



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 3C79 / pdb_00003c79
Title : Crystal structure of Aplysia californica AChBP in complex with the neonicotinoid imidacloprid
Authors : Talley, T.T.; Harel, M.; Hibbs, R.E.; Tomizawa, M.; Casida, J.E.; Taylor, P.W.
Deposited on : 2008-02-06
Resolution : 2.48 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

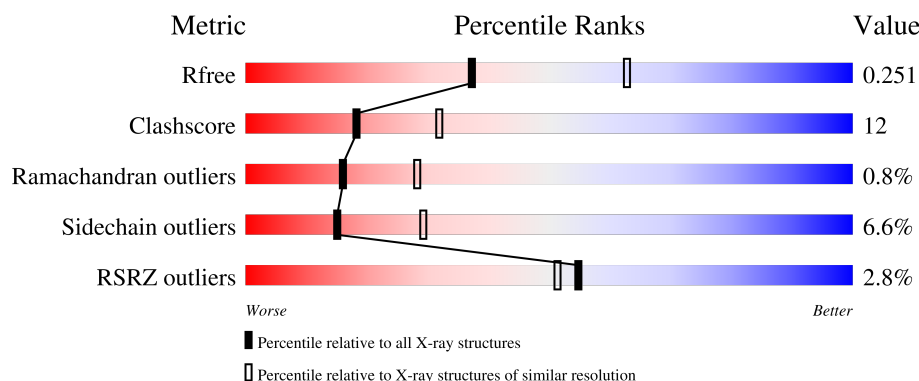
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	227	3% 69% 20% • 7%
1	B	227	2% 70% 20% • • 7%
1	C	227	2% 67% 22% • 8%
1	D	227	4% 68% 22% • 7%
1	E	227	2% 62% 24% 7% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8648 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	1	0
			1695	1069	282	335	9			
1	B	212	Total	C	N	O	S	0	1	0
			1703	1073	283	338	9			
1	C	208	Total	C	N	O	S	0	0	0
			1661	1049	275	329	8			
1	D	212	Total	C	N	O	S	0	0	0
			1692	1067	279	337	9			
1	E	211	Total	C	N	O	S	0	1	0
			1693	1067	281	336	9			

There are 40 discrepancies between the modelled and reference sequences:

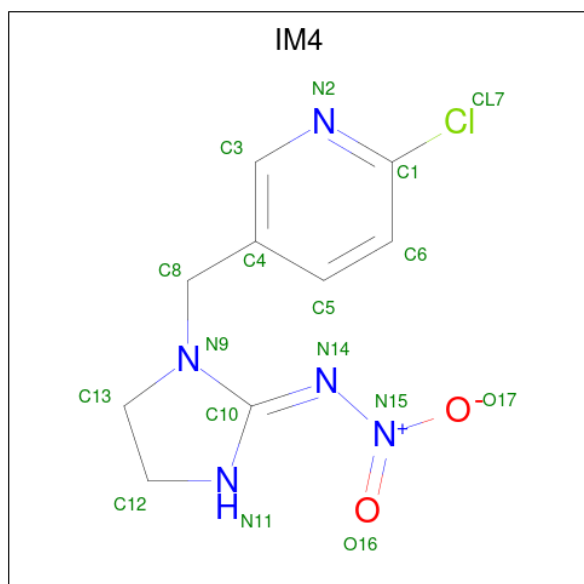
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8

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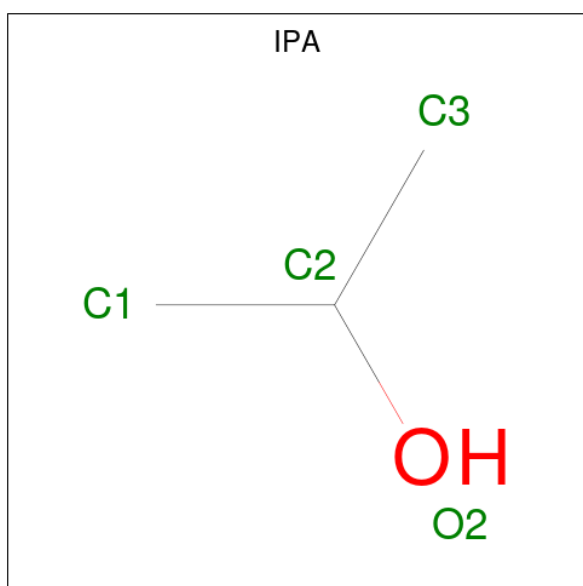
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is (2E)-1-[(6-chloropyridin-3-yl)methyl]-N-nitroimidazolidin-2-imine (CCD ID: IM4) (formula: C₉H₁₀ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	B	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	C	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	D	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	24	Total	O	0	0
			24	24		
4	C	29	Total	O	0	0
			29	29		

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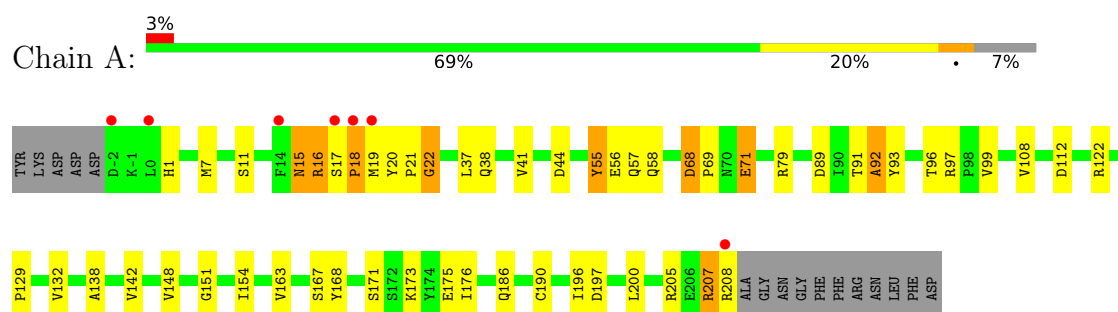
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	19	Total	O	0	0
			19	19		
4	E	29	Total	O	0	0
			29	29		

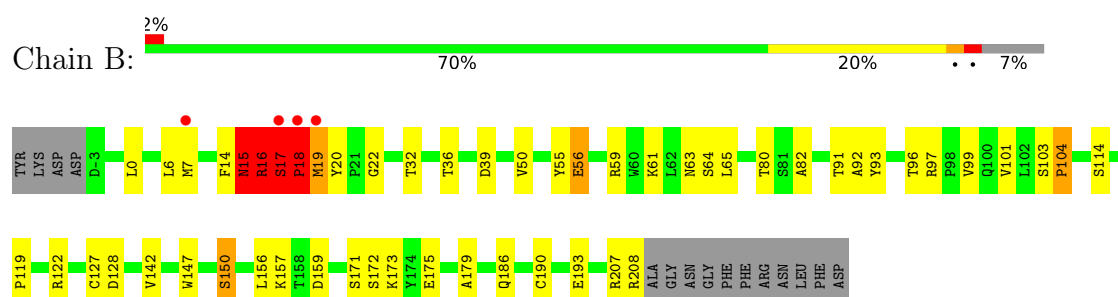
3 Residue-property plots [i](#)

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.

