	MET
1	B	136	VAL
1	B	150	LEU
1	B	156	SER
1	B	189	MET
1	B	209	LEU
1	B	248	GLU
1	B	254	THR
1	B	376	LEU
1	B	378	LEU
1	B	433	SER
1	B	513	VAL
1	B	662	LEU
1	B	712	VAL
1	B	714	GLU
1	B	773	VAL
1	B	847	SER
1	C	72	LEU
1	C	102	LEU
1	C	128	LEU
1	C	130	GLU
1	C	189	MET
1	C	209	LEU
1	C	248	GLU
1	C	379	VAL
1	C	406	ASN
1	C	411	VAL
1	C	437	ASP
1	C	597	GLU
1	C	609	GLU
1	C	617	SER
1	C	676	VAL
1	C	703	GLU
1	C	748	LYS

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Mol	Chain	Res	Type
1	D	25	GLN
1	D	128	LEU
1	D	184	CYS
1	D	189	MET
1	D	209	LEU
1	D	220	ARG
1	D	238	SER
1	D	248	GLU
1	D	280	VAL
1	D	319	LEU
1	D	378	LEU
1	D	393	GLU
1	D	618	ASP
1	D	624	MET
1	D	631	LEU
1	D	632	GLN
1	D	643	VAL
1	D	712	VAL
1	D	748	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	392	ASN
1	A	395	GLN
1	A	464	GLN
1	A	507	ASN
1	A	555	ASN
1	A	650	GLN
1	A	705	GLN
1	A	778	GLN
1	A	804	HIS
1	A	831	GLN
1	A	833	GLN
1	A	837	ASN
1	B	54	HIS
1	B	84	ASN
1	B	154	GLN
1	B	395	GLN
1	B	422	ASN
1	B	464	GLN

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Mol	Chain	Res	Type
1	B	507	ASN
1	B	548	HIS
1	B	562	HIS
1	B	695	ASN
1	B	705	GLN
1	B	804	HIS
1	B	831	GLN
1	C	70	HIS
1	C	84	ASN
1	C	247	GLN
1	C	406	ASN
1	C	464	GLN
1	C	507	ASN
1	C	548	HIS
1	C	612	HIS
1	C	650	GLN
1	C	804	HIS
1	C	812	HIS
1	D	27	GLN
1	D	29	HIS
1	D	113	GLN
1	D	154	GLN
1	D	157	ASN
1	D	161	HIS
1	D	205	ASN
1	D	548	HIS
1	D	684	GLN
1	D	695	ASN
1	D	705	GLN
1	D	804	HIS
1	D	822	GLN
1	D	831	GLN
1	D	837	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](#)

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	A	901	-	41,41,41	0.94	3 (7%)	55,58,58	1.35	6 (10%)
2	9XH	C	901	-	41,41,41	0.91	1 (2%)	55,58,58	1.45	11 (20%)
2	9XH	B	901	-	41,41,41	1.04	2 (4%)	55,58,58	1.53	10 (18%)
2	9XH	D	901	-	41,41,41	1.12	2 (4%)	55,58,58	1.81	12 (21%)

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	A	901	-	-	5/28/46/46	0/5/5/5
2	9XH	C	901	-	-	13/28/46/46	0/5/5/5
2	9XH	B	901	-	-	5/28/46/46	0/5/5/5
2	9XH	D	901	-	-	10/28/46/46	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:

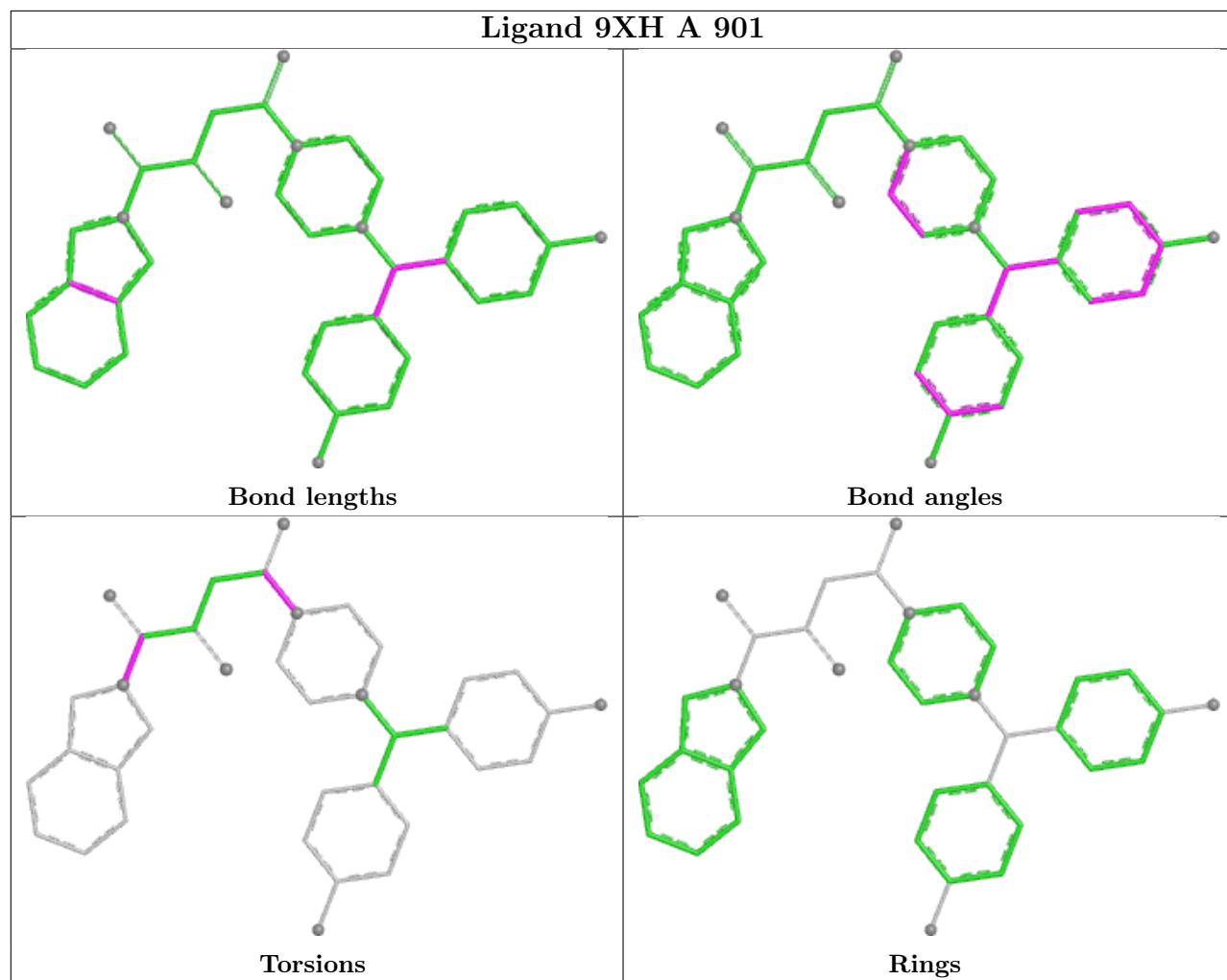
Mol	Chain	Res	Type	Atoms
2	A	901	9XH	C14-C15-N17-C18
2	A	901	9XH	C14-C15-N17-C22
2	A	901	9XH	O16-C15-N17-C18
2	A	901	9XH	O16-C15-N17-C22
2	B	901	9XH	O11-C10-C12-N13
2	B	901	9XH	C14-C15-N17-C18
2	B	901	9XH	C14-C15-N17-C22
2	B	901	9XH	O16-C15-N17-C18
2	B	901	9XH	O16-C15-N17-C22
2	C	901	9XH	C12-C10-N8-C7
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

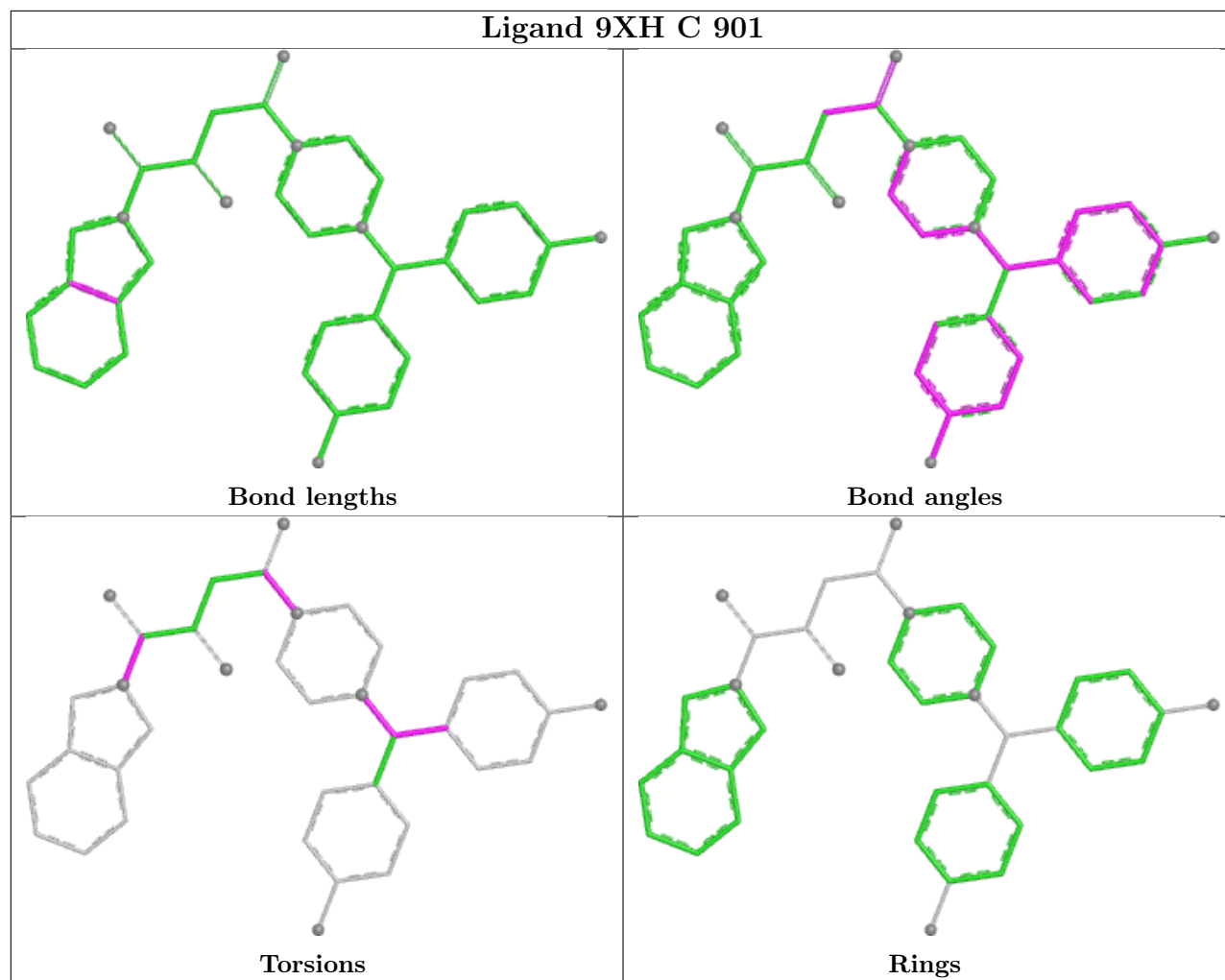
There are no ring outliers.

