



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 04:17 PM EDT

PDB ID : 7SVL  
Title : DPP9 IN COMPLEX WITH LIGAND ICeD-2  
Authors : Lammens, A.; Hollenstein, K.; Klein, D.J.  
Deposited on : 2021-11-19  
Resolution : 2.46 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

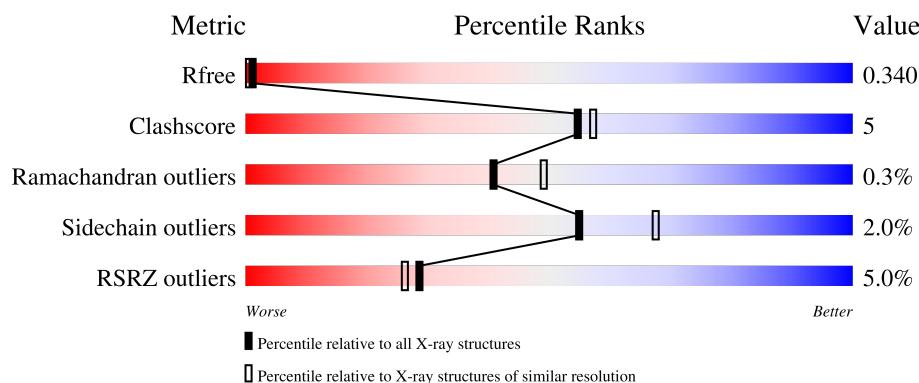
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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>4%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	B	869	<div> <div>4%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	C	869	<div> <div>6%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	D	869	<div> <div>4%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27997 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	824	Total	C	N	O	S	133	1	0
			6694	4304	1142	1220	28			
1	B	823	Total	C	N	O	S	164	0	0
			6677	4294	1140	1215	28			
1	C	830	Total	C	N	O	S	113	2	0
			6755	4346	1154	1227	28			
1	D	830	Total	C	N	O	S	104	1	0
			6744	4334	1153	1229	28			

There are 24 discrepancies between the modelled and reference sequences:

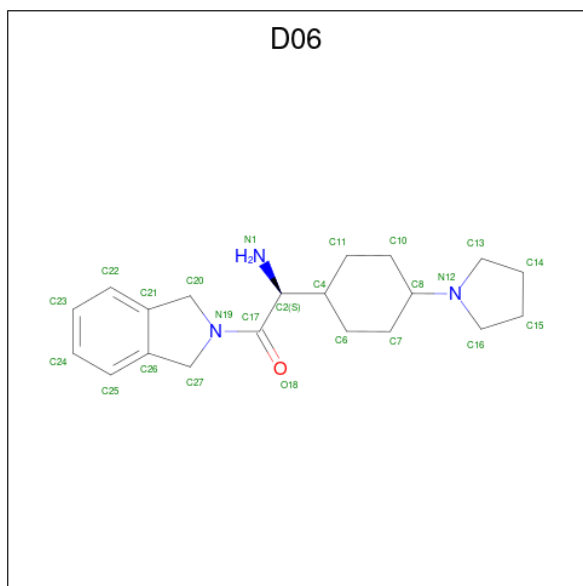
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	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 (2S)-2-amino-1-(1,3-dihydro-2H-isoindol-2-yl)-2-[(1R,4S)-4-(pyrrolidin-1-yl)cyclohexyl]ethan-1-one (three-letter code: D06) (formula: C<sub>20</sub>H<sub>29</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	20	3	1		
2	B	1	Total	C	N	O	0	0
			24	20	3	1		
2	C	1	Total	C	N	O	0	0
			24	20	3	1		
2	D	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	275	Total	O	0	0
			275	275		
3	B	223	Total	O	0	0
			223	223		
3	C	269	Total	O	0	0
			269	269		

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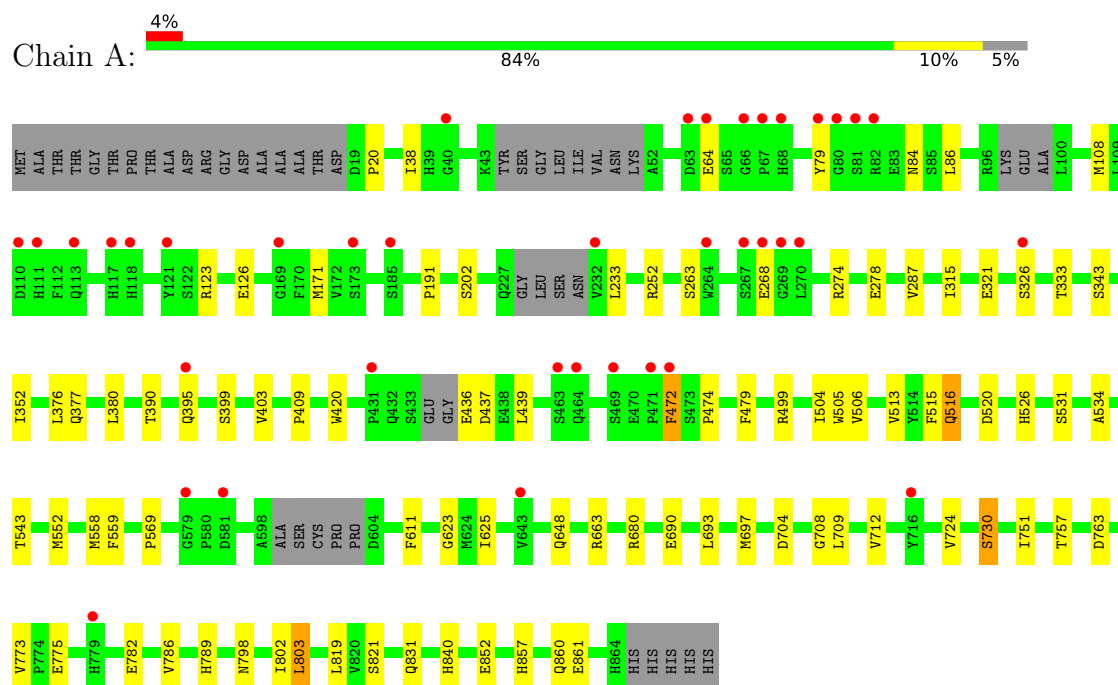
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	264	Total 264	O 264	0	0

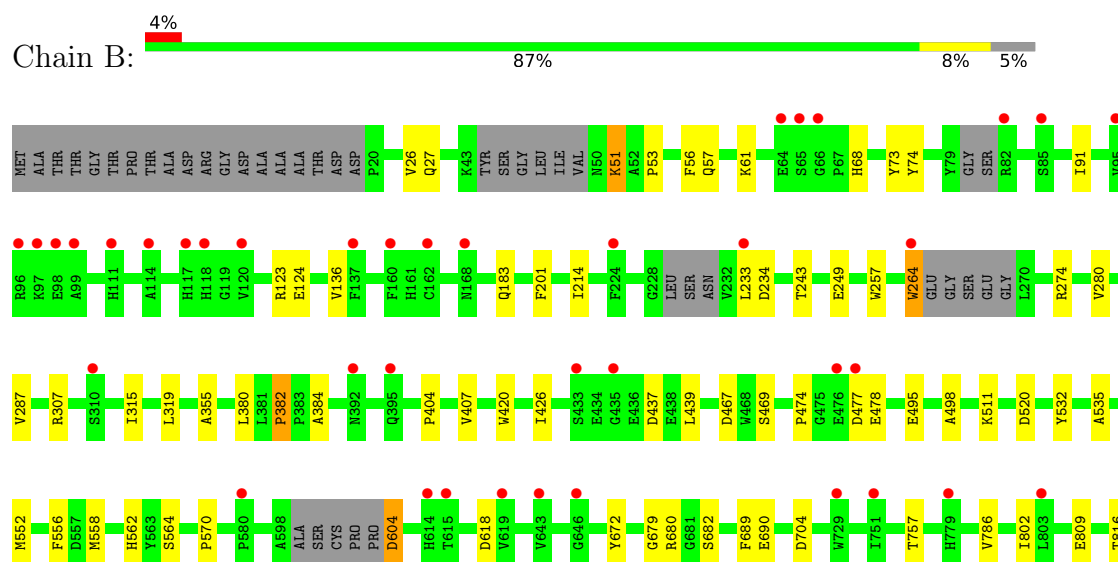
### 3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 9