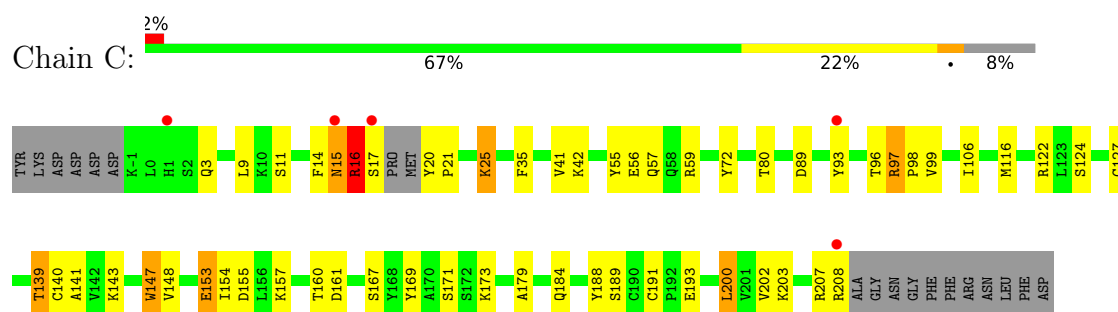
• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor

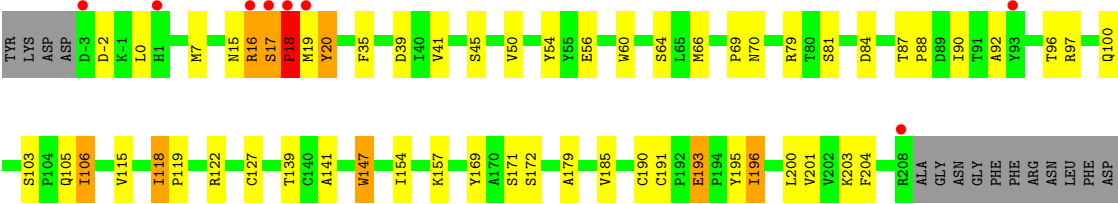


• Molecule 1: Soluble acetylcholine receptor

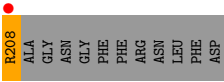
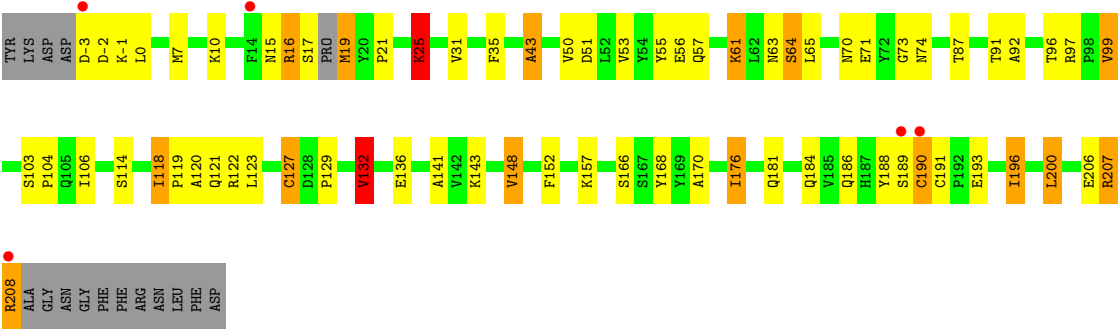


• Molecule 1: Soluble acetylcholine receptor





● Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 116.29Å 132.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.48 47.72 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.72-2.48) 97.6 (47.72-2.48)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.250 0.192 , 0.251	Depositor DCC
R_{free} test set	2353 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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: IM4, IPA

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	1.45	2/1736 (0.1%)	1.34	10/2366 (0.4%)
1	B	1.51	9/1744 (0.5%)	1.35	8/2377 (0.3%)
1	C	1.49	6/1700 (0.4%)	1.39	11/2315 (0.5%)
1	D	1.50	9/1733 (0.5%)	1.36	9/2362 (0.4%)
1	E	1.45	7/1735 (0.4%)	1.32	15/2362 (0.6%)
All	All	1.48	33/8648 (0.4%)	1.35	53/11782 (0.4%)

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	A	0	1
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	11

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ALA	CA-CB	-7.78	1.41	1.53
1	C	153	GLU	CA-C	7.12	1.59	1.52
1	E	196	ILE	C-O	-6.95	1.17	1.24
1	D	97	ARG	N-CA	6.90	1.52	1.45
1	E	103	SER	C-O	-6.53	1.18	1.24
1	E	31	VAL	CA-CB	-6.49	1.46	1.54
1	C	161	ASP	N-CA	-6.36	1.38	1.46
1	E	148	VAL	CA-CB	6.28	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	100	GLN	N-CA	6.20	1.53	1.46
1	B	101	VAL	CA-CB	6.18	1.61	1.54
1	E	35	PHE	CA-C	-6.15	1.45	1.52
1	B	99	VAL	N-CA	-5.96	1.38	1.46
1	A	99	VAL	CA-CB	-5.92	1.48	1.54
1	D	92	ALA	CA-CB	-5.78	1.43	1.53
1	E	53	VAL	N-CA	-5.74	1.39	1.46
1	B	103	SER	C-O	-5.54	1.19	1.24
1	C	139	THR	N-CA	-5.50	1.39	1.46
1	B	82	ALA	CA-C	5.46	1.60	1.52
1	D	103	SER	C-O	-5.43	1.18	1.24
1	C	179	ALA	CA-C	-5.37	1.46	1.52
1	B	32	THR	CA-CB	-5.35	1.45	1.53
1	B	179	ALA	CA-CB	-5.34	1.45	1.53
1	C	99	VAL	N-CA	-5.18	1.39	1.46
1	C	106	ILE	CG1-CD1	5.15	1.71	1.51
1	B	156	LEU	C-O	5.15	1.30	1.23
1	B	93	TYR	N-CA	-5.13	1.39	1.46
1	E	121	GLN	C-O	5.10	1.30	1.23
1	D	106	ILE	N-CA	-5.06	1.40	1.46
1	D	69	PRO	CA-C	5.06	1.59	1.52
1	D	87	THR	C-O	-5.04	1.19	1.24
1	D	115	VAL	N-CA	-5.04	1.40	1.46
1	B	104	PRO	C-O	5.02	1.29	1.23
1	D	7	MET	CG-SD	5.00	1.93	1.80