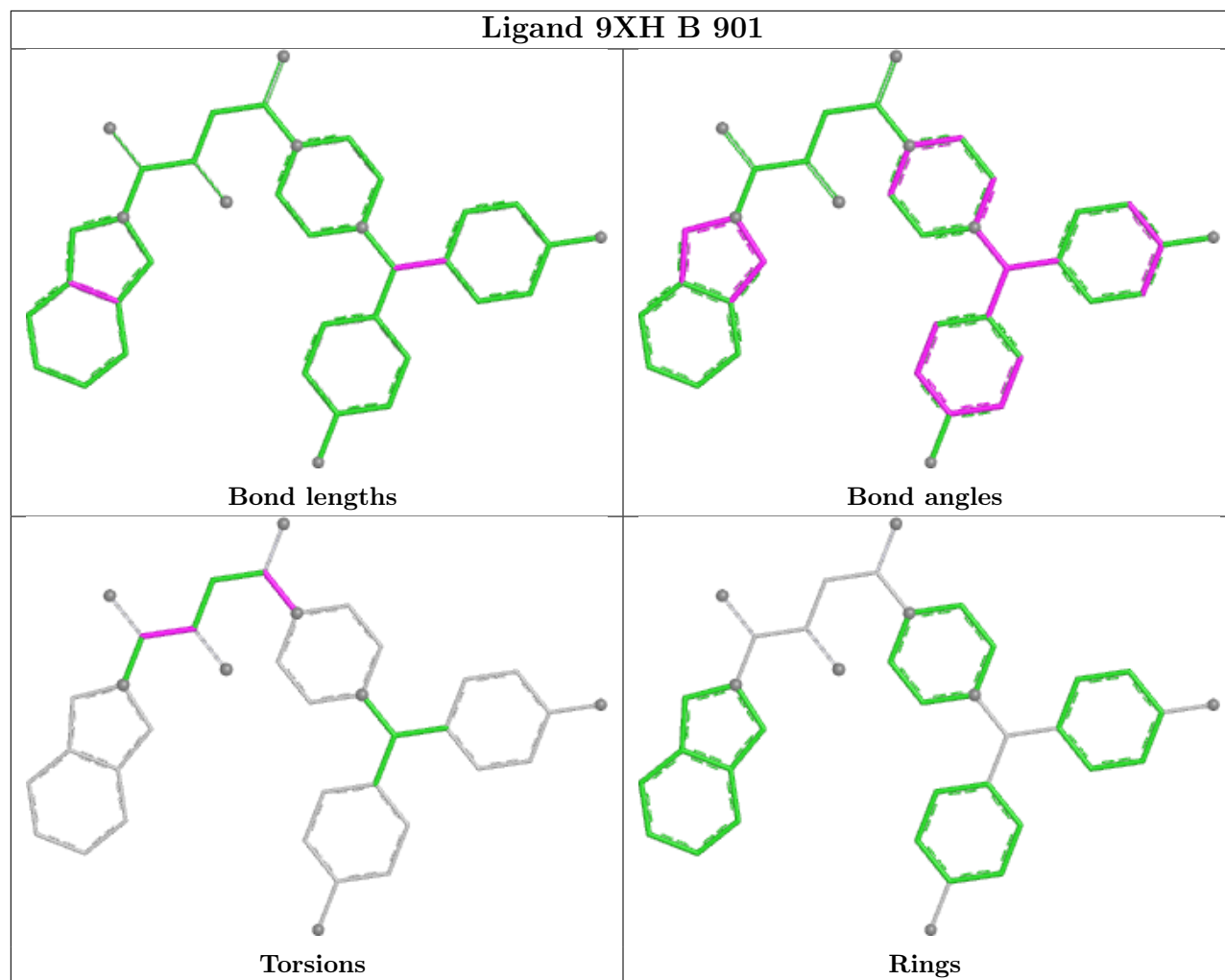
3 monomers are involved in 9 short contacts:

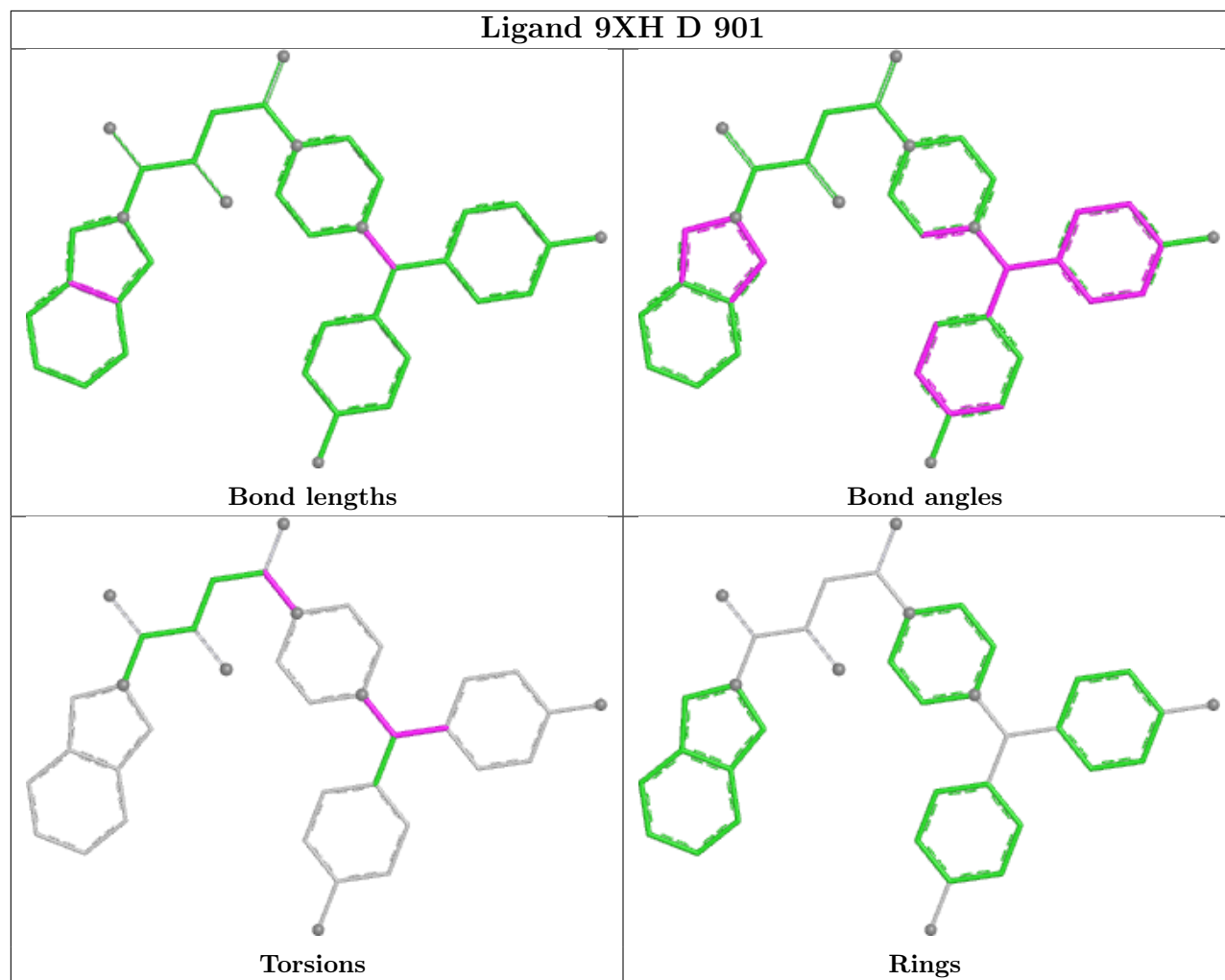
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	9XH	4	0
2	C	901	9XH	4	0
2	B	901	9XH	1	0

