



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:49 AM UTC

PDB ID : 7SVL / pdb_00007svl
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

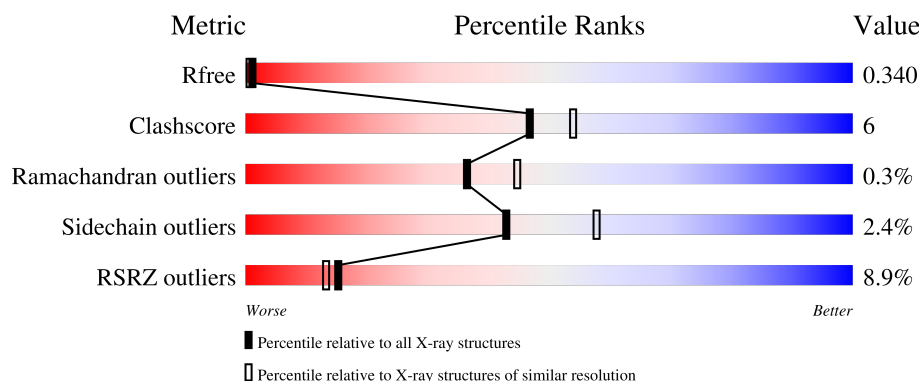
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	7% 83% 11% • 5%
1	B	869	8% 85% 9% • 5%
1	C	869	10% 79% 16% •
1	D	869	9% 75% 19% • •

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:

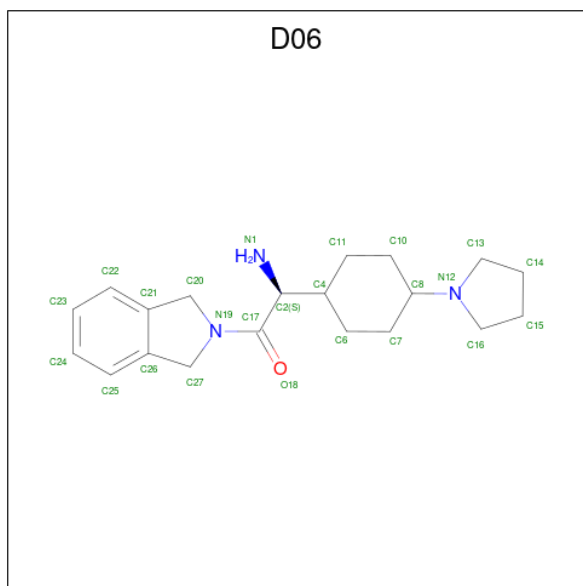
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	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 (CCD ID: D06) (formula: C₂₀H₂₉N₃O) (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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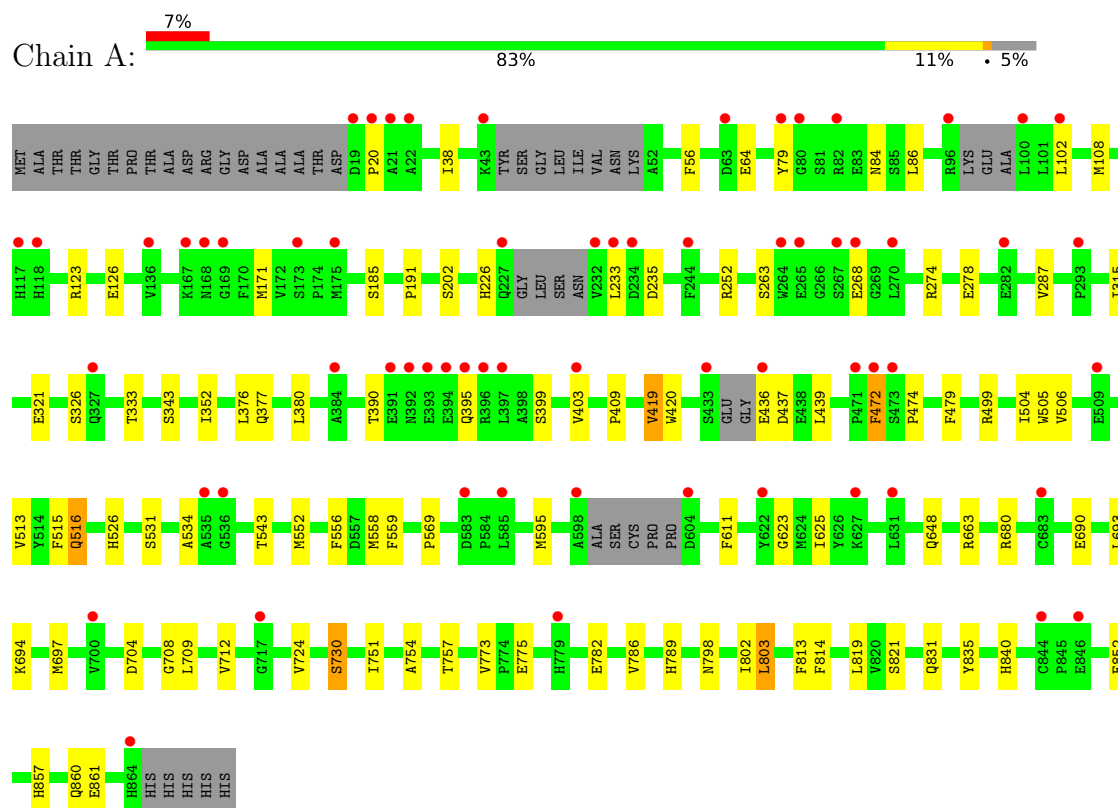
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	264	Total 264	O 264	0	0

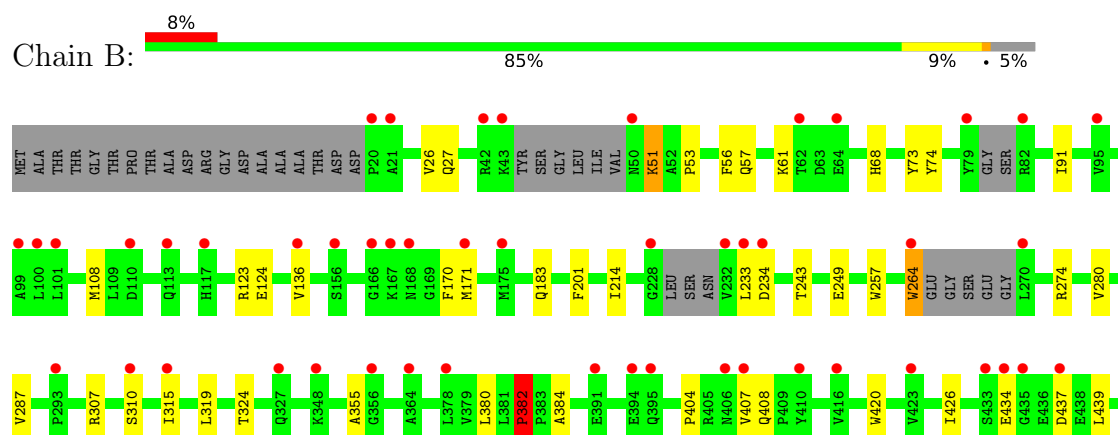
3 Residue-property plots [i](#)