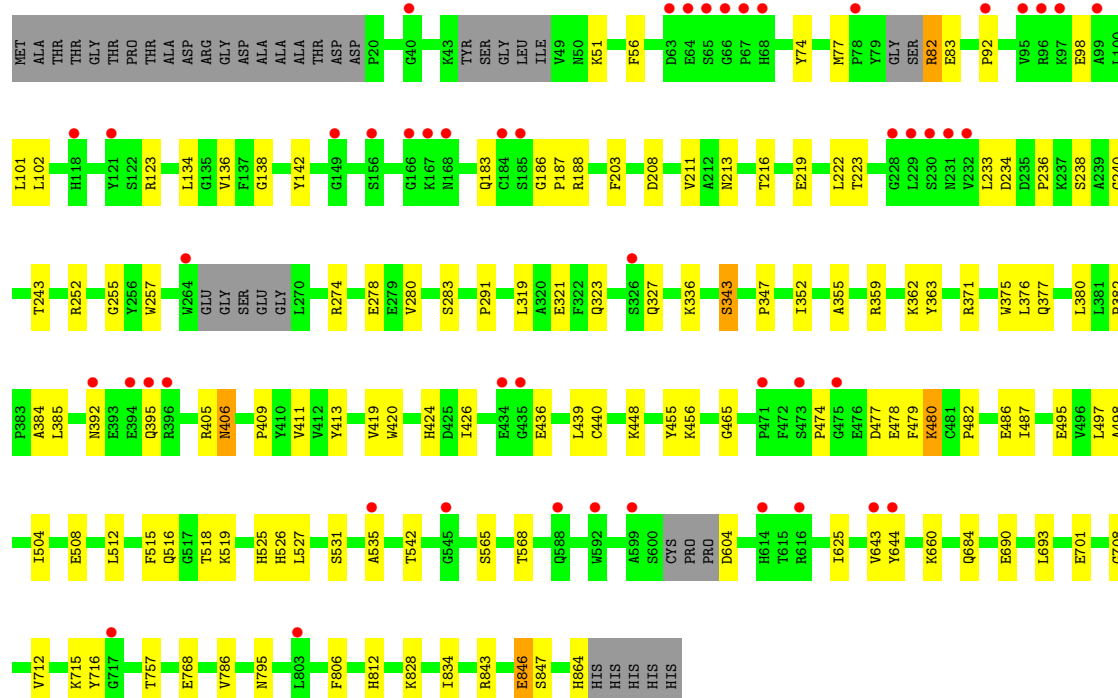
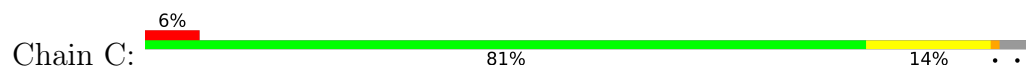


#### • Molecule 1: Dipeptidyl peptidase 9

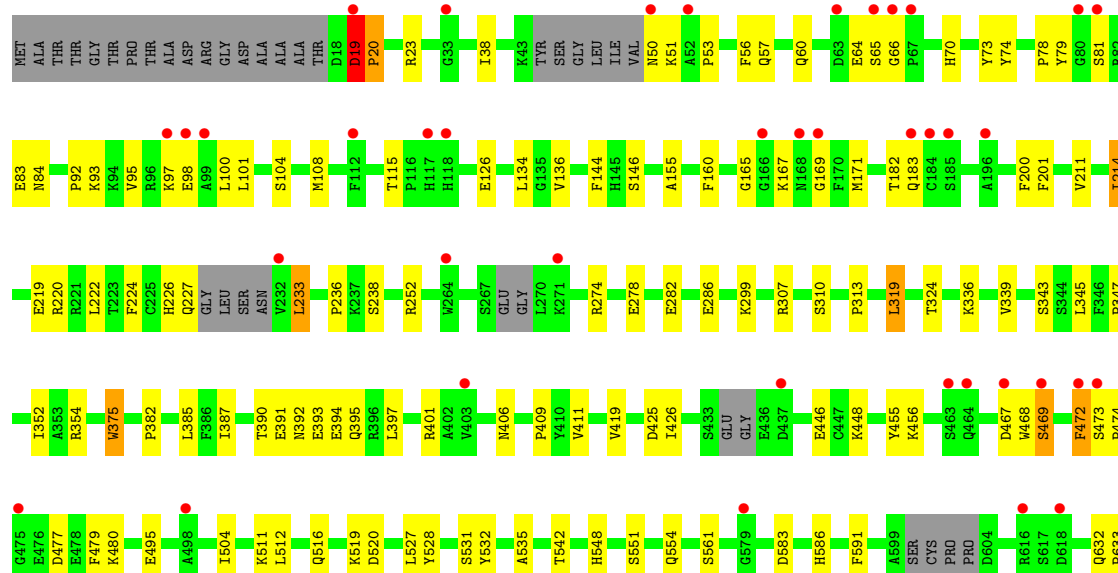
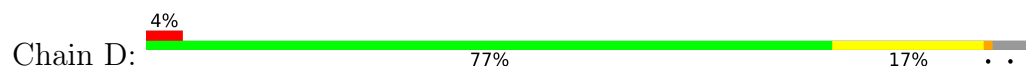


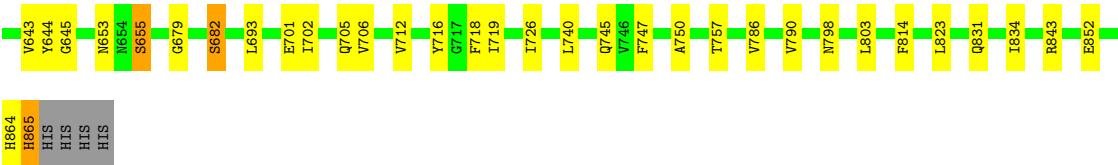


• Molecule 1: Dipeptidyl peptidase 9



• 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, $\alpha$ , $\beta$ , $\gamma$	119.72Å 117.40Å 163.69Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	157.66 – 2.46 45.99 – 2.46	Depositor EDS
% Data completeness (in resolution range)	95.6 (157.66-2.46) 95.6 (45.99-2.46)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.263 , 0.341 0.266 , 0.340	Depositor DCC
$R_{free}$ test set	1004 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 59.40 % 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 1.7758e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: D06

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	0.52	0/6895	0.71	2/9354 (0.0%)
1	B	0.53	0/6875	0.73	0/9323
1	C	0.51	0/6959	0.71	0/9442
1	D	0.50	0/6946	0.72	1/9422 (0.0%)
All	All	0.52	0/27675	0.72	3/37541 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	PRO	C-N-CD	6.81	142.70	128.40
1	D	19	ASP	C-N-CD	5.47	139.88	128.40
1	A	763	ASP	CB-CG-OD1	5.15	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	PRO	Mainchain

## 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	6694	0	6464	51	1
1	B	6677	0	6469	37	3
1	C	6755	0	6536	79	1
1	D	6744	0	6514	109	3
2	A	24	0	0	0	0
2	B	24	0	0	1	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
3	A	275	0	0	3	0
3	B	223	0	0	3	0
3	C	269	0	0	13	0
3	D	264	0	0	11	0
All	All	27997	0	25983	270	4

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 5.