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%)	0.95	93 (11%) 9 8	17, 38, 76, 100	0
1	B	805/869 (92%)	0.98	85 (10%) 11 9	17, 37, 70, 112	0
1	C	808/869 (92%)	0.90	96 (11%) 9 7	13, 33, 66, 84	0
1	D	812/869 (93%)	0.99	111 (13%) 6 5	14, 33, 67, 95	0
All	All	3233/3476 (93%)	0.95	385 (11%) 9 7	13, 36, 70, 112	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	HIS	6.5
1	A	232	VAL	6.3
1	A	135	GLY	6.2
1	A	233	LEU	5.8
1	D	399	SER	5.5
1	A	469	SER	5.4
1	C	475	GLY	5.2
1	D	232	VAL	5.2
1	A	101	LEU	5.2
1	C	232	VAL	5.1
1	D	118	HIS	4.8
1	D	185	SER	4.7
1	A	392	ASN	4.7
1	C	264	TRP	4.7
1	A	683	CYS	4.5
1	B	20	PRO	4.5
1	A	472	PHE	4.4
1	A	396	ARG	4.4
1	B	21	ALA	4.3
1	B	135	GLY	4.3
1	A	397	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	101	LEU	4.3
1	C	20	PRO	4.3
1	C	185	SER	4.2
1	C	473	SER	4.2
1	B	124	GLU	4.2
1	B	232	VAL	4.2
1	C	233	LEU	4.2
1	B	118	HIS	4.2
1	D	20	PRO	4.1
1	A	266	GLY	4.1
1	B	475	GLY	4.0
1	C	478	GLU	4.0
1	D	187	PRO	4.0
1	D	52	ALA	4.0
1	C	645	GLY	4.0
1	A	395	GLN	4.0
1	A	117	HIS	4.0
1	D	78	PRO	3.9
1	B	700	VAL	3.9
1	D	166	GLY	3.9
1	B	233	LEU	3.9
1	D	43	LYS	3.9
1	D	135	GLY	3.8
1	D	395	GLN	3.8
1	B	437	ASP	3.8
1	B	117	HIS	3.8
1	D	270	LEU	3.8
1	A	704	ASP	3.7
1	C	474	PRO	3.7
1	D	21	ALA	3.7
1	A	231	ASN	3.7
1	B	348	LYS	3.7
1	D	760	MET	3.6
1	D	464	GLN	3.6
1	A	65	SER	3.6
1	C	135	GLY	3.6
1	A	79	TYR	3.5
1	A	116	PRO	3.5
1	C	402	ALA	3.5
1	C	688	ARG	3.5
1	D	683	CYS	3.5
1	A	248	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	436	GLU	3.5
1	A	120	VAL	3.5
1	D	433	SER	3.5
1	B	78	PRO	3.5
1	C	53	PRO	3.5
1	D	437	ASP	3.5
1	A	113	GLN	3.4
1	B	438	GLU	3.4
1	D	471	PRO	3.4
1	A	158	SER	3.4
1	B	760	MET	3.4
1	C	378	LEU	3.3
1	D	700	VAL	3.3
1	D	324	THR	3.3
1	C	396	ARG	3.3
1	D	396	ARG	3.3
1	D	463	SER	3.3
1	B	264	TRP	3.3
1	C	545	GLY	3.3
1	B	683	CYS	3.2
1	D	375	TRP	3.2
1	B	371	ARG	3.2
1	B	554	GLN	3.2
1	B	425	ASP	3.2
1	D	117	HIS	3.2
1	C	62	THR	3.2
1	C	344	SER	3.1
1	B	598	ALA	3.1
1	C	112	PHE	3.1
1	B	394	GLU	3.1
1	B	185	SER	3.1
1	B	384	ALA	3.1
1	C	399	SER	3.1
1	C	437	ASP	3.1
1	A	115	THR	3.1
1	A	282	GLU	3.1
1	C	395	GLN	3.1
1	C	56	PHE	3.1
1	D	112	PHE	3.1
1	C	554	GLN	3.1
1	A	82	ARG	3.1
1	C	117	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	599	ALA	3.0
1	B	120	VAL	3.0
1	C	463	SER	3.0
1	C	483	ILE	3.0
1	D	113	GLN	3.0
1	D	266	GLY	3.0
1	D	170	PHE	3.0
1	D	122	SER	3.0
1	B	301	ASP	3.0
1	A	580	PRO	3.0
1	C	703	GLU	2.9
1	C	791	GLU	2.9
1	C	52	ALA	2.9
1	A	166	GLY	2.9
1	A	78	PRO	2.9
1	D	392	ASN	2.9
1	D	233	LEU	2.9
1	A	375	TRP	2.9
1	B	395	GLN	2.9
1	D	432	GLN	2.9
1	D	167	LYS	2.9
1	A	298	ARG	2.9
1	B	111	HIS	2.9
1	C	464	GLN	2.9
1	A	462	LYS	2.9
1	A	234	ASP	2.9
1	B	407	VAL	2.9
1	A	471	PRO	2.8
1	D	183	GLN	2.8
1	A	393	GLU	2.8
1	A	394	GLU	2.8
1	A	287	VAL	2.8
1	A	865	HIS	2.8
1	B	424	HIS	2.8
1	C	86	LEU	2.8
1	B	464	GLN	2.8
1	D	237	LYS	2.8
1	C	476	GLU	2.8
1	C	121	TYR	2.8
1	A	534	ALA	2.8
1	D	645	GLY	2.8
1	B	116	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	56	PHE	2.8
1	A	237	LYS	2.8
1	A	124	GLU	2.7
1	D	405	ARG	2.7
1	C	683	CYS	2.7
1	C	178	LEU	2.7
1	A	167	LYS	2.7
1	A	399	SER	2.7
1	B	169	GLY	2.7
1	C	118	HIS	2.7
1	A	185	SER	2.7
1	A	339	VAL	2.7
1	B	391	GLU	2.7
1	C	432	GLN	2.7
1	D	791	GLU	2.7
1	D	303	TYR	2.7
1	A	583	ASP	2.7
1	C	618	ASP	2.7
1	D	334	GLN	2.7
1	C	22	ALA	2.6
1	A	779	HIS	2.6
1	C	78	PRO	2.6
1	D	227	GLN	2.6
1	D	168	ASN	2.6
1	B	113	GLN	2.6
1	D	386	PHE	2.6
1	A	463	SER	2.6
1	D	500	HIS	2.6
1	A	174	PRO	2.6
1	D	165	GLY	2.6
1	A	136	VAL	2.6
1	C	270	LEU	2.6
1	A	286	GLU	2.6
1	B	487	ILE	2.6
1	B	427	PHE	2.6
1	D	148	SER	2.6
1	C	401	ARG	2.6
1	C	646	GLY	2.6
1	D	184	CYS	2.6
1	D	554	GLN	2.6
1	B	392	ASN	2.6
1	D	111	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	121	TYR	2.5
1	D	377	GLN	2.5
1	A	760	MET	2.5
1	A	126	GLU	2.5
1	B	396	ARG	2.5
1	A	289	HIS	2.5
1	A	165	GLY	2.5
1	D	248	GLU	2.5
1	D	234	ASP	2.5
1	D	558	MET	2.5
1	D	214	ILE	2.5
1	A	26	VAL	2.5
1	C	120	VAL	2.5
1	A	391	GLU	2.5
1	D	393	GLU	2.5
1	D	476	GLU	2.5
1	D	509	GLU	2.5
1	A	334	GLN	2.5
1	C	27	GLN	2.5
1	C	334	GLN	2.5
1	D	22	ALA	2.5
1	B	51	LYS	2.5
1	C	171	MET	2.4
1	C	584	PRO	2.4
1	D	842	ILE	2.4
1	D	82	ARG	2.4
1	B	300	THR	2.4
1	C	424	HIS	2.4
1	B	397	LEU	2.4
1	C	175	MET	2.4
1	A	431	PRO	2.4
1	B	604	ASP	2.4
1	C	234	ASP	2.4
1	D	335	GLU	2.4
1	D	472	PHE	2.4
1	B	294	ALA	2.4
1	B	840	HIS	2.4
1	C	461	LEU	2.4
1	B	172	VAL	2.4
1	C	136	VAL	2.4
1	C	700	VAL	2.4
1	C	717	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	2.4
1	A	401	ARG	2.4
1	B	122	SER	2.4
1	D	498	ALA	2.4
1	B	62	THR	2.4
1	C	189	MET	2.4
1	A	418	ASN	2.4
1	A	123	ARG	2.4
1	A	844	CYS	2.4
1	B	443	ARG	2.4
1	C	467	ASP	2.4
1	D	164	ASP	2.4
1	D	582	ASP	2.4
1	C	470	GLU	2.4
1	B	385	LEU	2.4
1	B	779	HIS	2.4
1	C	397	LEU	2.4
1	A	301	ASP	2.3
1	D	618	ASP	2.3
1	B	155	ALA	2.3
1	B	327	GLN	2.3
1	B	347	PRO	2.3
1	D	236	PRO	2.3
1	C	157	ASN	2.3
1	A	402	ALA	2.3
1	B	470	GLU	2.3
1	D	391	GLU	2.3
1	D	175	MET	2.3
1	C	111	HIS	2.3
1	A	660	LYS	2.3
1	B	260	PRO	2.3
1	B	328	GLY	2.3
1	A	175	MET	2.3
1	D	408	GLN	2.3
1	B	132	LYS	2.3
1	B	289	HIS	2.3
1	C	468	TRP	2.3
1	D	424	HIS	2.3
1	C	168	ASN	2.3
1	B	775	GLU	2.3
1	C	179	GLU	2.3
1	C	219	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	378	LEU	2.3
1	D	86	LEU	2.3
1	A	264	TRP	2.3
1	C	156	SER	2.3
1	D	680	ARG	2.3
1	D	388	PRO	2.3
1	D	412	VAL	2.3
1	B	479	PHE	2.2
1	C	760	MET	2.2
1	A	157	ASN	2.2
1	A	535	ALA	2.2
1	A	598	ALA	2.2
1	D	418	ASN	2.2
1	A	163	ARG	2.2
1	A	680	ARG	2.2
1	C	116	PRO	2.2
1	D	140	THR	2.2
1	B	535	ALA	2.2
1	C	21	ALA	2.2
1	D	64	GLU	2.2
1	D	462	LYS	2.2
1	A	214	ILE	2.2
1	D	387	ILE	2.2
1	A	111	HIS	2.2
1	D	26	VAL	2.2
1	D	67	PRO	2.2
1	A	173	SER	2.2
1	B	303	TYR	2.2
1	B	413	TYR	2.2
1	B	463	SER	2.2
1	B	171	MET	2.2
1	A	112	PHE	2.2
1	A	22	ALA	2.2
1	C	398	ALA	2.2
1	C	660	LYS	2.2
1	C	377	GLN	2.2
1	C	408	GLN	2.2
1	C	110	ASP	2.2
1	D	251	ASP	2.2
1	D	62	THR	2.2
1	B	717	GLY	2.2
1	C	303	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	472	PHE	2.2
1	D	402	ALA	2.2
1	A	168	ASN	2.2
1	C	43	LYS	2.2
1	D	398	ALA	2.2
1	D	474	PRO	2.1
1	A	618	ASP	2.1
1	B	618	ASP	2.1
1	B	338	LEU	2.1
1	C	386	PHE	2.1
1	D	103	LEU	2.1
1	D	376	LEU	2.1
1	D	661	TYR	2.1
1	B	393	GLU	2.1
1	C	139	ILE	2.1
1	A	177	PRO	2.1
1	D	359	ARG	2.1
1	A	327	GLN	2.1
1	B	431	PRO	2.1
1	C	94	LYS	2.1
1	C	412	VAL	2.1
1	D	136	VAL	2.1
1	B	270	LEU	2.1
1	C	438	GLU	2.1
1	D	219	GLU	2.1
1	A	424	HIS	2.1
1	A	290	VAL	2.1
1	A	403	VAL	2.1
1	B	157	ASN	2.1
1	A	693	LEU	2.1
1	B	662	LEU	2.1
1	B	66	GLY	2.1
1	C	501	GLY	2.1
1	D	475	GLY	2.1
1	C	115	THR	2.1
1	C	604	ASP	2.1
1	D	63	ASP	2.1
1	D	110	ASP	2.1
1	B	114	ALA	2.1
1	D	630	ALA	2.1
1	B	147	GLU	2.1
1	C	337	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	410	TYR	2.1
1	B	661	TYR	2.1
1	C	77	MET	2.0
1	C	840	HIS	2.0
1	D	411	VAL	2.0
1	B	580	PRO	2.0
1	A	512	LEU	2.0
1	A	590	ARG	2.0
1	D	659	ILE	2.0
1	B	509	GLU	2.0
1	D	470	GLU	2.0
1	A	644	TYR	2.0
1	B	43	LYS	2.0
1	D	660	LYS	2.0
1	A	586	HIS	2.0
1	D	158	SER	2.0
1	C	376	LEU	2.0
1	C	298	ARG	2.0
1	C	392	ASN	2.0
1	C	422	ASN	2.0
1	A	137	PHE	2.0
1	A	21	ALA	2.0
1	D	114	ALA	2.0
1	B	234	ASP	2.0
1	A	176	LYS	2.0
1	C	125	GLU	2.0
1	C	394	GLU	2.0
1	D	415	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.