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	SER	CA-C-N	-7.55	112.22	119.85
1	B	103	SER	C-N-CA	-7.55	112.22	119.85
1	A	22	GLY	CA-C-N	7.52	128.12	120.14
1	A	22	GLY	C-N-CA	7.52	128.12	120.14
1	E	193	GLU	CA-C-N	7.21	127.13	119.85
1	E	193	GLU	C-N-CA	7.21	127.13	119.85
1	C	202	VAL	CB-CA-C	-7.06	100.89	110.42
1	D	97	ARG	CA-C-N	-6.84	112.74	119.78
1	D	97	ARG	C-N-CA	-6.84	112.74	119.78
1	A	167	SER	CB-CA-C	-6.79	100.09	111.02
1	D	118	ILE	CA-C-N	-6.70	112.87	119.90
1	D	118	ILE	C-N-CA	-6.70	112.87	119.90
1	E	-2	ASP	N-CA-C	-6.64	104.44	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASP	CA-C-N	6.39	126.88	119.47
1	A	68	ASP	C-N-CA	6.39	126.88	119.47
1	C	147	TRP	N-CA-C	-6.34	103.64	112.45
1	C	148	VAL	CB-CA-C	-6.32	103.80	110.62
1	E	193	GLU	N-CA-C	6.31	117.85	109.83
1	E	132	VAL	CB-CA-C	-6.23	102.50	112.16
1	E	25	LYS	N-CA-C	-6.17	104.56	111.28
1	C	41	VAL	CB-CA-C	-6.16	103.99	112.24
1	C	193	GLU	CA-C-N	-6.07	114.37	120.31
1	C	193	GLU	C-N-CA	-6.07	114.37	120.31
1	E	87	THR	CA-C-N	-6.00	113.79	119.85
1	E	87	THR	C-N-CA	-6.00	113.79	119.85
1	B	128	ASP	CA-C-N	-5.97	114.74	120.83
1	B	128	ASP	C-N-CA	-5.97	114.74	120.83
1	C	15	ASN	N-CA-C	-5.89	106.09	113.28
1	A	41	VAL	CB-CA-C	-5.82	104.61	111.94
1	E	166	SER	CA-C-N	-5.76	114.04	122.86
1	E	166	SER	C-N-CA	-5.76	114.04	122.86
1	E	148	VAL	CB-CA-C	-5.57	104.60	110.62
1	A	92	ALA	N-CA-C	-5.44	101.61	110.20
1	E	43	ALA	CA-C-N	-5.42	115.42	123.11
1	E	43	ALA	C-N-CA	-5.42	115.42	123.11
1	B	99	VAL	N-CA-CB	-5.40	102.89	110.13
1	D	193	GLU	N-CA-C	5.37	116.46	109.64
1	A	112	ASP	N-CA-C	-5.35	106.73	113.20
1	C	191	CYS	CA-C-N	5.32	124.50	118.97
1	C	191	CYS	C-N-CA	5.32	124.50	118.97
1	B	56	GLU	N-CA-CB	-5.30	102.78	110.84
1	C	42	LYS	CB-CG-CD	-5.30	99.12	111.30
1	C	98	PRO	CB-CA-C	-5.26	104.68	111.46
1	D	41	VAL	CB-CA-C	-5.26	104.97	112.22
1	D	185	VAL	N-CA-C	5.25	116.15	108.53
1	A	55	TYR	CA-CB-CG	5.23	123.31	113.90
1	B	22	GLY	CA-C-N	5.18	125.39	120.31
1	B	22	GLY	C-N-CA	5.18	125.39	120.31
1	D	147	TRP	CA-C-N	-5.18	116.39	122.14
1	D	147	TRP	C-N-CA	-5.18	116.39	122.14
1	E	99	VAL	CA-C-N	-5.15	115.61	122.72
1	E	99	VAL	C-N-CA	-5.15	115.61	122.72
1	A	1	HIS	N-CA-C	5.09	116.91	111.36

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ASN	Peptide
1	B	15	ASN	Peptide
1	B	16	ARG	Peptide
1	B	17	SER	Peptide
1	B	18	PRO	Peptide
1	C	14	PHE	Peptide
1	C	16	ARG	Peptide
1	D	16	ARG	Peptide
1	D	18	PRO	Peptide
1	E	16	ARG	Peptide
1	E	189	SER	Peptide

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	1695	0	1630	41	0
1	B	1703	0	1634	42	0
1	C	1661	0	1598	38	0
1	D	1692	0	1621	34	0
1	E	1693	0	1626	59	0
2	A	17	0	10	4	0
2	B	17	0	10	3	0
2	C	17	0	10	2	0
2	D	17	0	10	5	0
3	A	4	0	8	3	0
3	C	4	0	8	0	0
3	D	4	0	8	1	0
4	A	23	0	0	0	0
4	B	24	0	0	0	0
4	C	29	0	0	3	0
4	D	19	0	0	0	0
4	E	29	0	0	0	0
All	All	8648	0	8173	200	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 12.