All (270) 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:C:123:ARG:NH1	3:C:1001:HOH:O	1.77	1.18
1:C:252:ARG:NH1	1:C:352:ILE:O	1.99	0.95
1:A:333:THR:O	1:C:405:ARG:NH2	2.02	0.92
1:A:648:GLN:NE2	3:A:1001:HOH:O	2.03	0.92
1:C:252:ARG:NH2	1:C:278:GLU:OE2	2.03	0.91
1:C:406:ASN:ND2	3:C:1003:HOH:O	2.06	0.89
1:D:19:ASP:OD1	1:D:23:ARG:NH1	2.06	0.88
1:C:321:GLU:CD	1:C:336:LYS:NZ	2.28	0.87
1:C:321:GLU:OE2	1:C:336:LYS:NZ	2.07	0.87
1:C:274:ARG:NH1	1:C:321:GLU:OE2	2.09	0.86
1:A:252:ARG:NH1	1:A:352:ILE:O	2.09	0.85
1:C:186:GLY:O	3:C:1002:HOH:O	1.96	0.84
1:C:321:GLU:CD	1:C:336:LYS:HZ1	1.82	0.81
1:B:680:ARG:NH2	1:B:704:ASP:OD1	2.17	0.77
1:B:474:PRO:HB3	1:B:478:GLU:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ARG:NH2	1:D:278:GLU:OE2	2.18	0.76
1:C:134:LEU:O	1:C:843:ARG:NH2	2.20	0.73
1:D:477:ASP:OD1	3:D:1001:HOH:O	2.06	0.72
1:D:632:GLN:HG2	3:D:1002:HOH:O	1.88	0.72
1:D:51:LYS:HD2	1:D:136:VAL:HG21	1.70	0.72
1:D:134:LEU:O	1:D:843:ARG:NH2	2.21	0.72
1:B:420:TRP:HZ2	1:B:690:GLU:HG2	1.56	0.71
1:C:795:ASN:OD1	1:C:828:LYS:NZ	2.24	0.70
1:D:339:VAL:HG23	1:D:385:LEU:O	1.92	0.70
1:C:708:GLY:O	1:C:712:VAL:HG23	1.93	0.69
1:C:376:LEU:HD23	1:C:377:GLN:N	2.09	0.68
1:D:390:THR:HG22	1:D:392:ASN:H	1.57	0.68
1:A:252:ARG:NH2	1:A:278:GLU:OE2	2.27	0.67
1:C:477:ASP:OD1	3:C:1004:HOH:O	2.12	0.67
1:D:679:GLY:O	1:D:682:SER:OG	2.13	0.66
1:D:745:GLN:OE1	1:D:745:GLN:N	2.23	0.66
1:C:834:ILE:HD11	1:D:834:ILE:HD11	1.77	0.65
1:D:633:PRO:O	3:D:1002:HOH:O	2.13	0.65
1:D:78:PRO:HD2	1:D:81:SER:CB	2.27	0.64
1:D:645:GLY:HA2	3:D:1178:HOH:O	1.97	0.64
1:C:274:ARG:HG2	1:C:319:LEU:HD21	1.80	0.64
1:C:142:TYR:O	3:C:1005:HOH:O	2.15	0.63
1:D:252:ARG:NH1	1:D:352:ILE:O	2.30	0.63
1:A:708:GLY:O	1:A:712:VAL:HG23	1.97	0.63
1:A:390:THR:HG21	1:A:395:GLN:OE1	1.98	0.63
1:D:467:ASP:OD1	1:D:469:SER:OG	2.16	0.62
1:D:375[A]:TRP:O	1:D:375[A]:TRP:CE3	2.53	0.62
1:D:95:VAL:CG2	1:D:101:LEU:HD22	2.30	0.62
1:D:51:LYS:NZ	3:D:1008:HOH:O	2.31	0.60
1:B:274:ARG:HD3	1:B:319:LEU:HD21	1.83	0.59
1:D:84:ASN:HB2	1:D:136:VAL:CG1	2.32	0.59
1:D:92:PRO:HG2	1:D:95:VAL:CG2	2.33	0.59
1:D:307:ARG:O	1:D:310:SER:OG	2.14	0.59
1:C:375[B]:TRP:O	1:C:375[B]:TRP:CE3	2.56	0.58
1:A:499:ARG:NH2	3:A:1004:HOH:O	2.36	0.58
1:D:472:PHE:HE1	1:D:474:PRO:HB3	1.68	0.58
1:A:860:GLN:NE2	1:A:861:GLU:OE2	2.24	0.58
1:C:359:ARG:NH2	1:C:508:GLU:OE1	2.37	0.58
1:A:802:ILE:HD13	1:A:819:LEU:HD23	1.84	0.57
1:A:108:MET:HA	1:A:171:MET:HE1	1.85	0.57
1:C:51:LYS:HD2	1:C:136:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:MET:HG2	1:D:171:MET:HE3	1.86	0.57
1:A:376:LEU:HD23	1:A:377:GLN:N	2.19	0.57
1:B:843:ARG:NH2	3:B:1008:HOH:O	2.37	0.57
1:D:864:HIS:O	1:D:865:HIS:HB2	2.03	0.57
1:D:57:GLN:HB2	1:D:73:TYR:HB2	1.86	0.57
1:A:693:LEU:HD22	1:A:697:MET:HG2	1.85	0.57
1:C:362:LYS:HD3	1:C:363:TYR:CE2	2.40	0.56
1:D:702:ILE:O	1:D:706:VAL:HG23	2.06	0.55
1:B:56:PHE:CD1	1:B:74:TYR:HB3	2.41	0.55
1:B:91:ILE:HG21	1:B:558:MET:HE1	1.87	0.55
1:C:236:PRO:HG2	1:C:283:SER:OG	2.06	0.55
1:D:50:ASN:HD22	1:D:79:TYR:HA	1.71	0.55
1:B:467:ASP:OD1	1:B:469:SER:OG	2.22	0.55
1:D:50:ASN:ND2	1:D:79:TYR:HA	2.22	0.55
1:C:380:LEU:HD11	1:C:439:LEU:HD22	1.88	0.54
1:B:233:LEU:CD1	1:B:287:VAL:HG21	2.38	0.54
1:D:548:HIS:HB3	1:D:561:SER:OG	2.07	0.54
1:C:375[B]:TRP:O	1:C:375[B]:TRP:HE3	1.90	0.54
1:C:497:LEU:HD11	1:C:525:HIS:CD2	2.42	0.54
1:D:78:PRO:HD2	1:D:81:SER:HB3	1.89	0.54
1:D:233:LEU:HD12	1:D:233:LEU:O	2.07	0.54
1:D:527:LEU:HB3	1:D:542:THR:HG23	1.90	0.54
1:A:472:PHE:CZ	1:A:474:PRO:HB3	2.42	0.54
1:B:53:PRO:HB3	1:B:74:TYR:CD2	2.42	0.54
1:C:512:LEU:HD23	1:C:531:SER:HA	1.89	0.54
1:B:380:LEU:HD11	1:B:439:LEU:HD22	1.89	0.53
1:D:233:LEU:HD12	1:D:233:LEU:C	2.28	0.53
1:D:375[A]:TRP:O	1:D:375[A]:TRP:HE3	1.89	0.53
1:D:425:ASP:OD2	3:D:1004:HOH:O	2.19	0.53
1:B:51:LYS:HD2	1:B:136:VAL:HG21	1.90	0.53
1:D:693:LEU:HD22	1:D:701:GLU:OE2	2.09	0.53
1:C:504:ILE:HG22	1:C:515:PHE:HB3	1.91	0.52
1:D:183:GLN:HG2	1:D:219:GLU:OE1	2.09	0.52
1:B:404:PRO:HD2	1:D:395:GLN:NE2	2.24	0.52
1:C:456:LYS:HB3	1:C:487:ILE:HG12	1.92	0.52
1:B:280:VAL:HG22	1:B:315:ILE:HG22	1.92	0.52
1:C:474:PRO:HB3	1:C:478:GLU:HG2	1.92	0.52
1:D:224:PHE:O	3:D:1005:HOH:O	2.19	0.52
1:D:757:THR:HA	1:D:786:VAL:CG2	2.40	0.52
1:A:505:TRP:CD1	1:A:552:MET:HB3	2.45	0.52
1:C:188:ARG:HG2	1:C:203:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:O	1:A:403:VAL:HG23	2.10	0.51
1:C:376:LEU:HD23	1:C:376:LEU:C	2.29	0.51
1:A:506:VAL:HG22	1:A:513:VAL:HG23	1.93	0.51
1:D:201:PHE:CD1	1:D:214:ILE:HG23	2.46	0.51
1:D:19:ASP:H	1:D:20:PRO:HD3	1.76	0.51
1:C:240:GLY:HA2	1:C:255:GLY:O	2.11	0.51
1:D:343:SER:O	1:D:347:PRO:HA	2.10	0.50
1:D:701:GLU:O	1:D:705:GLN:HG2	2.11	0.50
1:A:680:ARG:NH2	1:A:704:ASP:OD1	2.39	0.50
1:C:343:SER:O	1:C:347:PRO:HA	2.11	0.50
1:B:274:ARG:NH2	1:D:394:GLU:OE1	2.44	0.50
1:D:339:VAL:HG11	1:D:468:TRP:HB3	1.94	0.50
1:B:552:MET:HE1	1:B:556:PHE:HA	1.94	0.50
1:D:653:ASN:OD1	1:D:655:SER:OG	2.30	0.50
1:D:274:ARG:HG2	1:D:319:LEU:CD2	2.41	0.50
1:D:382:PRO:O	1:D:385:LEU:HB3	2.12	0.50
1:A:380:LEU:HD11	1:A:439:LEU:HD22	1.94	0.49
1:D:511:LYS:HA	1:D:532:TYR:CE2	2.47	0.49
1:A:516:GLN:HA	1:A:526:HIS:O	2.12	0.49
1:C:424:HIS:ND1	3:C:1012:HOH:O	2.32	0.49
1:D:83:GLU:OE1	1:D:115:THR:OG1	2.15	0.49
1:D:512:LEU:HD23	1:D:531:SER:HA	1.95	0.49
1:D:643:VAL:HG22	1:D:644:TYR:N	2.27	0.49
1:A:552:MET:CE	1:A:559:PHE:HB3	2.43	0.49
1:D:448:LYS:HD3	1:D:455:TYR:CE2	2.47	0.49
1:D:391:GLU:H	1:D:391:GLU:CD	2.16	0.48
1:C:519:LYS:HE2	3:C:1128:HOH:O	2.14	0.48
1:C:757:THR:HA	1:C:786:VAL:HG22	1.96	0.48
1:D:56:PHE:CD1	1:D:74:TYR:HB3	2.48	0.48
1:D:716:TYR:HB3	1:D:718:PHE:CE2	2.49	0.48
1:D:740:LEU:HD22	1:D:750:ALA:HB3	1.95	0.48
1:D:95:VAL:HG21	1:D:101:LEU:CD2	2.44	0.48
1:B:384:ALA:HB1	1:D:395:GLN:NE2	2.29	0.48
1:C:812:HIS:HB3	3:C:1192:HOH:O	2.13	0.48
1:D:84:ASN:HB2	1:D:136:VAL:HG12	1.95	0.48
1:A:505:TRP:CG	1:A:552:MET:HB3	2.49	0.48
1:B:426:ILE:HD12	1:B:498:ALA:HB2	1.95	0.48
1:D:95:VAL:HG21	1:D:101:LEU:HD22	1.94	0.48
1:D:456:LYS:HE2	3:D:1071:HOH:O	2.14	0.47
1:D:814:PHE:HA	3:D:1116:HOH:O	2.14	0.47
1:A:274:ARG:HG2	1:A:321:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:TRP:N	1:B:264:TRP:CD1	2.82	0.47
1:D:282:GLU:HG2	1:D:313:PRO:HB3	1.97	0.47
1:A:773:VAL:HG12	1:A:775:GLU:CD	2.35	0.47
1:C:321:GLU:CD	1:C:336:LYS:HZ2	2.00	0.47
1:D:95:VAL:HG22	1:D:101:LEU:HD22	1.95	0.47
1:D:97:LYS:O	1:D:98:GLU:HB2	2.15	0.47
1:D:519:LYS:HB3	1:D:528:TYR:CZ	2.49	0.47
1:A:611:PHE:CE1	1:A:623:GLY:HA3	2.50	0.47