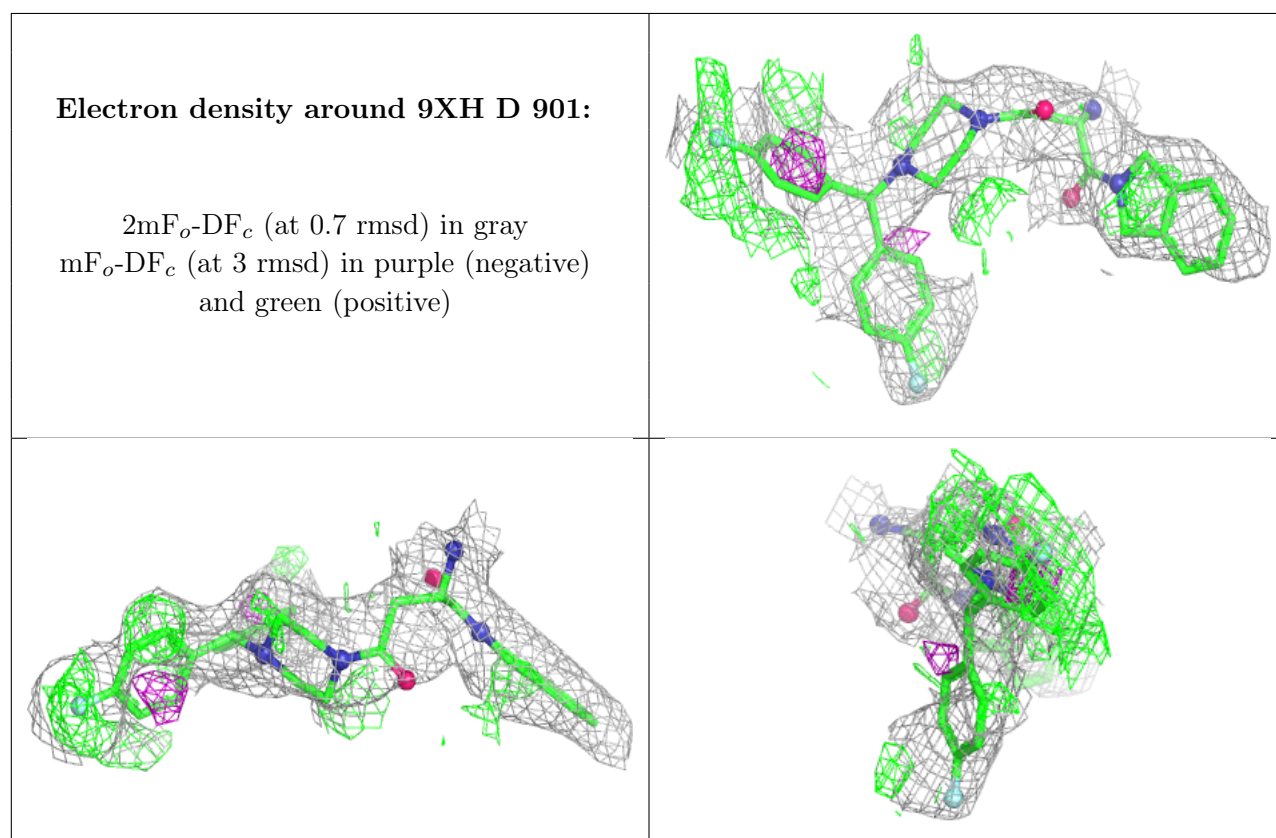
6.4 Ligands [i](#)