All (200) 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:A:301:IM4:O16	2:A:301:IM4:N15	1.57	1.38
1:D:15:ASN:O	1:D:16:ARG:HG3	1.37	1.20
1:C:127:CYS:CB	1:C:140:CYS:SG	2.36	1.13
1:A:93:TYR:HB2	3:A:404:IPA:H32	1.19	1.11
1:E:17:SER:C	1:E:19:MET:HG3	1.78	1.07
1:A:93:TYR:HB2	3:A:404:IPA:C3	1.86	1.04
1:C:97:ARG:HG2	1:C:97:ARG:HH11	0.92	1.04
1:E:17:SER:O	1:E:19:MET:HG3	1.57	1.03
1:C:127:CYS:SG	1:C:140:CYS:CB	2.48	1.01
1:C:97:ARG:HG2	1:C:97:ARG:NH1	1.68	1.00
1:E:15:ASN:O	1:E:16:ARG:HD2	1.62	0.99
1:C:97:ARG:HH11	1:C:97:ARG:CG	1.79	0.96
1:B:15:ASN:O	1:B:16:ARG:HG3	1.72	0.90
1:B:7:MET:HE3	1:C:20:TYR:N	1.88	0.87
1:E:15:ASN:ND2	1:E:16:ARG:HH11	1.72	0.87
1:A:68:ASP:HB3	1:A:71:GLU:OE2	1.75	0.86
1:B:15:ASN:C	1:B:16:ARG:HD2	2.00	0.85
1:E:208:ARG:HA	1:E:208:ARG:NH1	1.93	0.84
1:B:15:ASN:O	1:B:16:ARG:CG	2.30	0.79
1:E:15:ASN:O	1:E:16:ARG:CD	2.30	0.79
1:B:15:ASN:O	1:B:16:ARG:CD	2.30	0.79
1:B:15:ASN:O	1:B:16:ARG:HD2	1.80	0.79
1:C:35:PHE:CE1	1:C:56:GLU:HG3	2.19	0.77
2:D:304:IM4:N11	2:D:304:IM4:O16	2.09	0.76
1:E:17:SER:HB3	1:E:19:MET:N	2.02	0.75
1:C:93:TYR:CE2	1:C:188:TYR:OH	2.39	0.74
1:A:21:PRO:HD3	1:E:7:MET:HE3	1.69	0.74
1:C:93:TYR:HE2	1:C:188:TYR:OH	1.70	0.74
1:C:97:ARG:NH1	1:C:97:ARG:CG	2.41	0.73
1:A:190:CYS:HB3	2:A:301:IM4:O16	1.87	0.73
1:E:57:GLN:HG3	1:E:118:ILE:HD13	1.71	0.72
1:B:172:SER:N	1:B:207:ARG:NH2	2.38	0.72
1:A:168:TYR:CE1	1:A:176:ILE:HD11	2.25	0.72
1:E:15:ASN:HD22	1:E:16:ARG:HH11	1.37	0.72
1:C:173:LYS:HE3	1:D:45:SER:O	1.89	0.72
1:A:15:ASN:O	1:A:16:ARG:C	2.34	0.71
1:D:15:ASN:C	1:D:16:ARG:HG3	2.14	0.71
1:E:17:SER:CB	1:E:19:MET:N	2.54	0.70
1:E:97[B]:ARG:CG	1:E:97[B]:ARG:HH11	2.05	0.69
1:E:15:ASN:ND2	1:E:16:ARG:NH1	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:HB3	1:B:207:ARG:HH11	1.58	0.68
1:B:6:LEU:HD23	1:C:21:PRO:HG2	1.76	0.68
1:C:207:ARG:HD2	4:C:421:HOH:O	1.95	0.67
1:E:17:SER:C	1:E:19:MET:CG	2.63	0.67
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.35	0.67
1:B:172:SER:N	1:B:207:ARG:HH21	1.93	0.67
1:A:93:TYR:CB	3:A:404:IPA:H32	2.11	0.67
1:D:15:ASN:O	1:D:16:ARG:CG	2.30	0.66
1:B:104:PRO:HG3	1:C:89:ASP:HB2	1.77	0.66
1:E:15:ASN:O	1:E:16:ARG:CG	2.44	0.66
1:B:15:ASN:O	1:B:16:ARG:NH1	2.30	0.65
1:B:16:ARG:HD2	1:B:16:ARG:N	2.12	0.65
1:C:143:LYS:NZ	1:C:184:GLN:HE22	1.96	0.64
1:E:168:TYR:CE1	1:E:176:ILE:HD11	2.32	0.63
1:A:168:TYR:CE1	1:A:176:ILE:CD1	2.81	0.63
1:E:61:LYS:HD3	1:E:114:SER:HB3	1.81	0.63
2:A:301:IM4:O17	2:A:301:IM4:N11	2.21	0.63
1:E:57:GLN:HG3	1:E:118:ILE:CD1	2.29	0.62
1:A:207:ARG:HH21	1:A:207:ARG:HG3	1.65	0.61
1:B:7:MET:CE	1:C:20:TYR:N	2.62	0.61
1:E:208:ARG:HA	1:E:208:ARG:HH11	1.63	0.61
1:A:79:ARG:HG3	1:A:108:VAL:HG22	1.83	0.60
1:B:6:LEU:HD23	1:C:21:PRO:CG	2.32	0.60
1:E:63:ASN:C	1:E:65:LEU:H	2.10	0.59
1:A:122:ARG:HD2	1:B:96:THR:O	2.02	0.59
1:B:15:ASN:N	1:B:15:ASN:OD1	2.36	0.59
1:C:155:ASP:OD2	1:C:157:LYS:HE2	2.02	0.59
1:D:118:ILE:HD12	3:D:402:IPA:H13	1.84	0.59
1:A:207:ARG:O	1:A:208:ARG:HG3	2.03	0.58
1:C:139:THR:OG1	1:C:203:LYS:HG2	2.04	0.58
1:A:96:THR:O	1:E:122:ARG:HD2	2.04	0.58
1:C:25:LYS:HE3	1:C:153:GLU:OE2	2.03	0.57
1:B:36:THR:HG21	1:B:55:TYR:CZ	2.40	0.57
1:A:186:GLN:HG2	1:A:197:ASP:OD2	2.05	0.57
1:B:39:ASP:OD1	1:B:172:SER:HB2	2.05	0.57
1:B:14:PHE:C	1:B:15:ASN:OD1	2.49	0.56
1:E:17:SER:HB2	1:E:19:MET:N	2.21	0.56
1:E:168:TYR:CZ	1:E:176:ILE:CD1	2.88	0.56
1:E:71:GLU:HG2	1:E:71:GLU:O	2.06	0.56
1:D:139:THR:OG1	1:D:203:LYS:HG2	2.06	0.56
2:A:301:IM4:N2	1:E:118:ILE:HG13	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:TYR:CE1	2:D:304:IM4:O16	2.59	0.55
1:E:15:ASN:HD22	1:E:16:ARG:NH1	2.04	0.55
1:D:141:ALA:HA	1:D:200:LEU:O	2.06	0.54
1:D:88:PRO:HB2	1:D:90:ILE:HD12	1.88	0.54
1:B:15:ASN:HA	1:B:18:PRO:HG3	1.90	0.54
1:E:168:TYR:CZ	1:E:176:ILE:HD11	2.43	0.54
1:D:88:PRO:HB2	1:D:90:ILE:CD1	2.38	0.54
1:C:143:LYS:HZ3	1:C:184:GLN:HE22	1.55	0.53
1:D:122:ARG:HD2	1:E:96:THR:O	2.09	0.53
1:D:39:ASP:OD1	1:D:172:SER:HB2	2.07	0.53
2:B:302:IM4:O16	2:B:302:IM4:N11	2.38	0.53
1:A:207:ARG:HG3	1:A:207:ARG:NH2	2.23	0.53
1:B:91:THR:HG22	1:B:92:ALA:O	2.08	0.53
2:C:303:IM4:N11	2:C:303:IM4:O17	2.42	0.53
1:A:151:GLY:HA3	1:A:196:ILE:CD1	2.39	0.52
1:E:15:ASN:O	1:E:16:ARG:HG3	2.08	0.52
1:A:151:GLY:CA	1:A:196:ILE:HD12	2.40	0.52
1:D:35:PHE:CE1	1:D:56:GLU:HG3	2.45	0.52