1:D:236:PRO:HG3	3:D:1132:HOH:O	2.15	0.47
1:C:257:TRP:CZ2	1:C:355:ALA:HB3	2.49	0.47
1:D:472:PHE:CE1	1:D:474:PRO:HB3	2.48	0.47
1:B:382:PRO:HG2	1:B:407:VAL:HG13	1.95	0.47
1:D:211:VAL:HG13	1:D:222:LEU:CD1	2.45	0.47
1:A:504:ILE:HG22	1:A:515:PHE:HB3	1.95	0.46
1:A:798:ASN:OD1	1:A:831:GLN:NE2	2.48	0.46
1:B:679:GLY:O	1:B:682:SER:OG	2.21	0.46
1:B:249:GLU:OE1	2:B:901:D06:N1	2.48	0.46
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.51	0.46
1:A:625:ILE:HD12	1:A:712:VAL:HG11	1.98	0.46
1:D:64:GLU:O	1:D:93:LYS:NZ	2.49	0.46
1:C:465:GLY:N	3:C:1013:HOH:O	2.40	0.46
1:D:726:ILE:HB	1:D:747:PHE:CD1	2.51	0.46
1:A:409:PRO:HD2	1:A:479:PHE:CE1	2.51	0.46
1:A:436:GLU:HG2	1:A:437:ASP:H	1.81	0.46
1:B:511:LYS:HA	1:B:532:TYR:CE2	2.51	0.46
1:D:211:VAL:HG13	1:D:222:LEU:HD12	1.98	0.46
1:A:857:HIS:CE1	1:A:861:GLU:HG3	2.51	0.45
1:C:77:MET:HE2	1:C:82:ARG:N	2.31	0.45
1:C:327:GLN:N	1:C:327:GLN:OE1	2.49	0.45
1:D:57:GLN:NE2	1:D:144:PHE:CD2	2.84	0.45
1:D:319:LEU:O	1:D:336:LYS:HB2	2.16	0.45
1:C:420:TRP:HZ2	1:C:690:GLU:HG2	1.82	0.45
1:D:345:LEU:HD21	1:D:468:TRP:CZ3	2.52	0.45
1:D:409:PRO:HD2	1:D:479:PHE:CE1	2.52	0.45
1:C:183:GLN:HG2	1:C:219:GLU:OE1	2.17	0.45
1:A:395:GLN:NE2	1:C:384:ALA:HB1	2.32	0.45
1:B:124:GLU:O	3:B:1002:HOH:O	2.20	0.45
1:C:409:PRO:HD2	1:C:479:PHE:CE1	2.51	0.45
1:B:680:ARG:HA	1:B:689:PHE:CE1	2.52	0.44
1:C:243:THR:HG21	1:C:280:VAL:HG11	1.98	0.44
1:B:61:LYS:HE3	1:B:68:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:LYS:HE3	1:C:716:TYR:CZ	2.52	0.44
1:B:257:TRP:CZ2	1:B:355:ALA:HB3	2.53	0.44
1:C:518:THR:HA	3:C:1028:HOH:O	2.17	0.44
3:C:1060:HOH:O	1:D:299:LYS:HE3	2.16	0.44
1:A:730:SER:OG	1:A:840:HIS:NE2	2.38	0.44
1:B:802:ILE:HG21	1:B:816:THR:HG23	1.99	0.44
1:D:57:GLN:N	1:D:73:TYR:O	2.48	0.44
1:C:213:ASN:OD1	1:C:216:THR:N	2.33	0.44
1:C:516:GLN:HA	1:C:526:HIS:O	2.16	0.44
1:B:233:LEU:HD12	1:B:287:VAL:HG21	1.99	0.44
1:C:291:PRO:HG2	1:C:806:PHE:CE2	2.53	0.44
1:A:757:THR:HA	1:A:786:VAL:HG22	1.99	0.44
1:D:51:LYS:HD2	1:D:136:VAL:CG2	2.44	0.44
1:A:782:GLU:O	1:A:789:HIS:NE2	2.43	0.43
1:D:712:VAL:HG12	1:D:719:ILE:HG13	1.99	0.43
1:B:26:VAL:HG21	1:B:672:TYR:CZ	2.54	0.43
1:A:552:MET:HE3	1:A:558:MET:O	2.18	0.43
1:C:413:TYR:OH	1:C:486:GLU:OE2	2.21	0.43
1:C:846:GLU:HG2	1:C:847:SER:N	2.33	0.43
1:D:411:VAL:HG23	1:D:479:PHE:HB2	2.00	0.43
1:A:751:ILE:CG2	1:A:803:LEU:HD11	2.48	0.43
1:C:382:PRO:O	1:C:385:LEU:HB3	2.18	0.43
1:C:527:LEU:HB3	1:C:542:THR:HG23	2.01	0.43
1:D:426:ILE:HD13	1:D:504:ILE:HG23	2.00	0.43
1:C:92:PRO:HG3	1:C:101:LEU:CD2	2.49	0.43
1:C:660:LYS:O	1:C:660:LYS:HG3	2.17	0.43
1:D:679:GLY:HA3	3:D:1044:HOH:O	2.18	0.43
1:A:775:GLU:OE1	1:A:775:GLU:N	2.43	0.43
1:C:257:TRP:CE2	1:C:355:ALA:HB3	2.53	0.43
1:C:625:ILE:HD12	1:C:712:VAL:HG11	2.00	0.43
1:D:446:GLU:O	1:D:446:GLU:HG2	2.18	0.43
1:D:200:PHE:CZ	1:D:324:THR:HG21	2.54	0.43
1:A:86:LEU:HB3	1:A:108:MET:HE3	2.01	0.43
1:A:123:ARG:NE	1:A:126:GLU:OE1	2.51	0.42
1:A:531:SER:HB3	1:A:534:ALA:O	2.19	0.42
1:D:354:ARG:NH2	1:D:425:ASP:OD1	2.52	0.42
1:A:611:PHE:CZ	1:A:623:GLY:HA3	2.54	0.42
1:C:448:LYS:HD3	1:C:455:TYR:CE2	2.55	0.42
1:D:393:GLU:HA	1:D:393:GLU:OE1	2.20	0.42
1:A:315:ILE:HD12	1:A:352:ILE:HG13	2.00	0.42
1:C:56:PHE:CD1	1:C:74:TYR:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLU:HG3	1:C:138:GLY:HA3	2.00	0.42
1:D:60:GLN:HG2	1:D:70:HIS:CD2	2.54	0.42
1:D:165:GLY:N	1:D:169:GLY:O	2.46	0.42
1:A:709:LEU:HD21	1:A:724:VAL:HG11	2.01	0.42
1:D:53:PRO:HB2	1:D:56:PHE:CZ	2.55	0.42
1:D:401:ARG:HG2	1:D:469:SER:HB3	1.99	0.42
1:C:208:ASP:OD1	1:C:223:THR:OG1	2.27	0.42
1:C:693:LEU:HD22	1:C:701:GLU:OE2	2.19	0.42
1:D:554:GLN:OE1	1:D:554:GLN:N	2.50	0.42
1:A:233:LEU:CD2	1:A:287:VAL:HG21	2.50	0.42
1:A:420:TRP:HZ2	1:A:690:GLU:HG2	1.85	0.42
1:B:307:ARG:O	3:B:1001:HOH:O	2.21	0.42
1:C:392:ASN:HD22	1:C:395:GLN:CG	2.33	0.42
1:C:426:ILE:HD12	1:C:498:ALA:HB2	2.01	0.42
1:C:643:VAL:HG22	1:C:644:TYR:N	2.35	0.42
1:D:397:LEU:O	1:D:401:ARG:HG3	2.19	0.42
1:A:191:PRO:HA	1:A:202:SER:O	2.19	0.41
1:C:371:ARG:NH2	1:C:768:GLU:OE2	2.46	0.41
1:D:286:GLU:OE1	1:D:307:ARG:NH2	2.53	0.41
1:C:684:GLN:HG3	3:C:1090:HOH:O	2.20	0.41
1:C:257:TRP:CH2	1:C:355:ALA:HB3	2.55	0.41
1:D:286:GLU:CD	1:D:307:ARG:HE	2.23	0.41
1:D:583:ASP:OD2	1:D:586:HIS:HB2	2.20	0.41
1:B:564:SER:HB3	1:B:570:PRO:HA	2.03	0.41
1:D:339:VAL:HG22	1:D:387:ILE:HG23	2.03	0.41
1:D:643:VAL:CG2	1:D:644:TYR:N	2.83	0.41
1:A:552:MET:HE3	1:A:559:PHE:HB3	2.03	0.41
1:C:440:CYS:SG	1:C:456:LYS:HE2	2.60	0.41
1:D:155:ALA:HB3	1:D:160:PHE:CD1	2.56	0.41
1:A:663:ARG:NH2	3:A:1019:HOH:O	2.52	0.41
1:B:243:THR:HG21	1:B:280:VAL:HG11	2.02	0.41
1:C:211:VAL:HG13	1:C:222:LEU:CD1	2.51	0.41
1:C:643:VAL:CG2	1:C:644:TYR:N	2.84	0.41
1:D:757:THR:HA	1:D:786:VAL:HG22	2.02	0.41
1:C:323:GLN:NE2	3:C:1038:HOH:O	2.54	0.41
1:C:565:SER:OG	1:C:568:THR:OG1	2.19	0.41
1:D:38:ILE:HD12	1:D:852:GLU:HB3	2.03	0.41
1:D:798:ASN:ND2	1:D:831:GLN:OE1	2.54	0.41
1:B:757:THR:HA	1:B:786:VAL:HG22	2.03	0.40
1:C:319:LEU:O	1:C:336:LYS:HB2	2.21	0.40
1:B:57:GLN:HB2	1:B:73:TYR:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:GLU:OE1	1:B:809:GLU:N	2.43	0.40
1:A:38:ILE:HD12	1:A:852:GLU:HB3	2.02	0.40
1:A:472:PHE:CD1	1:A:472:PHE:C	2.94	0.40
1:D:66:GLY:O	1:D:93:LYS:NZ	2.36	0.40
1:D:790:VAL:HG11	1:D:823:LEU:HA	2.03	0.40
1:A:233:LEU:HD21	1:A:287:VAL:HG21	2.03	0.40
1:D:226:HIS:C	1:D:227:GLN:HG3	2.40	0.40
1:C:411:VAL:HB	1:C:480:LYS:HA	2.03	0.40
1:D:182:THR:OG1	1:D:219:GLU:OE2	2.30	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:ASP:OD1	1:D:167:LYS:O[2_546]	2.02	0.18
1:A:64:GLU:CG	1:B:183:GLN:O[2_456]	2.13	0.07
1:B:27:GLN:NE2	1:D:65:SER:OG[2_546]	2.15	0.05
1:C:98:GLU:OE1	1:D:591:PHE:N[2_547]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	813/869 (94%)	785 (97%)	27 (3%)	1 (0%)	51	64
1	B	811/869 (93%)	774 (95%)	35 (4%)	2 (0%)	47	57
1	C	822/869 (95%)	793 (96%)	26 (3%)	3 (0%)	34	41
1	D	819/869 (94%)	790 (96%)	24 (3%)	5 (1%)	25	29
All	All	3265/3476 (94%)	3142 (96%)	112 (3%)	11 (0%)	41	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	ALA
1	A	20	PRO
1	B	51	LYS
1	C	480	LYS
1	C	535	ALA
1	D	480	LYS
1	D	535	ALA
1	D	19	ASP
1	D	20	PRO
1	C	419	VAL
1	D	419	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	727/759 (96%)	714 (98%)	13 (2%)	59	71
1	B	725/759 (96%)	715 (99%)	10 (1%)	67	77
1	C	733/759 (97%)	719 (98%)	14 (2%)	57	69
1	D	732/759 (96%)	709 (97%)	23 (3%)	40	52
All	All	2917/3036 (96%)	2857 (98%)	60 (2%)	55	66