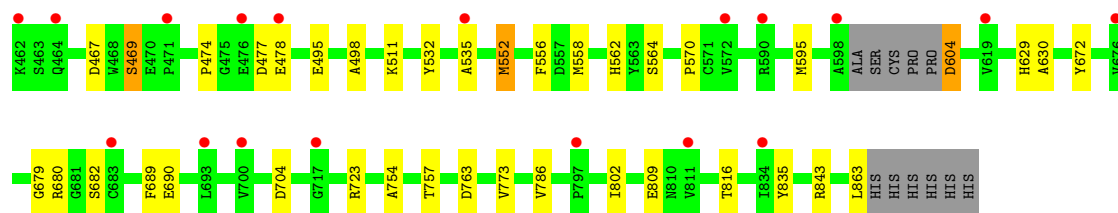
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

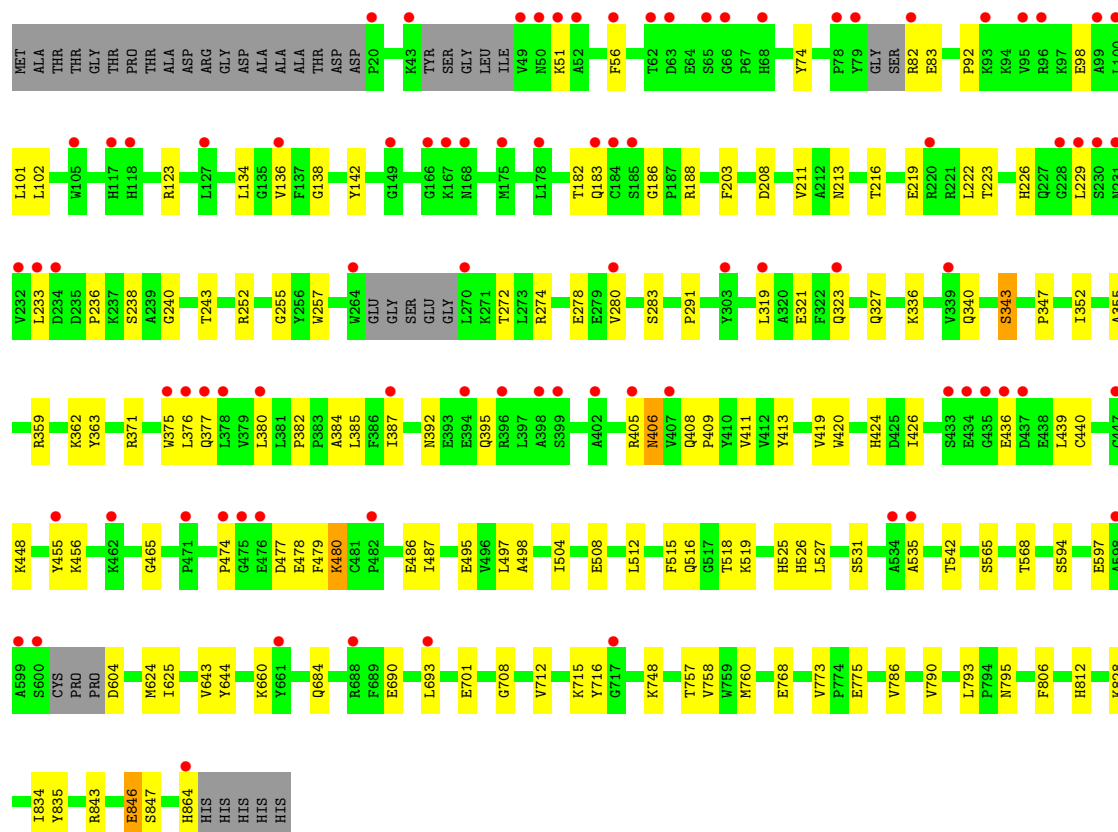
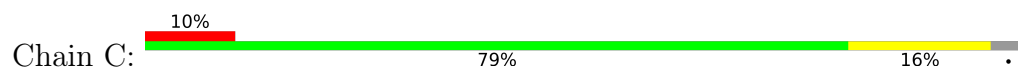


• Molecule 1: Dipeptidyl peptidase 9

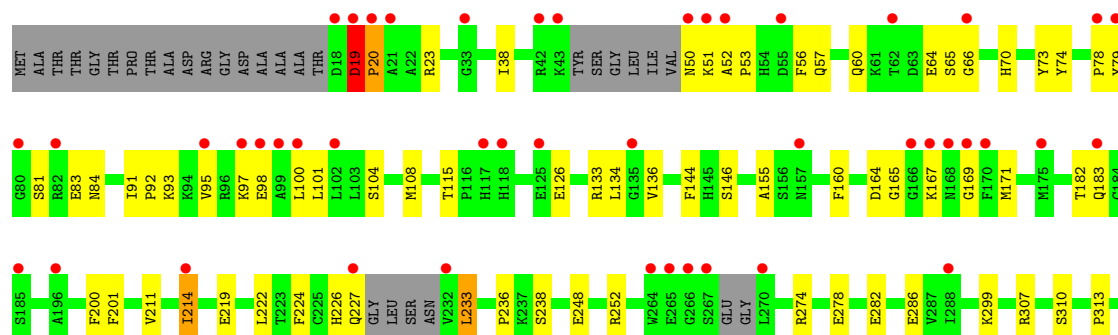
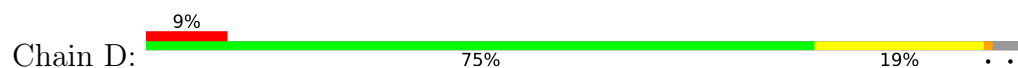