1:D:147:TRP:O	2:D:304:IM4:H13	2.09	0.52
1:D:56:GLU:O	1:D:119:PRO:HD2	2.10	0.52
1:A:56:GLU:OE2	1:A:58:GLN:NE2	2.36	0.51
1:A:175:GLU:OE2	1:A:205:ARG:NH2	2.42	0.51
1:D:191:CYS:HB3	1:D:193:GLU:OE1	2.11	0.51
1:E:97[B]:ARG:HH11	1:E:97[B]:ARG:HG3	1.76	0.50
1:E:91:THR:HG22	1:E:92:ALA:O	2.12	0.50
1:A:17:SER:O	1:A:18:PRO:O	2.30	0.50
1:E:176:ILE:HD12	1:E:176:ILE:N	2.27	0.50
1:E:181:GLN:HG3	1:E:181:GLN:O	2.11	0.50
1:C:122:ARG:HD2	1:D:96:THR:O	2.12	0.50
1:B:16:ARG:CD	1:B:16:ARG:N	2.74	0.49
1:D:54:TYR:CD1	1:D:54:TYR:C	2.89	0.49
1:A:19:MET:O	1:E:7:MET:HE2	2.11	0.49
1:D:190:CYS:C	1:D:191:CYS:SG	2.95	0.49
1:E:63:ASN:C	1:E:65:LEU:N	2.71	0.49
1:B:59:ARG:NH1	1:B:159:ASP:OD1	2.46	0.49
1:E:168:TYR:CE1	1:E:176:ILE:CD1	2.95	0.49
1:E:129:PRO:O	1:E:132:VAL:HG22	2.13	0.49
1:B:17:SER:O	1:B:18:PRO:O	2.30	0.48
1:A:129:PRO:O	1:A:132:VAL:HB	2.13	0.48
1:A:175:GLU:HB3	1:A:207:ARG:NH2	2.29	0.48
1:B:56:GLU:O	1:B:119:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.54	0.48
1:A:15:ASN:O	1:A:17:SER:C	2.57	0.47
1:E:56:GLU:O	1:E:119:PRO:HD2	2.14	0.47
1:C:97:ARG:NH1	4:C:402:HOH:O	2.23	0.47
1:E:170:ALA:O	1:E:207:ARG:NH1	2.46	0.47
1:B:171:SER:C	1:B:207:ARG:HH21	2.22	0.47
1:D:60:TRP:CH2	1:D:88:PRO:HD2	2.50	0.47
1:A:91:THR:HG22	1:A:92:ALA:O	2.15	0.47
1:C:93:TYR:HE2	1:C:188:TYR:CZ	2.33	0.47
1:D:17:SER:HA	1:D:18:PRO:HD3	1.29	0.47
1:A:7:MET:HE2	1:B:18:PRO:O	2.15	0.47
1:A:37:LEU:HD23	1:A:176:ILE:HD13	1.97	0.47
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.55	0.47
1:B:15:ASN:C	1:B:16:ARG:CD	2.77	0.46
1:C:147:TRP:CH2	2:C:303:IM4:H12	2.50	0.46
1:A:89:ASP:HB2	1:E:104:PRO:HG2	1.96	0.46
1:E:141:ALA:HA	1:E:200:LEU:O	2.16	0.46
1:B:190:CYS:HB3	2:B:302:IM4:O17	2.14	0.46
1:E:188:TYR:O	1:E:191:CYS:N	2.40	0.46
1:C:93:TYR:HE2	1:C:188:TYR:HH	1.40	0.46
1:E:73:GLY:O	1:E:74:ASN:HB2	2.16	0.46
1:A:151:GLY:CA	1:A:196:ILE:CD1	2.93	0.46
1:C:9:LEU:HB2	1:C:72:TYR:CD1	2.51	0.46
1:D:204:PHE:N	1:D:204:PHE:CD2	2.84	0.46
1:B:122:ARG:HD2	1:C:96:THR:O	2.16	0.46
1:D:16:ARG:O	1:D:17:SER:O	2.34	0.46
1:D:179:ALA:HA	1:D:201:VAL:O	2.16	0.46
1:D:81:SER:O	1:D:84:ASP:HB2	2.16	0.45
1:D:106:ILE:HB	1:E:148:VAL:HG11	1.98	0.45
1:A:207:ARG:HH21	1:A:207:ARG:CG	2.28	0.45
1:D:195:TYR:CE1	2:D:304:IM4:H8	2.52	0.45
1:A:20:TYR:CE1	1:A:22:GLY:HA2	2.52	0.45
1:D:195:TYR:C	1:D:196:ILE:HD13	2.42	0.45
1:C:139:THR:HG1	1:C:203:LYS:HG2	1.81	0.44
1:A:173:LYS:HA	1:A:173:LYS:HD2	1.70	0.44
1:B:173:LYS:HA	1:B:173:LYS:HD2	1.83	0.44
1:B:50:VAL:CG2	1:B:127:CYS:SG	3.03	0.44
1:E:143:LYS:NZ	1:E:184:GLN:HE22	2.16	0.44
1:B:18:PRO:O	1:B:19:MET:C	2.61	0.43
1:E:188:TYR:O	1:E:190:CYS:N	2.51	0.43
1:E:190:CYS:C	1:E:191:CYS:SG	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	1:B:18:PRO:HD3	1.80	0.43
1:B:61:LYS:HA	1:B:114:SER:HA	2.01	0.43
1:E:97[B]:ARG:HH11	1:E:97[B]:ARG:HG2	1.82	0.43
1:C:59:ARG:HD3	1:C:116:MET:HE3	1.99	0.43
1:A:16:ARG:O	1:A:17:SER:HB2	2.18	0.43
1:A:163:VAL:HG21	1:A:200:LEU:CD1	2.48	0.43
1:C:3:GLN:HE21	1:D:20:TYR:HD2	1.65	0.43
1:E:25:LYS:HE3	1:E:152:PHE:CD1	2.54	0.43
1:C:169:TYR:CZ	1:C:171:SER:HB2	2.53	0.43
1:E:208:ARG:HA	1:E:208:ARG:CZ	2.48	0.43
1:A:151:GLY:HA3	1:A:196:ILE:HD12	1.99	0.42
1:D:147:TRP:CZ3	2:D:304:IM4:H12	2.54	0.42
1:B:150:SER:HB2	1:B:193:GLU:HG2	2.01	0.42
1:B:15:ASN:C	1:B:16:ARG:HH11	2.24	0.42
1:E:51:ASP:HA	1:E:123:LEU:O	2.19	0.42
1:E:70:ASN:ND2	1:E:74:ASN:OD1	2.52	0.42
1:A:68:ASP:HA	1:A:69:PRO:HD2	1.68	0.41
1:B:147:TRP:CH2	2:B:302:IM4:H12	2.55	0.41
1:C:3:GLN:NE2	1:D:20:TYR:HD2	2.17	0.41
1:C:141:ALA:HA	1:C:200:LEU:O	2.20	0.41
1:E:-3:ASP:C	1:E:-1:LYS:N	2.78	0.41
1:A:148:VAL:HG21	1:E:106:ILE:HG21	2.02	0.41
1:B:97[B]:ARG:HG3	1:B:97[B]:ARG:HH11	1.85	0.41
1:E:65:LEU:HD23	1:E:65:LEU:HA	1.89	0.41
1:A:68:ASP:CB	1:A:71:GLU:OE2	2.57	0.41
1:C:11:SER:HA	1:C:15:ASN:HD22	1.85	0.41
1:D:79:ARG:N	1:D:79:ARG:HD2	2.36	0.41
1:E:61:LYS:HD3	1:E:114:SER:CB	2.50	0.41
1:C:15:ASN:C	1:C:16:ARG:HG3	2.43	0.41
1:D:66:MET:HE2	1:D:66:MET:HB3	1.91	0.40
1:E:55:TYR:HB3	1:E:120:ALA:HA	2.03	0.40
1:A:97[B]:ARG:HH21	1:A:97[B]:ARG:HG2	1.86	0.40
1:B:63:ASN:C	1:B:65:LEU:H	2.29	0.40
1:C:57:GLN:HB2	4:C:427:HOH:O	2.20	0.40
1:E:43:ALA:HA	1:E:50:VAL:HG22	2.03	0.40
1:A:44:ASP:C	1:A:44:ASP:OD2	2.65	0.40
1:D:169:TYR:CZ	1:D:171:SER:HB2	2.57	0.40