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	TYR
1	A	84	ASN
1	A	263	SER
1	A	268	GLU
1	A	326	SER
1	A	343	SER
1	A	472	PHE
1	A	516	GLN
1	A	520	ASP
1	A	543	THR
1	A	730	SER

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Mol	Chain	Res	Type
1	A	803	LEU
1	A	821	SER
1	B	123	ARG
1	B	234	ASP
1	B	264	TRP
1	B	437	ASP
1	B	477	ASP
1	B	495	GLU
1	B	520	ASP
1	B	562	HIS
1	B	604	ASP
1	B	618	ASP
1	C	82	ARG
1	C	102	LEU
1	C	187	PRO
1	C	233	LEU
1	C	234	ASP
1	C	238	SER
1	C	343	SER
1	C	406	ASN
1	C	436	GLU
1	C	482	PRO
1	C	495	GLU
1	C	604	ASP
1	C	846	GLU
1	C	864	HIS
1	D	100	LEU
1	D	104	SER
1	D	126	GLU
1	D	146	SER
1	D	214	ILE
1	D	220	ARG
1	D	233	LEU
1	D	238	SER
1	D	319	LEU
1	D	375[A]	TRP
1	D	375[B]	TRP
1	D	406	ASN
1	D	469	SER
1	D	472	PHE
1	D	473	SER
1	D	495	GLU

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Mol	Chain	Res	Type
1	D	516	GLN
1	D	520	ASP
1	D	551	SER
1	D	655	SER
1	D	682	SER
1	D	803	LEU
1	D	865	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	798	ASN
1	A	831	GLN
1	B	312	ASN
1	C	60	GLN
1	C	111	HIS
1	C	392	ASN
1	C	555	ASN
1	D	57	GLN