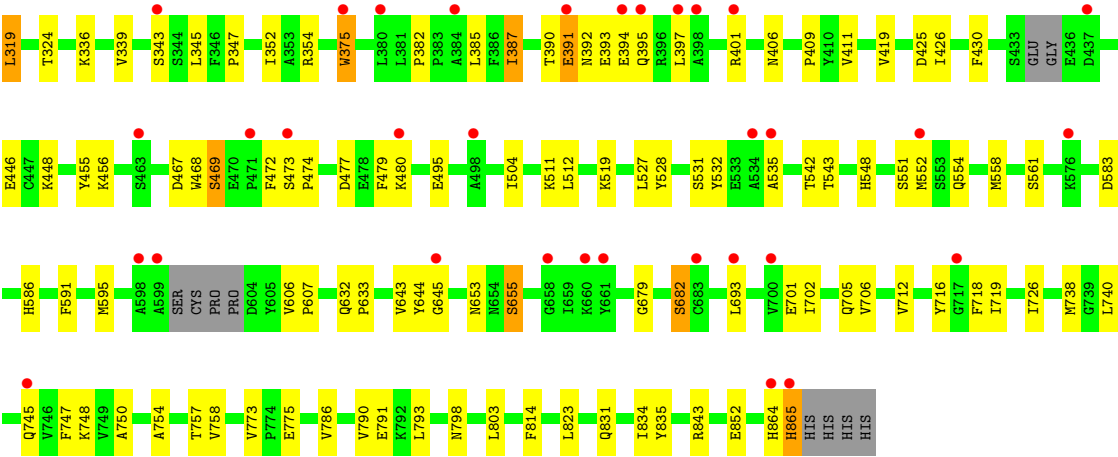


• Molecule 1: Dipeptidyl peptidase 9



• 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, α , β , γ	119.72Å 117.40Å 163.69Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	157.66 – 2.46 157.66 – 2.46	Depositor EDS
% Data completeness (in resolution range)	95.6 (157.66-2.46) 95.6 (157.66-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.45Å)	Xtrriage
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 (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtrriage
Anisotropy	0.595	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27997	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 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.*

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: 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	0.73	2/6895 (0.0%)	0.95	5/9354 (0.1%)
1	B	0.74	1/6875 (0.0%)	0.94	8/9323 (0.1%)
1	C	0.72	0/6959	0.95	9/9442 (0.1%)
1	D	0.72	0/6946	0.99	16/9422 (0.2%)
All	All	0.73	3/27675 (0.0%)	0.96	38/37541 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	PRO	C-N	5.90	1.40	1.33
1	B	382	PRO	CA-C	5.69	1.57	1.52
1	A	235	ASP	C-N	5.00	1.37	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	PRO	CA-C-N	-14.62	105.56	120.03
1	A	569	PRO	C-N-CA	-14.62	105.56	120.03
1	D	835	TYR	CB-CA-C	8.09	118.58	110.33
1	B	382	PRO	O-C-N	-7.34	112.80	121.46
1	B	763	ASP	N-CA-C	6.98	119.00	110.41
1	B	408	GLN	N-CA-C	6.54	114.01	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	TYR	CB-CA-C	6.51	116.97	110.33
1	C	835	TYR	CB-CA-C	6.27	116.73	110.33
1	A	754	ALA	CA-C-N	-6.10	114.01	120.66
1	A	754	ALA	C-N-CA	-6.10	114.01	120.66
1	A	835	TYR	CB-CA-C	6.09	116.54	110.33
1	B	310	SER	N-CA-C	5.99	116.19	108.34
1	D	606	VAL	CA-C-N	-5.98	115.36	119.66
1	D	606	VAL	C-N-CA	-5.98	115.36	119.66
1	C	408	GLN	CA-C-N	-5.66	114.13	119.85
1	C	408	GLN	C-N-CA	-5.66	114.13	119.85
1	C	408	GLN	N-CA-C	5.56	113.13	108.13
1	D	793	LEU	CA-C-N	-5.45	114.97	120.31
1	D	793	LEU	C-N-CA	-5.45	114.97	120.31
1	B	754	ALA	CA-C-N	-5.38	114.80	120.66
1	B	754	ALA	C-N-CA	-5.38	114.80	120.66
1	D	607	PRO	N-CA-C	5.33	116.29	110.58
1	C	793	LEU	CA-C-N	-5.25	115.17	120.31
1	C	793	LEU	C-N-CA	-5.25	115.17	120.31
1	D	52	ALA	CA-C-N	-5.20	114.60	119.90
1	D	52	ALA	C-N-CA	-5.20	114.60	119.90
1	C	340	GLN	CA-C-N	-5.20	114.41	119.76
1	C	340	GLN	C-N-CA	-5.20	114.41	119.76
1	D	430	PHE	CA-C-N	-5.17	114.91	120.03
1	D	430	PHE	C-N-CA	-5.17	114.91	120.03
1	D	387	ILE	CA-C-N	-5.11	114.50	119.76
1	D	387	ILE	C-N-CA	-5.11	114.50	119.76
1	D	19	ASP	CA-C-N	-5.10	113.47	119.84
1	D	19	ASP	C-N-CA	-5.10	113.47	119.84
1	C	387	ILE	N-CA-C	5.09	113.49	107.84
1	D	754	ALA	CA-C-N	-5.08	115.12	120.66
1	D	754	ALA	C-N-CA	-5.08	115.12	120.66
1	B	170	PHE	N-CA-C	5.01	116.48	108.41

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	54	1
1	B	6677	0	6469	43	3
1	C	6755	0	6536	84	1
1	D	6744	0	6514	121	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	14	0
3	D	264	0	0	11	0
All	All	27997	0	25983	296	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 6.