There are no symmetry-related clashes.

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	210/227 (92%)	202 (96%)	6 (3%)	2 (1%)	12	22
1	B	211/227 (93%)	203 (96%)	6 (3%)	2 (1%)	14	25
1	C	204/227 (90%)	199 (98%)	5 (2%)	0	100	100
1	D	210/227 (92%)	203 (97%)	5 (2%)	2 (1%)	12	22
1	E	208/227 (92%)	197 (95%)	9 (4%)	2 (1%)	12	22
All	All	1043/1135 (92%)	1004 (96%)	31 (3%)	8 (1%)	16	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	D	18	PRO
1	A	16	ARG
1	D	17	SER
1	B	19	MET
1	B	18	PRO
1	E	64	SER
1	E	21	PRO

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	193/205 (94%)	184 (95%)	9 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/205 (95%)	182 (94%)	12 (6%)	16	32
1	C	189/205 (92%)	177 (94%)	12 (6%)	16	31
1	D	193/205 (94%)	183 (95%)	10 (5%)	21	39
1	E	193/205 (94%)	173 (90%)	20 (10%)	7	12
All	All	962/1025 (94%)	899 (94%)	63 (6%)	15	30

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	38	GLN
1	A	55	TYR
1	A	57	GLN
1	A	71	GLU
1	A	142	VAL
1	A	154	ILE
1	A	171	SER
1	A	207	ARG
1	B	0	LEU
1	B	15	ASN
1	B	16	ARG
1	B	17	SER
1	B	20	TYR
1	B	64	SER
1	B	80	THR
1	B	142	VAL
1	B	150	SER
1	B	157	LYS
1	B	186	GLN
1	B	208	ARG
1	C	16	ARG
1	C	17	SER
1	C	25	LYS
1	C	80	THR
1	C	97	ARG
1	C	124	SER
1	C	154	ILE
1	C	160	THR
1	C	167	SER
1	C	189	SER
1	C	200	LEU

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Mol	Chain	Res	Type
1	C	208	ARG
1	D	-2	ASP
1	D	0	LEU
1	D	19	MET
1	D	20	TYR
1	D	64	SER
1	D	70	ASN
1	D	105	GLN
1	D	154	ILE
1	D	157	LYS
1	D	196	ILE
1	E	0	LEU
1	E	10	LYS
1	E	19	MET
1	E	25	LYS
1	E	61	LYS
1	E	64	SER
1	E	99	VAL
1	E	118	ILE
1	E	127	CYS
1	E	132	VAL
1	E	136	GLU
1	E	157	LYS
1	E	176	ILE
1	E	186	GLN
1	E	190	CYS
1	E	196	ILE
1	E	200	LEU
1	E	206	GLU
1	E	207	ARG
1	E	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	74	ASN
1	A	121	GLN
1	A	184	GLN
1	A	187	HIS
1	B	1	HIS
1	B	70	ASN