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.

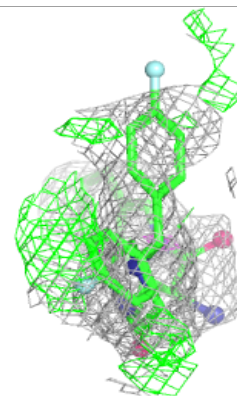
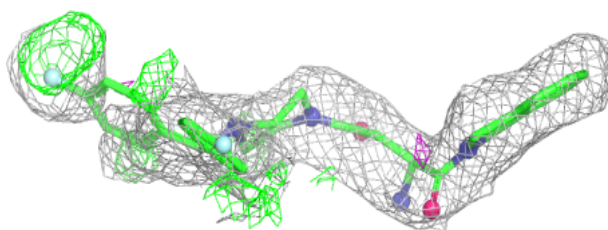
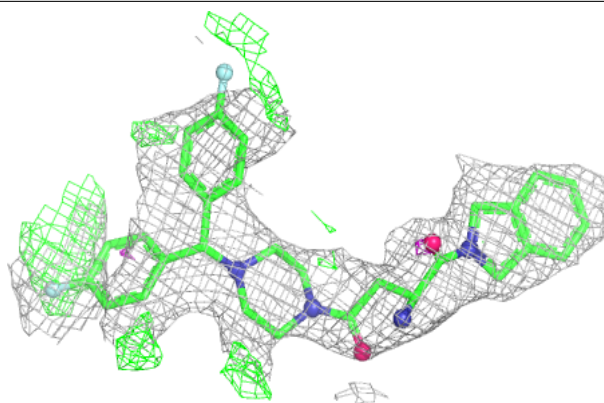
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9XH	D	901	37/37	0.66	0.30	44,65,80,82	0
2	9XH	C	901	37/37	0.72	0.26	37,65,83,87	0
2	9XH	B	901	37/37	0.77	0.25	48,68,98,102	0
2	9XH	A	901	37/37	0.78	0.23	40,79,93,93	0

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.