All (296) 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:D:108:MET:HE3	1:D:171:MET:HE1	1.38	1.04
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:C:321:GLU:CD	1:C:336:LYS:NZ	2.28	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: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:C:321:GLU:CD	1:C:336:LYS:HZ2	1.81	0.85
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:B:680:ARG:NH2	1:B:704:ASP:OD1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:PRO:HB3	1:B:478:GLU:HG2	1.67	0.76
1:D:252:ARG:NH2	1:D:278:GLU:OE2	2.18	0.76
1:B:56:PHE:CE1	1:B:595:MET:HE1	2.21	0.75
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:B:56:PHE:HE1	1:B:595:MET:HE1	1.57	0.69
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:C:321:GLU:OE1	1:C:336:LYS:NZ	2.27	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:748:LYS:NZ	3:C:1008:HOH:O	2.29	0.65
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:D:70:HIS:CE1	1:D:558:MET:HE3	2.32	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:D:164:ASP:CG	1:D:171:MET:HE2	2.27	0.60
1:D:108:MET:CE	1:D:171:MET:HE1	2.25	0.59
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:74:TYR:CE1	1:D:595:MET:HE1	2.38	0.59
1:D:92:PRO:HG2	1:D:95:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:108:MET:HA	1:A:171:MET:HE1	1.84	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:C:51:LYS:HD2	1:C:136:VAL:HG21	1.87	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:D:233:LEU:C	1:D:233:LEU:HD12	2.28	0.57
1:D:83:GLU:OE1	1:D:115:THR:OG1	2.15	0.57
1:B:679:GLY:O	1:B:682:SER:OG	2.21	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:C:376:LEU:HD23	1:C:376:LEU:C	2.29	0.56
1:D:702:ILE:O	1:D:706:VAL:HG23	2.06	0.55
1:D:738:MET:HE2	1:D:786:VAL:HG13	1.89	0.55
1:B:56:PHE:CD1	1:B:74:TYR:HB3	2.41	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:375[A]:TRP:O	1:D:375[A]:TRP:HE3	1.89	0.53
1:D:391:GLU:H	1:D:391:GLU:CD	2.16	0.53
1:D:425:ASP:OD2	3:D:1004:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:TYR:OH	1:D:164:ASP:OD2	2.22	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
1:A:399:SER:O	1:A:403:VAL:HG23	2.10	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:A:773:VAL:HG12	1:A:775:GLU:CD	2.35	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:C:321:GLU:CD	1:C:336:LYS:HZ1	2.01	0.50
1:D:339:VAL:HG11	1:D:468:TRP:HB3	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: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:B:91:ILE:HG21	1:B:558:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:594:SER:OG	1:C:597:GLU:OE1	2.29	0.46
1:B:249:GLU:OE1	2:B:901:D06:N1	2.48	0.46
1:D:66:GLY:O	1:D:93:LYS:NZ	2.36	0.46
1:D:91:ILE:HG21	1:D:558:MET:HE1	1.96	0.46
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.51	0.46
1:D:286:GLU:CD	1:D:307:ARG:HE	2.23	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:226:HIS:C	1:D:227:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:552:MET:HE1	1:B:556:PHE:HA	1.98	0.45
1:C:420:TRP:HZ2	1:C:690:GLU:HG2	1.82	0.45
1:A:472:PHE:CD1	1:A:472:PHE:C	2.94	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
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:D:133:ARG:HH12	1:D:248:GLU:CD	2.25	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:D:375[B]:TRP:CD1	1:D:375[B]:TRP:C	2.96	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:D:472:PHE:CD1	1:D:472:PHE:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:ASP:OD2	1:D:171:MET:HE2	2.18	0.43
1:D:679:GLY:HA3	3:D:1044:HOH:O	2.18	0.43
1:A:552:MET:HE3	1:A:558:MET:O	2.19	0.43
1:B:108:MET:HA	1:B:171:MET:HE1	2.00	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:200:PHE:CZ	1:D:324:THR:HG21	2.54	0.43
1:C:773:VAL:CG1	1:C:775:GLU:CD	2.92	0.43
1:A:123:ARG:NE	1:A:126:GLU:OE1	2.51	0.42
1:A:419:VAL:O	1:A:694:LYS:NZ	2.44	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
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:A:552:MET:HE2	1:A:556:PHE:HA	2.02	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:446:GLU:O	1:D:446:GLU:HG2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:GLN:HG3	3:C:1090:HOH:O	2.20	0.41
1:D:773:VAL:CG1	1:D:775:GLU:CD	2.93	0.41
1:A:813:PHE:O	1:A:814:PHE:C	2.63	0.41
1:B:56:PHE:CZ	1:B:595:MET:HE1	2.55	0.41
1:C:257:TRP:CH2	1:C:355:ALA:HB3	2.55	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: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:56:PHE:HE1	1:A:595:MET:HE1	1.86	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:629:HIS:O	1:B:630:ALA:C	2.64	0.40
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
1:B:723:ARG:C	1:B:863:LEU:HD11	2.46	0.40
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: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:C:760:MET:HE2	1:C:760:MET:HB3	1.88	0.40
1:A:86:LEU:HD22	1:A:108:MET:HE1	2.03	0.40
1:C:182:THR:OG1	1:C:219:GLU:OE2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	813/869 (94%)	785 (97%)	27 (3%)	1 (0%)	48	61
1	B	811/869 (93%)	774 (95%)	35 (4%)	2 (0%)	43	54
1	C	822/869 (95%)	793 (96%)	26 (3%)	3 (0%)	30	37
1	D	819/869 (94%)	790 (96%)	24 (3%)	5 (1%)	21	27
All	All	3265/3476 (94%)	3142 (96%)	112 (3%)	11 (0%)	36	45

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%)	711 (98%)	16 (2%)	45	60
1	B	725/759 (96%)	712 (98%)	13 (2%)	51	65
1	C	733/759 (97%)	716 (98%)	17 (2%)	44	59
1	D	732/759 (96%)	707 (97%)	25 (3%)	32	47
All	All	2917/3036 (96%)	2846 (98%)	71 (2%)	43	58

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	TYR
1	A	84	ASN
1	A	102	LEU
1	A	185	SER
1	A	226	HIS
1	A	263	SER
1	A	268	GLU
1	A	326	SER
1	A	343	SER
1	A	419	VAL
1	A	472	PHE
1	A	516	GLN
1	A	543	THR
1	A	730	SER
1	A	803	LEU
1	A	821	SER
1	B	123	ARG
1	B	234	ASP
1	B	264	TRP
1	B	324	THR
1	B	434	GLU
1	B	437	ASP
1	B	469	SER
1	B	477	ASP

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Mol	Chain	Res	Type
1	B	495	GLU
1	B	552	MET
1	B	562	HIS
1	B	604	ASP
1	B	773	VAL
1	C	82	ARG
1	C	102	LEU
1	C	226	HIS
1	C	229	LEU
1	C	233	LEU
1	C	238	SER
1	C	272	THR
1	C	343	SER
1	C	406	ASN
1	C	436	GLU
1	C	495	GLU
1	C	604	ASP
1	C	624	MET
1	C	758	VAL
1	C	790	VAL
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	233	LEU
1	D	238	SER
1	D	319	LEU
1	D	375[A]	TRP
1	D	375[B]	TRP
1	D	391	GLU
1	D	406	ASN
1	D	469	SER
1	D	473	SER
1	D	495	GLU
1	D	543	THR
1	D	551	SER
1	D	552	MET
1	D	655	SER
1	D	682	SER