### 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 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	D06	D	901	-	27,27,27	0.87	1 (3%)	33,38,38	2.81	7 (21%)
2	D06	A	901	-	27,27,27	0.95	1 (3%)	33,38,38	3.05	5 (15%)
2	D06	C	901	-	27,27,27	0.86	1 (3%)	33,38,38	2.80	6 (18%)
2	D06	B	901	-	27,27,27	0.64	0	33,38,38	3.01	7 (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	D06	D	901	-	-	0/16/41/41	0/4/4/4
2	D06	A	901	-	-	0/16/41/41	0/4/4/4
2	D06	C	901	-	-	0/16/41/41	0/4/4/4
2	D06	B	901	-	-	0/16/41/41	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	D06	C2-C17	-3.50	1.49	1.53
2	D	901	D06	C2-C17	-2.46	1.50	1.53
2	C	901	D06	C2-C17	-2.12	1.51	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	D06	C26-C27-N19	11.47	107.88	102.46
2	A	901	D06	C26-C27-N19	11.35	107.83	102.46
2	D	901	D06	C26-C27-N19	11.14	107.73	102.46
2	B	901	D06	C21-C20-N19	10.93	107.63	102.46
2	A	901	D06	C21-C20-N19	10.69	107.52	102.46
2	B	901	D06	C26-C27-N19	10.13	107.25	102.46
2	C	901	D06	C21-C20-N19	9.09	106.76	102.46
2	D	901	D06	C21-C20-N19	9.00	106.72	102.46
2	B	901	D06	C11-C4-C2	-5.03	105.15	111.86
2	A	901	D06	C17-C2-N1	-4.25	103.73	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	D06	O18-C17-N19	-3.28	117.82	121.67
2	D	901	D06	C27-C26-C21	-2.71	108.39	110.53
2	B	901	D06	C20-C21-C26	-2.65	108.43	110.53
2	B	901	D06	C10-C8-N12	-2.63	105.69	112.52
2	A	901	D06	C27-C26-C21	-2.60	108.47	110.53
2	C	901	D06	C27-C26-C21	-2.58	108.48	110.53
2	D	901	D06	C17-C2-N1	-2.51	106.39	110.22
2	D	901	D06	C10-C11-C4	-2.42	106.80	112.24
2	A	901	D06	C20-C21-C26	-2.39	108.64	110.53
2	C	901	D06	C13-N12-C8	-2.35	111.85	114.12
2	C	901	D06	C10-C11-C4	-2.23	107.21	112.24
2	D	901	D06	C13-N12-C8	-2.17	112.02	114.12
2	B	901	D06	C6-C7-C8	2.17	114.31	109.81
2	C	901	D06	C7-C6-C4	-2.06	107.61	112.24
2	D	901	D06	C7-C8-N12	-2.05	107.19	112.52

There are no chirality outliers.

There are no torsion outliers.

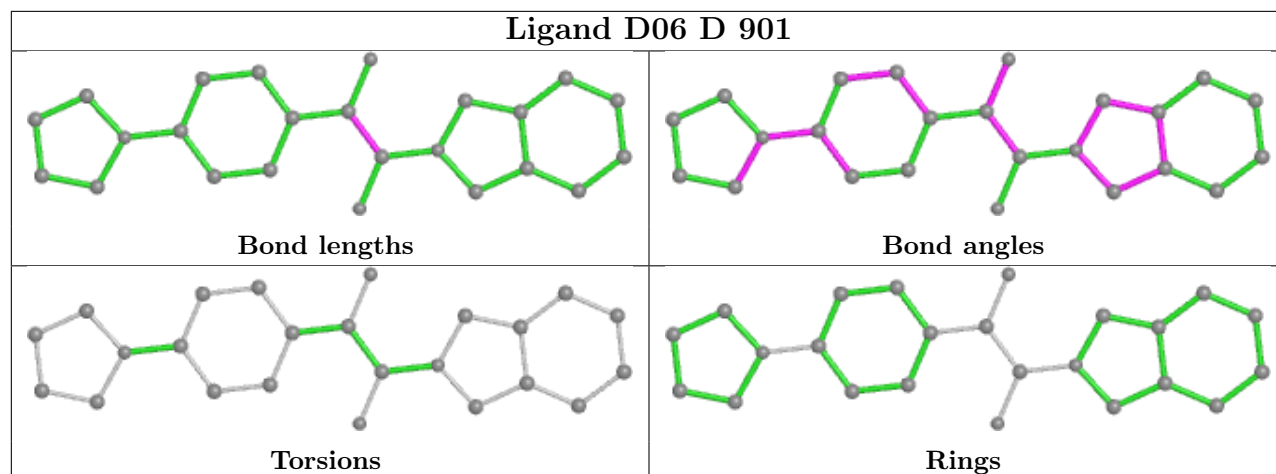
There are no ring outliers.

1 monomer is involved in 1 short contact:

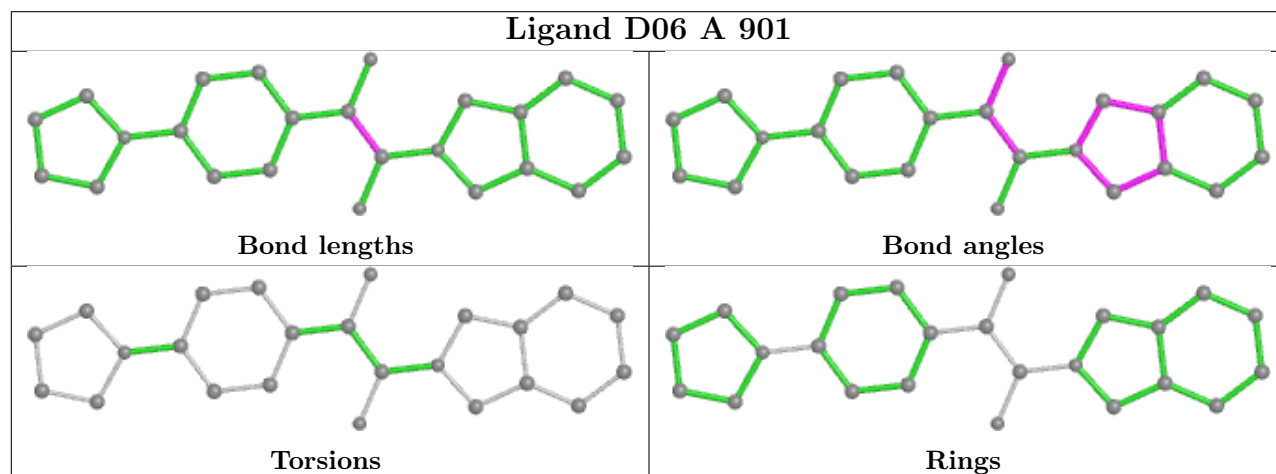
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	D06	1	0

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.