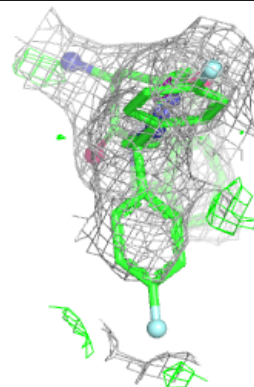
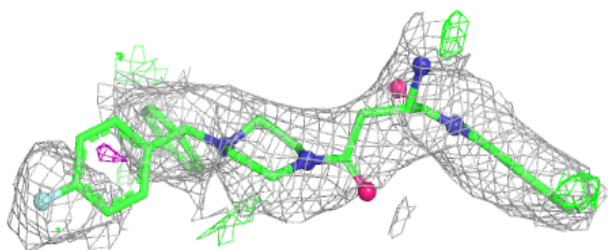
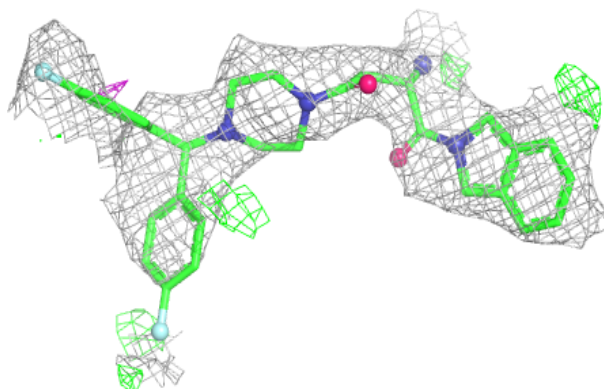


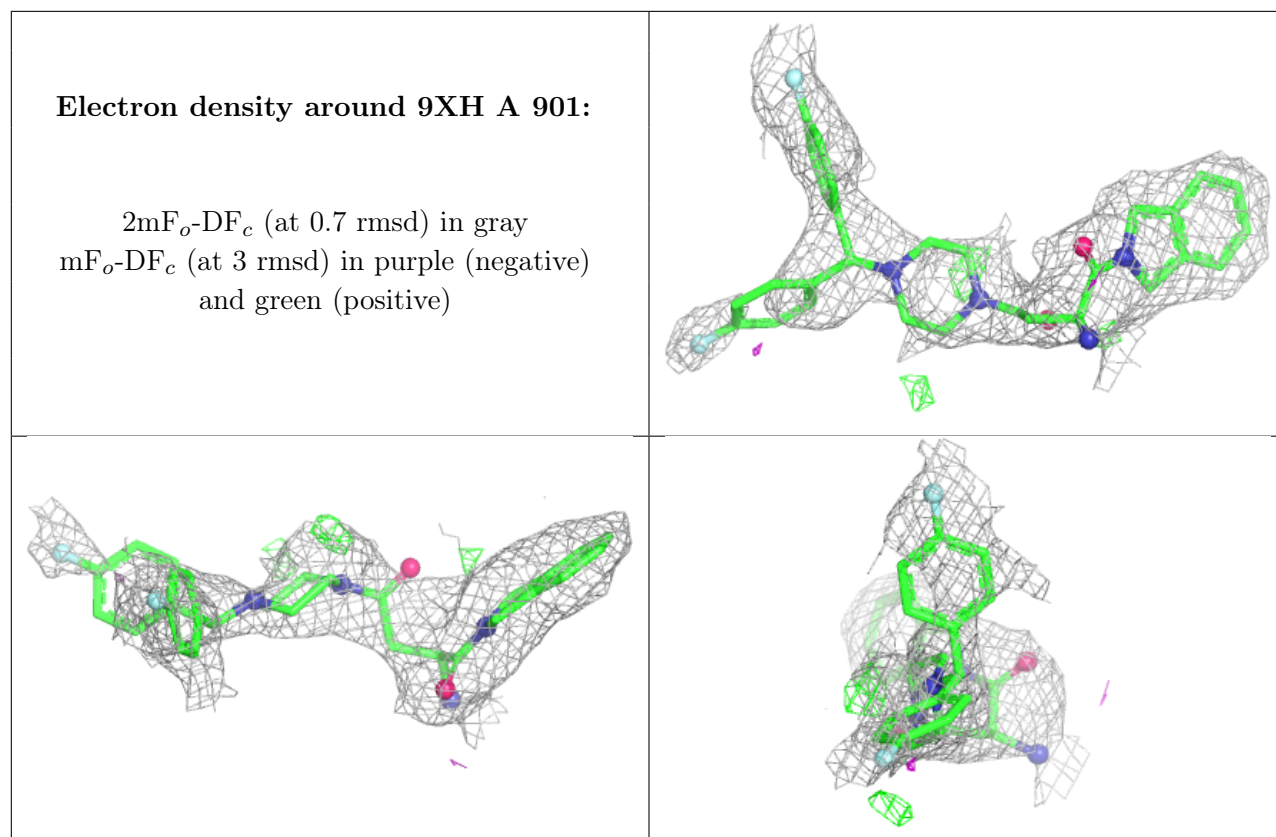
Electron density around 9XH C 901:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.