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Mol	Chain	Res	Type
1	D	748	LYS
1	D	758	VAL
1	D	791	GLU
1	D	803	LEU
1	D	865	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	60	GLN
1	A	822	GLN
1	B	226	HIS
1	B	422	ASN
1	B	648	GLN
1	B	665	ASN
1	B	684	GLN
1	B	833	GLN
1	C	60	GLN
1	C	111	HIS
1	C	392	ASN
1	C	395	GLN
1	C	500	HIS
1	C	525	HIS
1	C	555	ASN
1	C	648	GLN
1	C	798	ASN
1	C	815	HIS
1	C	831	GLN
1	D	25	GLN
1	D	57	GLN
1	D	340	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 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	D06	B	901	-	27,27,27	0.65	0	33,38,38	2.99	6 (18%)
2	D06	C	901	-	27,27,27	0.90	1 (3%)	33,38,38	2.81	5 (15%)
2	D06	D	901	-	27,27,27	0.92	1 (3%)	33,38,38	2.81	6 (18%)
2	D06	A	901	-	27,27,27	0.99	1 (3%)	33,38,38	3.03	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D06	B	901	-	-	0/16/41/41	0/4/4/4
2	D06	C	901	-	-	0/16/41/41	0/4/4/4
2	D06	D	901	-	-	0/16/41/41	0/4/4/4
2	D06	A	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	-3.71	1.49	1.53
2	D	901	D06	C2-C17	-2.61	1.50	1.53
2	C	901	D06	C2-C17	-2.24	1.51	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	D06	C26-C27-N19	11.62	107.88	102.42
2	A	901	D06	C26-C27-N19	11.50	107.83	102.42
2	D	901	D06	C26-C27-N19	11.29	107.73	102.42
2	B	901	D06	C21-C20-N19	11.08	107.63	102.42
2	A	901	D06	C21-C20-N19	10.84	107.52	102.42
2	B	901	D06	C26-C27-N19	10.28	107.25	102.42
2	C	901	D06	C21-C20-N19	9.23	106.76	102.42
2	D	901	D06	C21-C20-N19	9.14	106.72	102.42
2	B	901	D06	C11-C4-C2	-4.52	105.15	111.80
2	A	901	D06	C17-C2-N1	-3.78	103.73	110.09
2	B	901	D06	O18-C17-N19	-3.17	117.82	121.61
2	B	901	D06	C10-C8-N12	-2.72	105.69	112.66
2	D	901	D06	C10-C11-C4	-2.49	106.80	112.29
2	C	901	D06	C13-N12-C8	-2.35	111.85	114.12
2	C	901	D06	C10-C11-C4	-2.30	107.21	112.29
2	B	901	D06	C6-C7-C8	2.24	114.31	109.98
2	D	901	D06	C17-C2-N1	-2.20	106.39	110.09
2	D	901	D06	C13-N12-C8	-2.17	112.02	114.12
2	D	901	D06	C7-C8-N12	-2.14	107.19	112.66
2	C	901	D06	C7-C6-C4	-2.12	107.61	112.29
2	A	901	D06	C7-C8-N12	-2.02	107.48	112.66

There are no chirality outliers.

There are no torsion outliers.

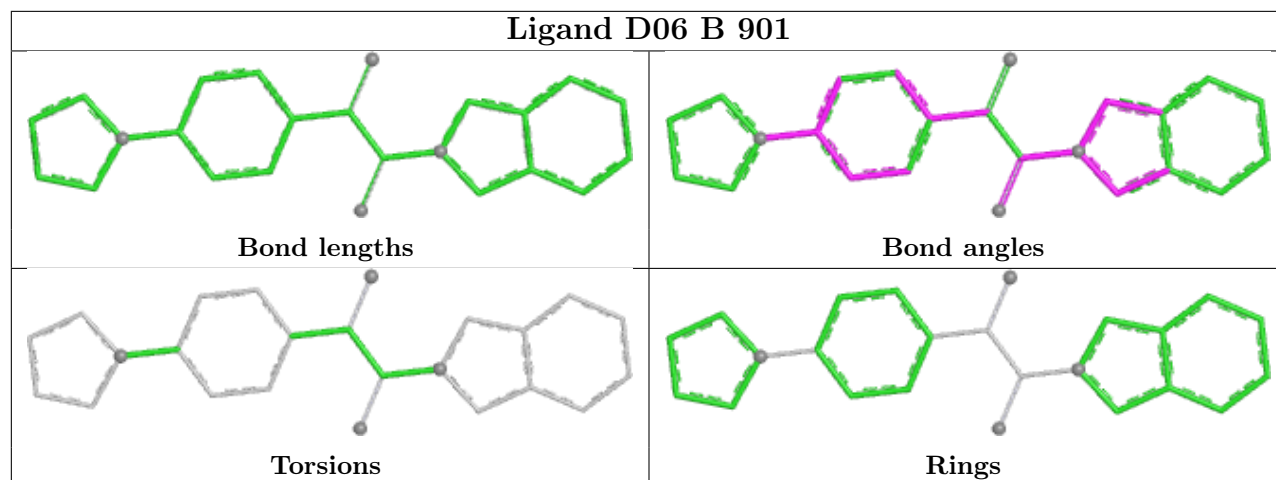
There are no ring outliers.

1 monomer is involved in 1 short contact:

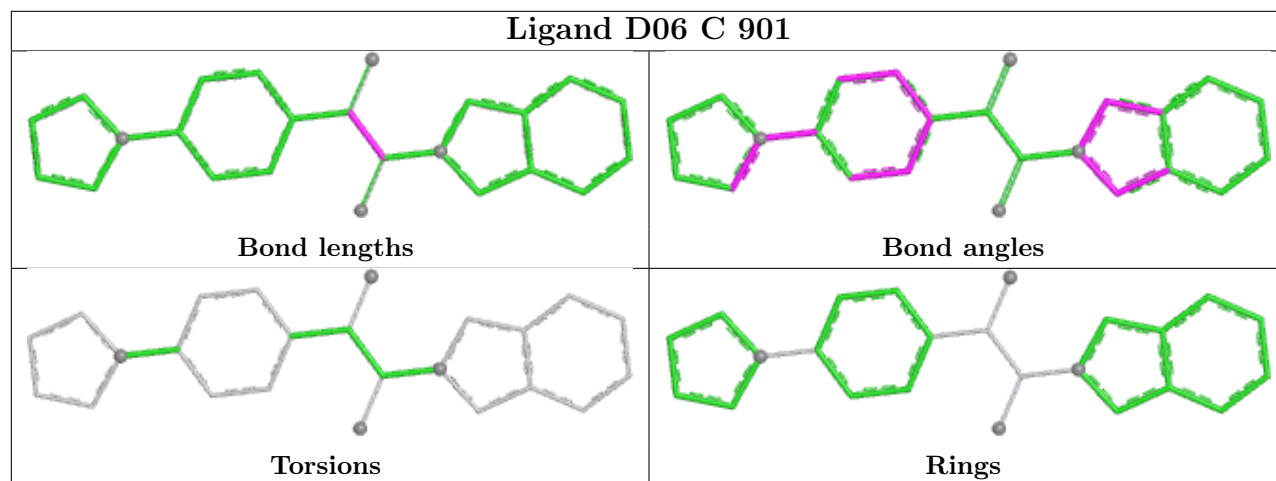
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	D06	1	0

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.