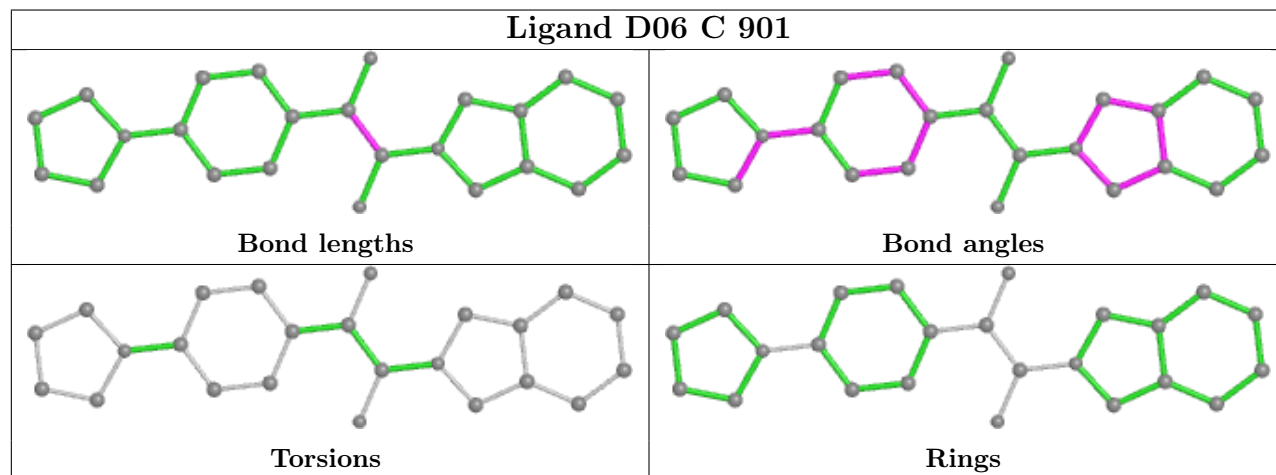
## Ligand D06 D 901



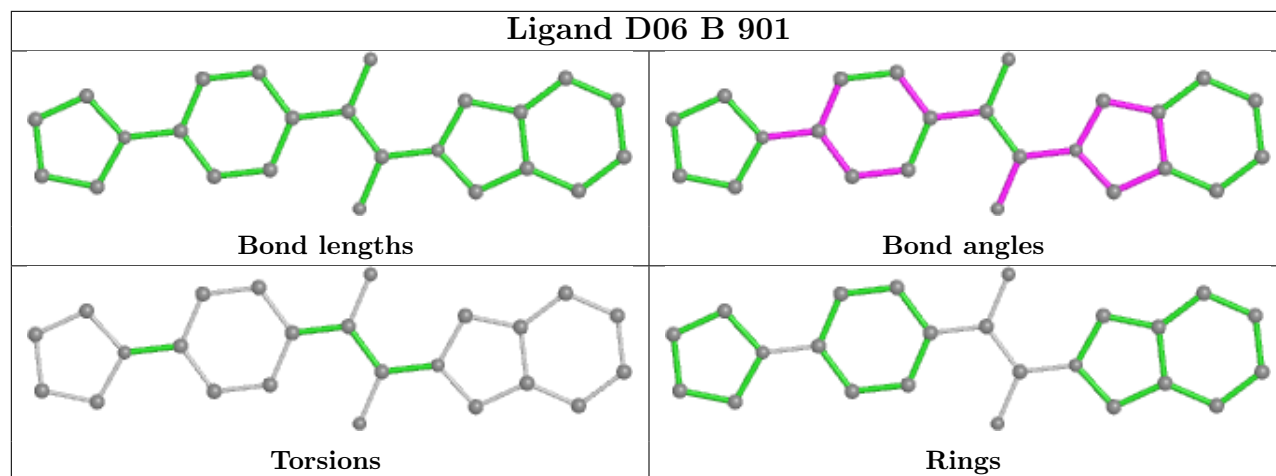
## Ligand D06 A 901



## Ligand D06 C 901







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	824/869 (94%)	0.35	38 (4%)	32	30	15, 38, 73, 111	54 (6%)
1	B	823/869 (94%)	0.41	39 (4%)	31	29	15, 38, 72, 110	58 (7%)
1	C	830/869 (95%)	0.39	49 (5%)	22	19	11, 36, 73, 111	42 (5%)
1	D	830/869 (95%)	0.32	39 (4%)	31	29	14, 36, 74, 121	39 (4%)
All	All	3307/3476 (95%)	0.37	165 (4%)	28	26	11, 37, 73, 121	193 (5%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	GLU	7.2
1	D	98	GLU	7.1
1	C	95	VAL	6.5
1	C	231	ASN	5.6
1	C	230	SER	5.6
1	C	96	ARG	5.2
1	A	395	GLN	5.0
1	C	66	GLY	5.0
1	C	229	LEU	4.8
1	D	19	ASP	4.7
1	B	476	GLU	4.7
1	A	169	GLY	4.7
1	A	472	PHE	4.7
1	B	435	GLY	4.5
1	A	264	TRP	4.4
1	C	232	VAL	4.4
1	D	118	HIS	4.4
1	A	81	SER	4.4
1	C	599	ALA	4.3
1	C	63	ASP	4.2
1	A	118	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	228	GLY	4.1
1	B	118	HIS	4.1
1	A	269	GLY	4.1
1	D	81	SER	3.8
1	C	99	ALA	3.8
1	C	97	LYS	3.7
1	B	111	HIS	3.7
1	A	471	PRO	3.6
1	D	184	CYS	3.6
1	A	80	GLY	3.6
1	C	65	SER	3.6
1	C	185	SER	3.5
1	D	80	GLY	3.5
1	C	118	HIS	3.5
1	D	66	GLY	3.4
1	D	472	PHE	3.4
1	C	717	GLY	3.3
1	C	473	SER	3.3
1	C	68	HIS	3.3
1	C	184	CYS	3.3
1	B	619	VAL	3.3
1	B	66	GLY	3.2
1	D	65	SER	3.2
1	B	117	HIS	3.2
1	A	270	LEU	3.2
1	B	98	GLU	3.1
1	D	97	LYS	3.1
1	A	79	TYR	3.0
1	A	111	HIS	3.0
1	C	475	GLY	3.0
1	A	113	GLN	3.0
1	D	473	SER	3.0
1	A	232	VAL	3.0
1	A	779	HIS	3.0
1	A	469	SER	2.9
1	D	169	GLY	2.9
1	D	475	GLY	2.9
1	B	96	ARG	2.9
1	D	168	ASN	2.9
1	D	196	ALA	2.9
1	B	114	ALA	2.9
1	B	97	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	173	SER	2.8
1	A	63	ASP	2.8
1	B	168	ASN	2.8
1	C	545	GLY	2.8
1	B	120	VAL	2.8
1	C	264	TRP	2.8
1	B	233	LEU	2.8
1	A	463	SER	2.7
1	B	65	SER	2.7
1	B	160	PHE	2.7
1	D	264	TRP	2.7
1	B	433	SER	2.6
1	C	592	TRP	2.6
1	A	579	GLY	2.6
1	D	579	GLY	2.6
1	C	616	ARG	2.6
1	C	64	GLU	2.6
1	C	394	GLU	2.6
1	D	112	PHE	2.5
1	A	68	HIS	2.5
1	B	64	GLU	2.5
1	D	50	ASN	2.5
1	C	166	GLY	2.5
1	C	435	GLY	2.5
1	D	52	ALA	2.5
1	B	392	ASN	2.5
1	B	779	HIS	2.5
1	A	64	GLU	2.5
1	C	395	GLN	2.5
1	A	185	SER	2.5
1	C	78	PRO	2.5
1	A	66	GLY	2.5
1	A	267	SER	2.4
1	B	264	TRP	2.4
1	A	67	PRO	2.4
1	B	646	GLY	2.4
1	C	392	ASN	2.4
1	D	166	GLY	2.4
1	C	643	VAL	2.4
1	C	535	ALA	2.4
1	C	121	TYR	2.4
1	D	498	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	VAL	2.4
1	D	183	GLN	2.4
1	D	464	GLN	2.4
1	B	395	GLN	2.4
1	A	121	TYR	2.4
1	C	644	TYR	2.4
1	D	467	ASP	2.4
1	D	403	VAL	2.3
1	B	82	ARG	2.3
1	D	67	PRO	2.3
1	B	224	PHE	2.3
1	D	437	ASP	2.3
1	C	167	LYS	2.3
1	B	729	TRP	2.3
1	B	85	SER	2.3
1	C	67	PRO	2.2
1	C	92	PRO	2.2
1	B	310	SER	2.2
1	D	63	ASP	2.2
1	A	117	HIS	2.2
1	D	271	LYS	2.2
1	C	326	SER	2.2
1	B	615	THR	2.2
1	B	162	CYS	2.2
1	B	99	ALA	2.2
1	A	268	GLU	2.2
1	B	137	PHE	2.2
1	A	40	GLY	2.2
1	A	581	ASP	2.2
1	C	168	ASN	2.2
1	C	149	GLY	2.2
1	B	803	LEU	2.2
1	B	614	HIS	2.2
1	D	185	SER	2.2
1	B	477	ASP	2.1
1	A	643	VAL	2.1
1	D	463	SER	2.1
1	A	110	ASP	2.1
1	C	471	PRO	2.1
1	D	469	SER	2.1
1	B	643	VAL	2.1
1	D	99	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	396	ARG	2.1
1	D	618	ASP	2.1
1	C	40	GLY	2.1
1	D	33	GLY	2.1
1	D	117	HIS	2.1
1	A	464	GLN	2.1
1	A	431	PRO	2.0
1	A	326	SER	2.0
1	B	751	ILE	2.0
1	C	156	SER	2.0
1	C	803	LEU	2.0
1	D	616	ARG	2.0
1	B	580	PRO	2.0
1	C	614	HIS	2.0
1	C	588	GLN	2.0
1	A	82	ARG	2.0
1	A	716	TYR	2.0
1	D	232	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