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Mol	Chain	Res	Type
1	B	100	GLN
1	B	199	ASN
1	C	15	ASN
1	C	58	GLN
1	C	162	GLN
1	C	184	GLN
1	C	186	GLN
1	C	187	HIS
1	C	199	ASN
1	D	58	GLN
1	D	70	ASN
1	D	105	GLN
1	D	187	HIS
1	E	15	ASN
1	E	58	GLN
1	E	70	ASN
1	E	184	GLN
1	E	186	GLN
1	E	199	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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	IPA	C	401	-	3,3,3	0.56	0	3,3,3	0.39	0
2	IM4	B	302	-	15,18,18	2.70	3 (20%)	20,24,24	4.11	8 (40%)
2	IM4	C	303	-	15,18,18	2.92	6 (40%)	20,24,24	3.88	9 (45%)
3	IPA	D	402	-	3,3,3	0.79	0	3,3,3	0.34	0
3	IPA	A	404	-	3,3,3	0.18	0	3,3,3	0.75	0
2	IM4	A	301	-	15,18,18	3.05	4 (26%)	20,24,24	4.18	9 (45%)
2	IM4	D	304	-	15,18,18	3.22	6 (40%)	20,24,24	3.72	12 (60%)

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	IM4	A	301	-	-	0/6/18/18	0/2/2/2
2	IM4	B	302	-	-	0/6/18/18	0/2/2/2
2	IM4	C	303	-	-	0/6/18/18	0/2/2/2
2	IM4	D	304	-	-	0/6/18/18	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	IM4	C1-CL7	-10.32	1.52	1.74
2	D	304	IM4	C1-CL7	-10.08	1.53	1.74
2	C	303	IM4	C1-CL7	-9.52	1.54	1.74
2	B	302	IM4	C1-CL7	-9.32	1.54	1.74
2	D	304	IM4	C8-C4	3.46	1.57	1.51
2	A	301	IM4	C6-C5	3.08	1.43	1.38
2	A	301	IM4	C8-C4	3.05	1.56	1.51
2	C	303	IM4	C1-N2	3.03	1.38	1.32
2	D	304	IM4	C3-C4	2.89	1.45	1.38
2	A	301	IM4	C1-N2	2.88	1.38	1.32
2	C	303	IM4	C8-N9	2.85	1.51	1.46
2	D	304	IM4	C1-N2	2.60	1.38	1.32
2	B	302	IM4	C1-N2	2.51	1.37	1.32
2	C	303	IM4	C10-N9	-2.19	1.31	1.35
2	C	303	IM4	C8-C4	2.15	1.55	1.51
2	C	303	IM4	C6-C1	2.12	1.42	1.37
2	D	304	IM4	C6-C5	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	IM4	C6-C5	2.02	1.42	1.38
2	D	304	IM4	C10-N9	-2.01	1.31	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	IM4	N11-C10-N14	-10.12	122.70	132.61
2	C	303	IM4	C3-N2-C1	9.47	127.71	116.33
2	B	302	IM4	N9-C10-N14	9.12	122.53	117.27
2	A	301	IM4	C3-N2-C1	8.85	126.96	116.33
2	A	301	IM4	C6-C1-N2	-8.33	112.78	124.87
2	A	301	IM4	N11-C10-N14	-7.93	124.85	132.61
2	D	304	IM4	N11-C10-N9	7.91	114.98	110.00
2	B	302	IM4	N11-C10-N9	7.58	114.77	110.00
2	A	301	IM4	N9-C10-N14	6.89	121.24	117.27
2	C	303	IM4	N11-C10-N14	-6.62	126.13	132.61
2	D	304	IM4	C5-C6-C1	6.21	123.58	117.36
2	A	301	IM4	N11-C10-N9	6.09	113.84	110.00
2	C	303	IM4	C6-C1-N2	-6.01	116.14	124.87
2	C	303	IM4	N11-C10-N9	5.91	113.72	110.00
2	D	304	IM4	C3-N2-C1	5.61	123.06	116.33
2	B	302	IM4	C3-N2-C1	5.55	123.00	116.33
2	D	304	IM4	CL7-C1-N2	5.45	126.18	115.98
2	C	303	IM4	C4-C3-N2	-5.41	115.95	123.99
2	D	304	IM4	C6-C1-N2	-5.39	117.05	124.87
2	D	304	IM4	N11-C10-N14	-5.20	127.52	132.61
2	C	303	IM4	N9-C10-N14	4.98	120.14	117.27
2	B	302	IM4	C6-C1-N2	-4.98	117.64	124.87
2	C	303	IM4	CL7-C1-N2	4.58	124.56	115.98
2	A	301	IM4	C5-C6-C1	4.25	121.61	117.36
2	D	304	IM4	C8-N9-C10	-3.77	121.44	124.97
2	B	302	IM4	C5-C6-C1	3.73	121.09	117.36
2	D	304	IM4	C8-N9-C13	3.67	130.45	121.00
2	A	301	IM4	CL7-C1-N2	3.48	122.50	115.98
2	D	304	IM4	C6-C5-C4	-2.87	117.22	121.00
2	A	301	IM4	C6-C1-CL7	2.66	124.70	119.18
2	D	304	IM4	C8-C4-C5	-2.62	115.91	120.75
2	B	302	IM4	CL7-C1-N2	2.29	120.27	115.98
2	C	303	IM4	C5-C4-C3	2.26	120.42	117.10
2	B	302	IM4	C8-N9-C13	2.25	126.79	121.00
2	D	304	IM4	C4-C3-N2	-2.23	120.68	123.99
2	D	304	IM4	C8-C4-C3	2.16	125.75	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	IM4	C8-N9-C13	2.13	126.47	121.00
2	C	303	IM4	C8-N9-C13	2.04	126.25	121.00

There are no chirality outliers.