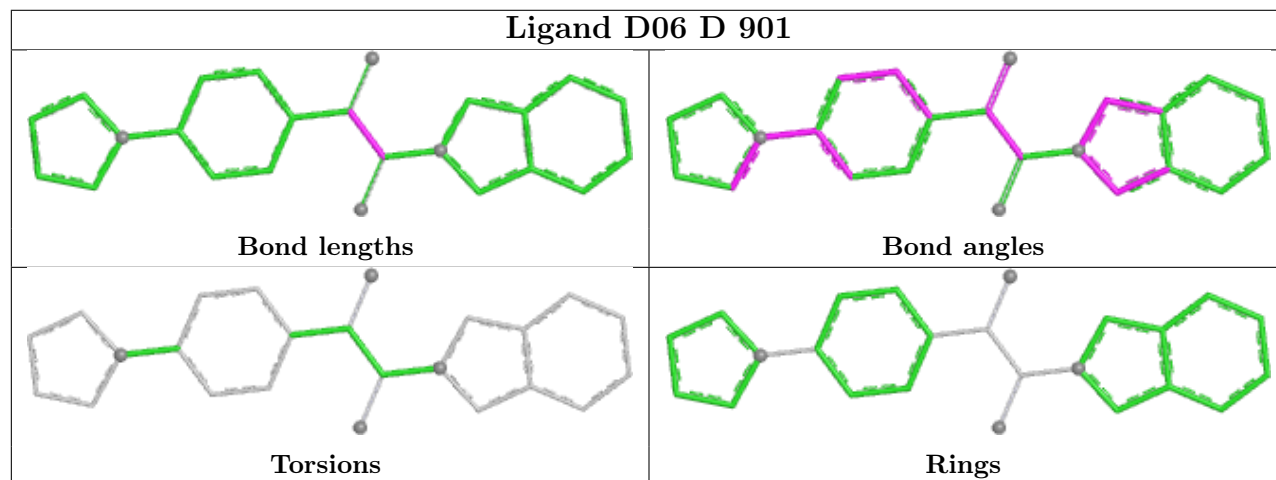
Ligand D06 B 901

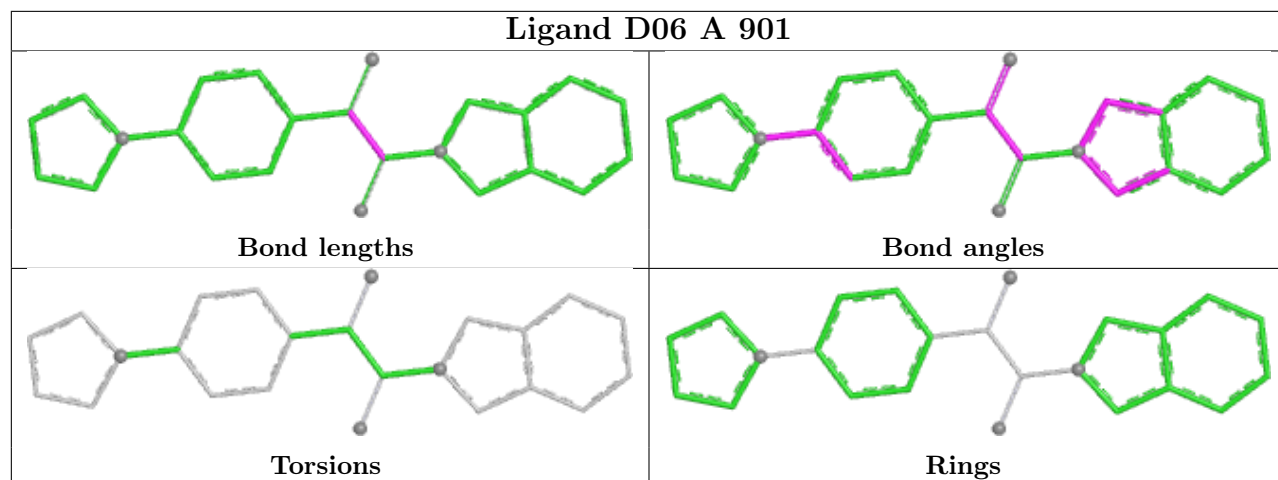


Ligand D06 C 901



Ligand D06 D 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, 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	824/869 (94%)	0.68	64 (7%) 19 16	15, 38, 70, 111	55 (6%)
1	B	823/869 (94%)	0.71	67 (8%) 18 16	15, 37, 66, 98	58 (7%)
1	C	830/869 (95%)	0.82	85 (10%) 12 10	11, 36, 68, 109	44 (5%)
1	D	830/869 (95%)	0.76	79 (9%) 14 11	14, 35, 72, 108	40 (4%)
All	All	3307/3476 (95%)	0.74	295 (8%) 15 13	11, 37, 70, 111	197 (5%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLU	5.8
1	D	168	ASN	5.7
1	A	395	GLN	5.6
1	C	434	GLU	5.6
1	C	168	ASN	5.5
1	C	20	PRO	5.5
1	A	232	VAL	5.3
1	D	232	VAL	5.1
1	B	20	PRO	5.1
1	D	19	ASP	5.0
1	A	79	TYR	5.0
1	B	228	GLY	4.9
1	A	20	PRO	4.6
1	D	20	PRO	4.5
1	B	233	LEU	4.5
1	A	604	ASP	4.4
1	C	475	GLY	4.3
1	C	375[A]	TRP	4.3
1	A	233	LEU	4.3
1	B	598	ALA	4.2
1	C	599	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	266	GLY	4.1
1	A	472	PHE	4.1
1	C	231	ASN	4.1
1	D	97	LYS	4.1
1	C	229	LEU	4.0
1	C	598	ALA	4.0
1	D	175	MET	4.0
1	C	51	LYS	3.9
1	B	168	ASN	3.9
1	D	51	LYS	3.9
1	A	21	ALA	3.9
1	A	82	ARG	3.9
1	A	392	ASN	3.8
1	C	230	SER	3.7
1	D	375[A]	TRP	3.7
1	D	645	GLY	3.7
1	C	166	GLY	3.7
1	C	433	SER	3.7
1	C	232	VAL	3.6
1	D	700	VAL	3.6
1	B	21	ALA	3.6
1	D	43	LYS	3.6
1	D	598	ALA	3.6
1	A	100	LEU	3.6
1	C	49	VAL	3.6
1	C	99	ALA	3.5
1	B	435	GLY	3.5
1	C	435	GLY	3.5
1	D	267	SER	3.5
1	A	43	LYS	3.4
1	A	864	HIS	3.4
1	C	118	HIS	3.4
1	A	535	ALA	3.4
1	C	377	GLN	3.3
1	A	471	PRO	3.3
1	D	599	ALA	3.3
1	C	95	VAL	3.3
1	B	43	LYS	3.3
1	B	310	SER	3.3
1	B	232	VAL	3.2
1	A	393	GLU	3.2
1	C	436	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	865	HIS	3.2
1	B	167	LYS	3.2
1	C	339	VAL	3.2
1	D	62	THR	3.2
1	A	598	ALA	3.2
1	A	118	HIS	3.2
1	B	478	GLU	3.2
1	D	102	LEU	3.1
1	B	407	VAL	3.1
1	B	700	VAL	3.1
1	C	693	LEU	3.1
1	D	50	ASN	3.1
1	C	535	ALA	3.1
1	D	864	HIS	3.0
1	B	619	VAL	3.0
1	C	323	GLN	3.0
1	D	52	ALA	3.0
1	C	117	HIS	3.0
1	C	717	GLY	3.0
1	C	43	LYS	3.0
1	C	864	HIS	3.0
1	C	270	LEU	3.0
1	A	19	ASP	3.0
1	C	407	VAL	2.9
1	C	264	TRP	2.9
1	C	534	ALA	2.9
1	C	78	PRO	2.9
1	C	471	PRO	2.9
1	B	270	LEU	2.9
1	C	476	GLU	2.9
1	C	378	LEU	2.9
1	D	183	GLN	2.9
1	A	234	ASP	2.9
1	D	552	MET	2.9
1	C	228	GLY	2.9
1	A	396	ARG	2.9
1	C	96	ARG	2.9
1	C	437	ASP	2.9
1	C	79	TYR	2.9
1	A	96	ARG	2.8
1	C	185	SER	2.8
1	C	405	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	2.8
1	C	482	PRO	2.8
1	B	535	ALA	2.8
1	C	303	TYR	2.8
1	B	471	PRO	2.8
1	C	462	LYS	2.8
1	D	21	ALA	2.8
1	D	397	LEU	2.8
1	D	227	GLN	2.8
1	C	387	ILE	2.8
1	B	95	VAL	2.8
1	A	175	MET	2.8
1	C	175	MET	2.8
1	B	64	GLU	2.8
1	D	658	GLY	2.7
1	C	600	SER	2.7
1	D	185	SER	2.7
1	A	700	VAL	2.7
1	A	167	LYS	2.7
1	A	173	SER	2.7
1	D	463	SER	2.7
1	C	688	ARG	2.7
1	C	100	LEU	2.7
1	D	82	ARG	2.7
1	C	394	GLU	2.7
1	B	811	VAL	2.7
1	D	343	SER	2.7
1	A	268	GLU	2.7