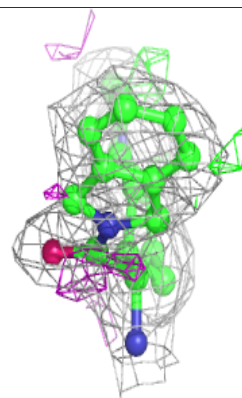
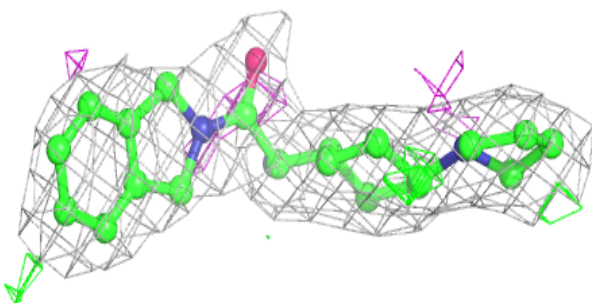
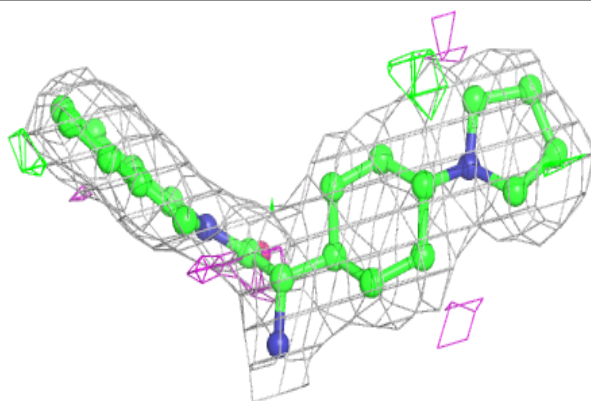
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	D06	B	901	24/24	0.88	0.27	21,28,35,41	0
2	D06	D	901	24/24	0.90	0.27	17,28,37,42	0
2	D06	C	901	24/24	0.92	0.26	12,24,30,32	0
2	D06	A	901	24/24	0.93	0.23	22,27,33,33	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.

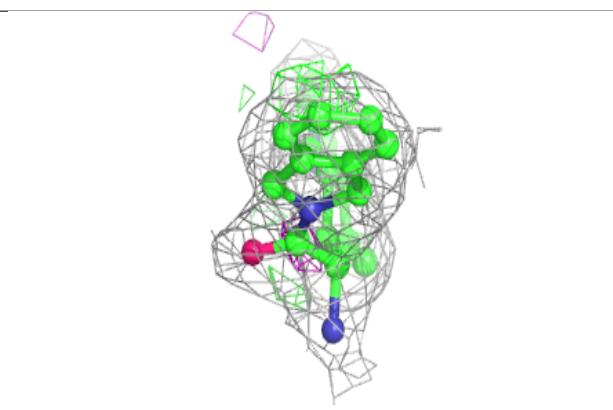
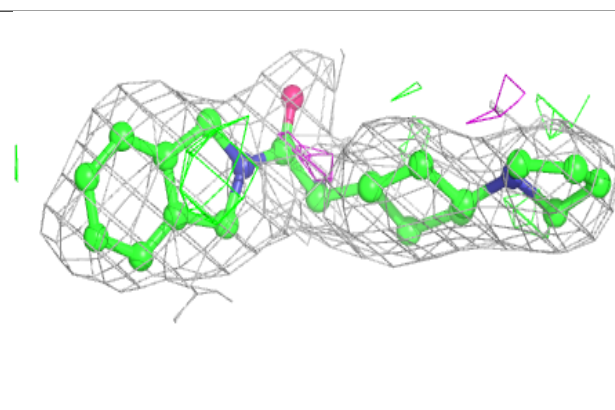
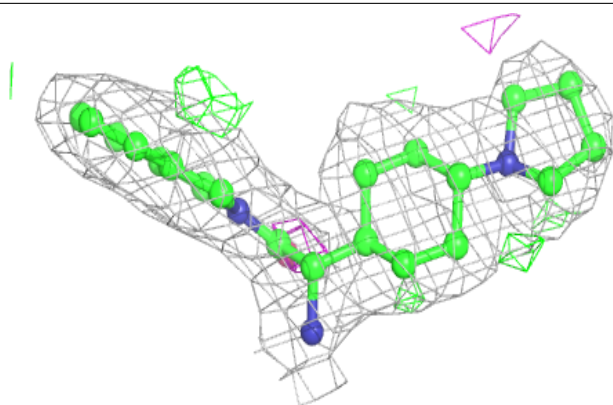
**Electron density around D06 B 901:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

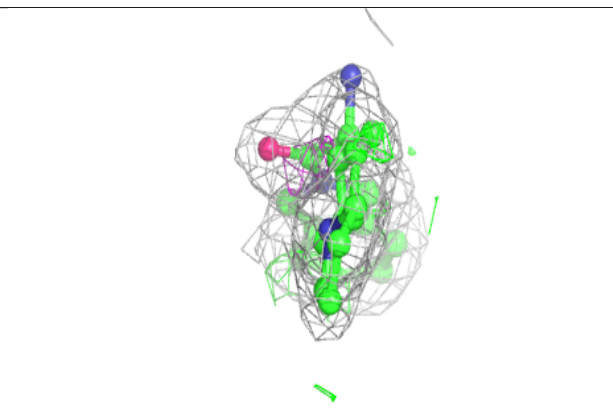
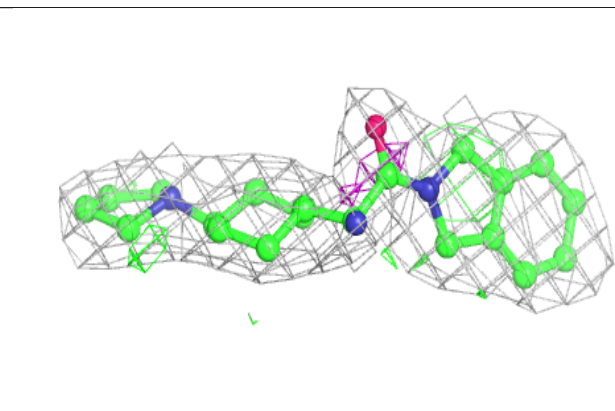
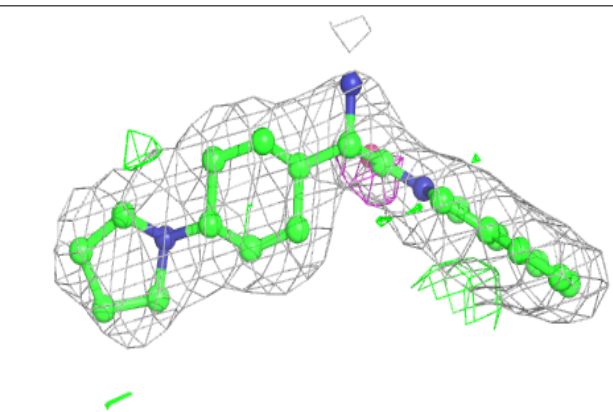


**Electron density around D06 D 901:**

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

**Electron density around D06 C 901:**

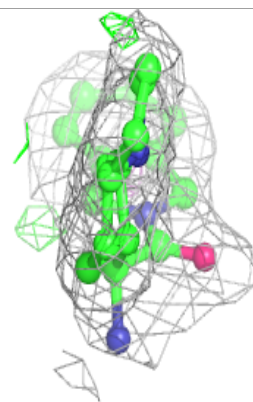
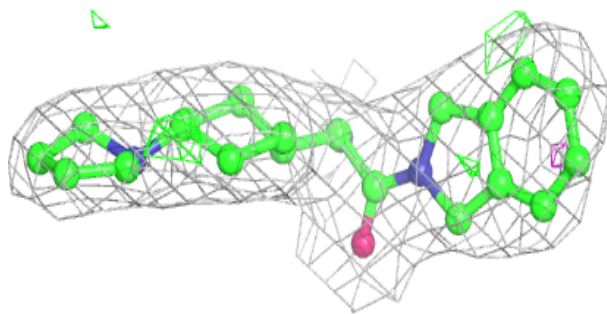
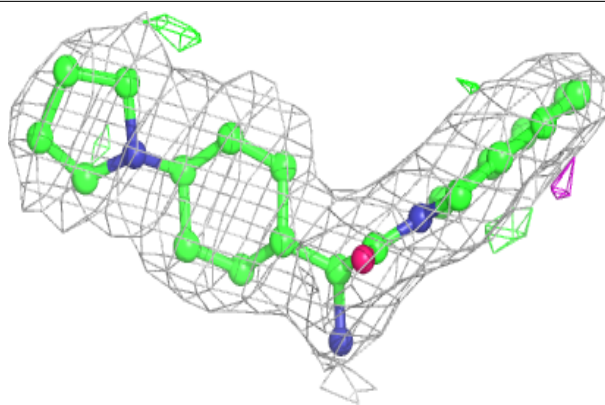
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around D06 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.