1	B	464	GLN	2.7
1	B	117	HIS	2.7
1	C	234	ASP	2.6
1	B	82	ARG	2.6
1	B	406	ASN	2.6
1	D	401	ARG	2.6
1	D	100	LEU	2.6
1	A	846	GLU	2.6
1	B	433	SER	2.6
1	B	79	TYR	2.6
1	A	264	TRP	2.6
1	B	264	TRP	2.6
1	D	118	HIS	2.6
1	A	80	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	2.6
1	A	436	GLU	2.6
1	D	99	ALA	2.6
1	A	270	LEU	2.6
1	A	136	VAL	2.6
1	A	227	GLN	2.6
1	B	683	CYS	2.6
1	C	398	ALA	2.6
1	D	264	TRP	2.5
1	C	63	ASP	2.5
1	B	676	VAL	2.5
1	C	380	LEU	2.5
1	A	267	SER	2.5
1	A	394	GLU	2.5
1	B	234	ASP	2.5
1	B	391	GLU	2.5
1	A	102	LEU	2.5
1	D	395	GLN	2.5
1	B	572	VAL	2.5
1	D	683	CYS	2.5
1	A	536	GLY	2.5
1	D	125	GLU	2.5
1	D	391	GLU	2.5
1	D	18	ASP	2.5
1	A	117	HIS	2.5
1	D	117	HIS	2.5
1	D	95	VAL	2.5
1	C	167	LYS	2.4
1	C	661	TYR	2.4
1	A	631	LEU	2.4
1	B	423	VAL	2.4
1	C	52	ALA	2.4
1	D	471	PRO	2.4
1	D	80	GLY	2.4
1	B	42	ARG	2.4
1	A	391	GLU	2.4
1	A	473	SER	2.4
1	A	717	GLY	2.4
1	C	184	CYS	2.4
1	D	437	ASP	2.4
1	C	82	ARG	2.4
1	D	384	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	62	THR	2.4
1	C	183	GLN	2.3
1	C	233	LEU	2.3
1	D	380	LEU	2.3
1	D	79	TYR	2.3
1	C	280	VAL	2.3
1	D	167	LYS	2.3
1	C	178	LEU	2.3
1	B	175	MET	2.3
1	C	65	SER	2.3
1	D	166	GLY	2.3
1	D	270	LEU	2.3
1	A	244	PHE	2.3
1	B	136	VAL	2.3
1	A	168	ASN	2.3
1	C	62	THR	2.3
1	B	378	LEU	2.3
1	B	834	ILE	2.3
1	C	319	LEU	2.3
1	B	394	GLU	2.3
1	A	844	CYS	2.3
1	D	78	PRO	2.3
1	D	498	ALA	2.2
1	D	661	TYR	2.3
1	C	149	GLY	2.2
1	A	627	LYS	2.2
1	C	127	LEU	2.2
1	A	63	ASP	2.2
1	A	282	GLU	2.2
1	D	170	PHE	2.2
1	B	50	ASN	2.2
1	A	779	HIS	2.2
1	D	33	GLY	2.2
1	D	480	LYS	2.2
1	D	576	LYS	2.2
1	A	397	LEU	2.2
1	B	693	LEU	2.2
1	B	110	ASP	2.2
1	B	437	ASP	2.2
1	C	136	VAL	2.2
1	B	364	ALA	2.2
1	C	93	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	GLY	2.2
1	D	473	SER	2.2
1	B	476	GLU	2.2
1	C	396	ARG	2.2
1	B	293	PRO	2.2
1	D	535	ALA	2.2
1	A	327	GLN	2.2
1	B	395	GLN	2.2
1	C	66	GLY	2.2
1	D	135	GLY	2.2
1	A	433	SER	2.2
1	D	42	ARG	2.2
1	C	56	PHE	2.2
1	B	416	VAL	2.1
1	B	113	GLN	2.1
1	B	327	GLN	2.1
1	D	534	ALA	2.1
1	D	745	GLN	2.1
1	B	717	GLY	2.1
1	D	288	ILE	2.1
1	B	434	GLU	2.1
1	A	293	PRO	2.1
1	C	50	ASN	2.1
1	A	169	GLY	2.1
1	A	585	LEU	2.1
1	B	101	LEU	2.1
1	B	356	GLY	2.1
1	C	376	LEU	2.1
1	B	315	ILE	2.1
1	B	410	TYR	2.1
1	D	394	GLU	2.1
1	C	447	CYS	2.1
1	B	156	SER	2.1
1	B	171	MET	2.1
1	A	22	ALA	2.1
1	D	196	ALA	2.1
1	B	590	ARG	2.1
1	B	348	LYS	2.1
1	B	462	LYS	2.1
1	D	660	LYS	2.1
1	A	683	CYS	2.1
1	C	402	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	398	ALA	2.1
1	D	693	LEU	2.1
1	D	66	GLY	2.1
1	C	474	PRO	2.1
1	C	68	HIS	2.1
1	D	157	ASN	2.0
1	C	105	TRP	2.0
1	D	717	GLY	2.0
1	A	583	ASP	2.0
1	A	622	TYR	2.0
1	C	455	TYR	2.0
1	D	55	ASP	2.0
1	C	220	ARG	2.0
1	A	384	ALA	2.0
1	B	99	ALA	2.0
1	A	265	GLU	2.0
1	A	509	GLU	2.0
1	D	265	GLU	2.0
1	D	169	GLY	2.0
1	D	214	ILE	2.0
1	B	797	PRO	2.0
1	C	399	SER	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	D06	B	901	24/24	0.84	0.14	21,28,35,41	0

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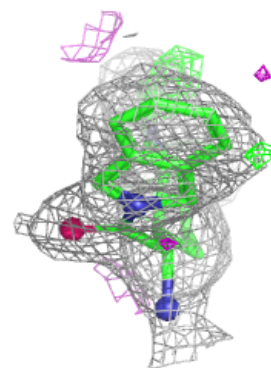
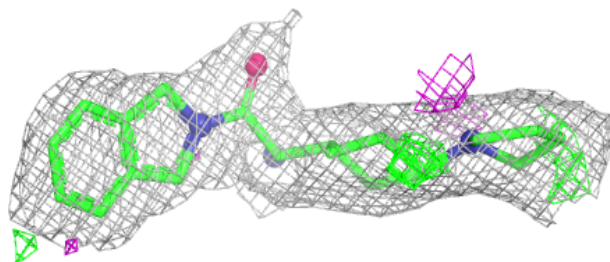
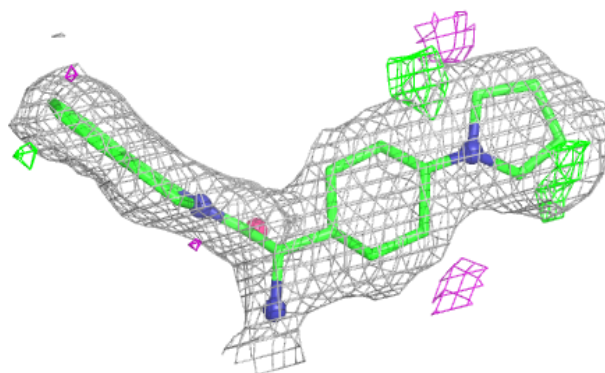
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	D06	D	901	24/24	0.87	0.13	17,28,37,42	0
2	D06	C	901	24/24	0.89	0.12	12,24,30,32	0
2	D06	A	901	24/24	0.91	0.11	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.

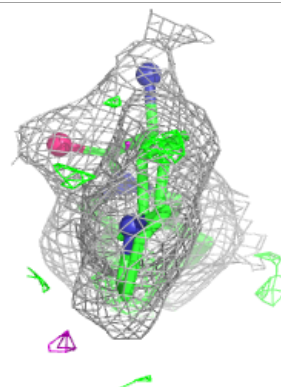
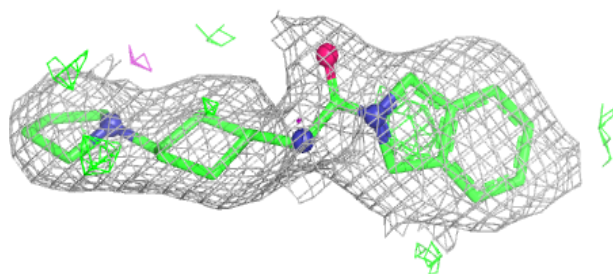
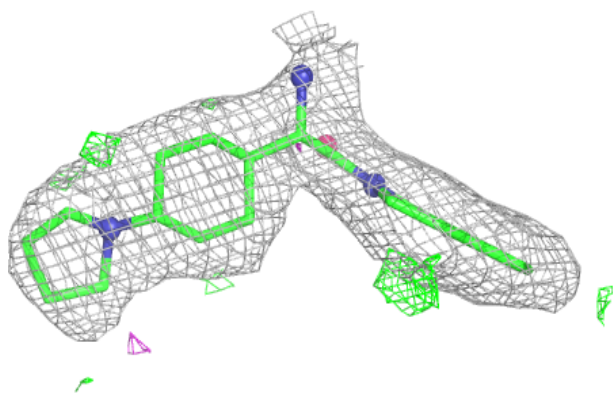
Electron density around D06 B 901:

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

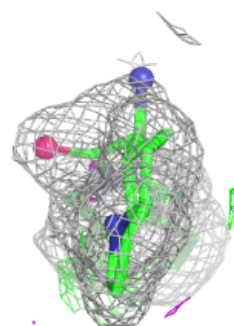
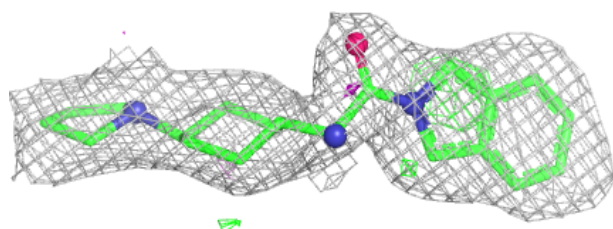
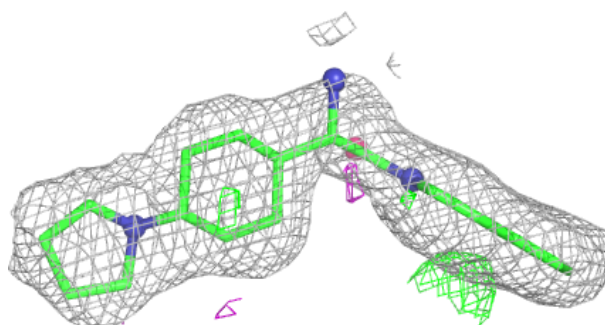


Electron density around D06 D 901:

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

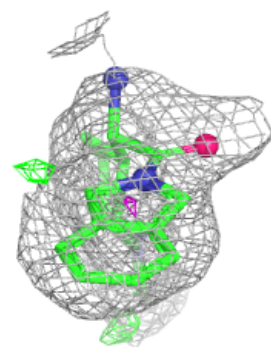
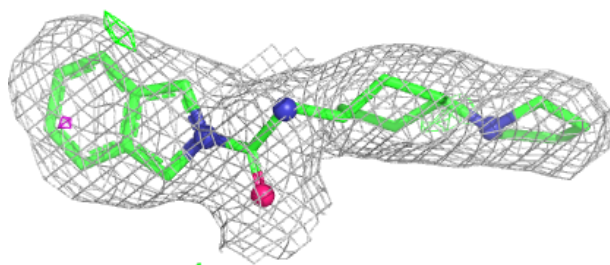
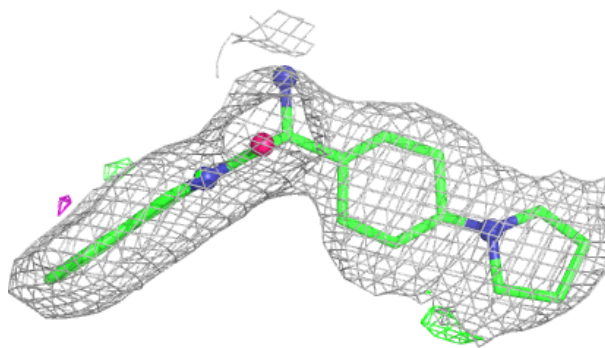
**Electron density around D06 C 901:**

$2mF_o-DF_c$ (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.