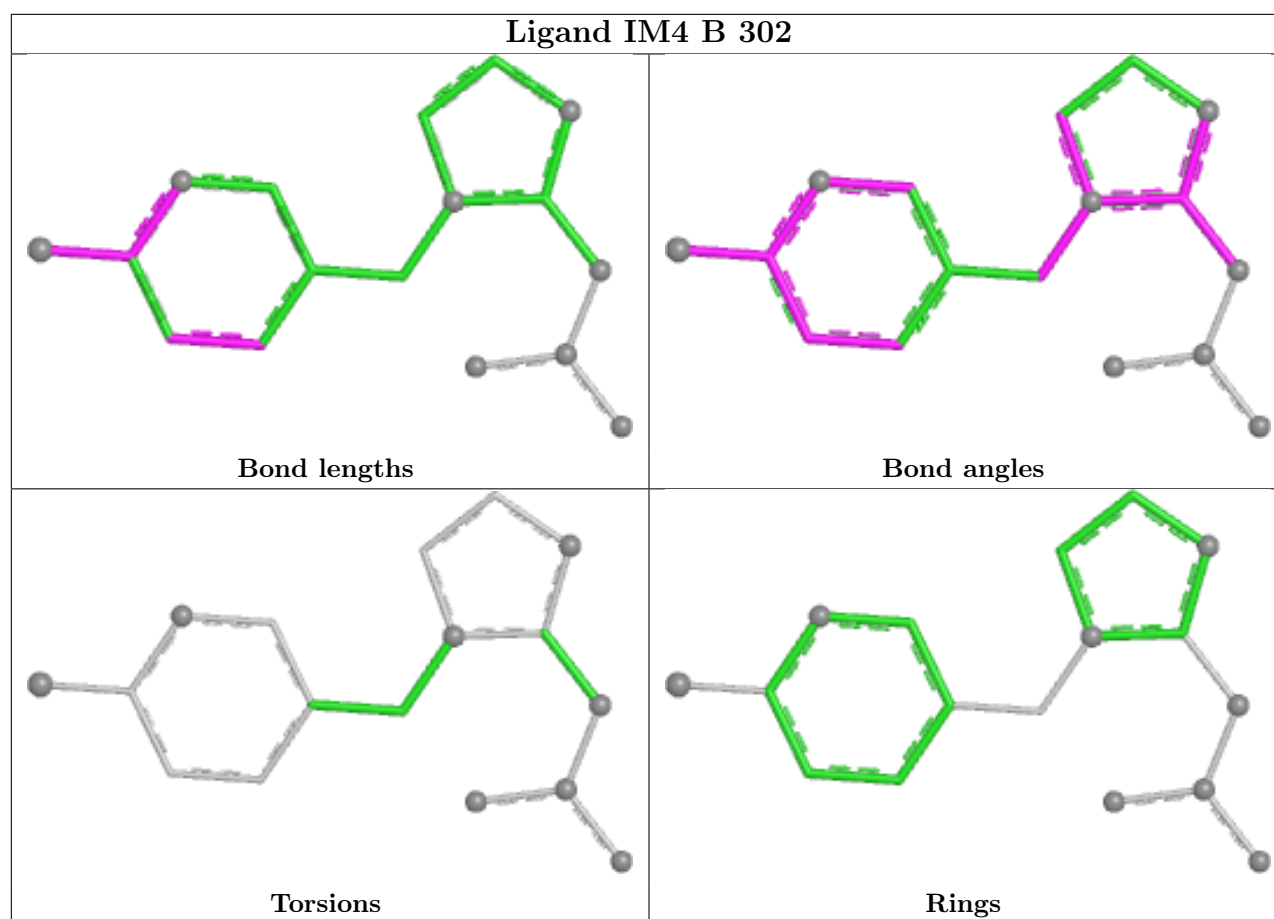
There are no torsion outliers.

There are no ring outliers.

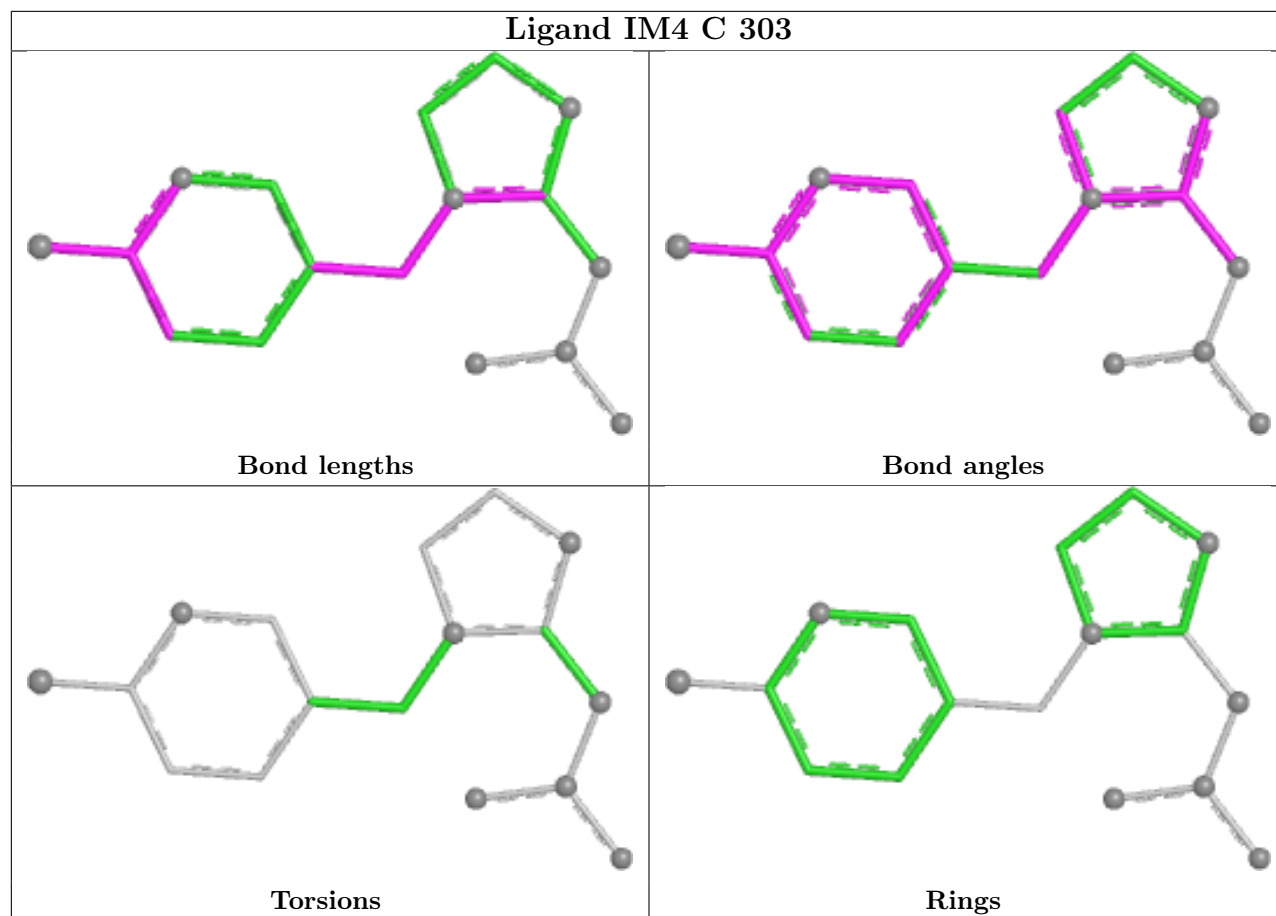
6 monomers are involved in 18 short contacts:

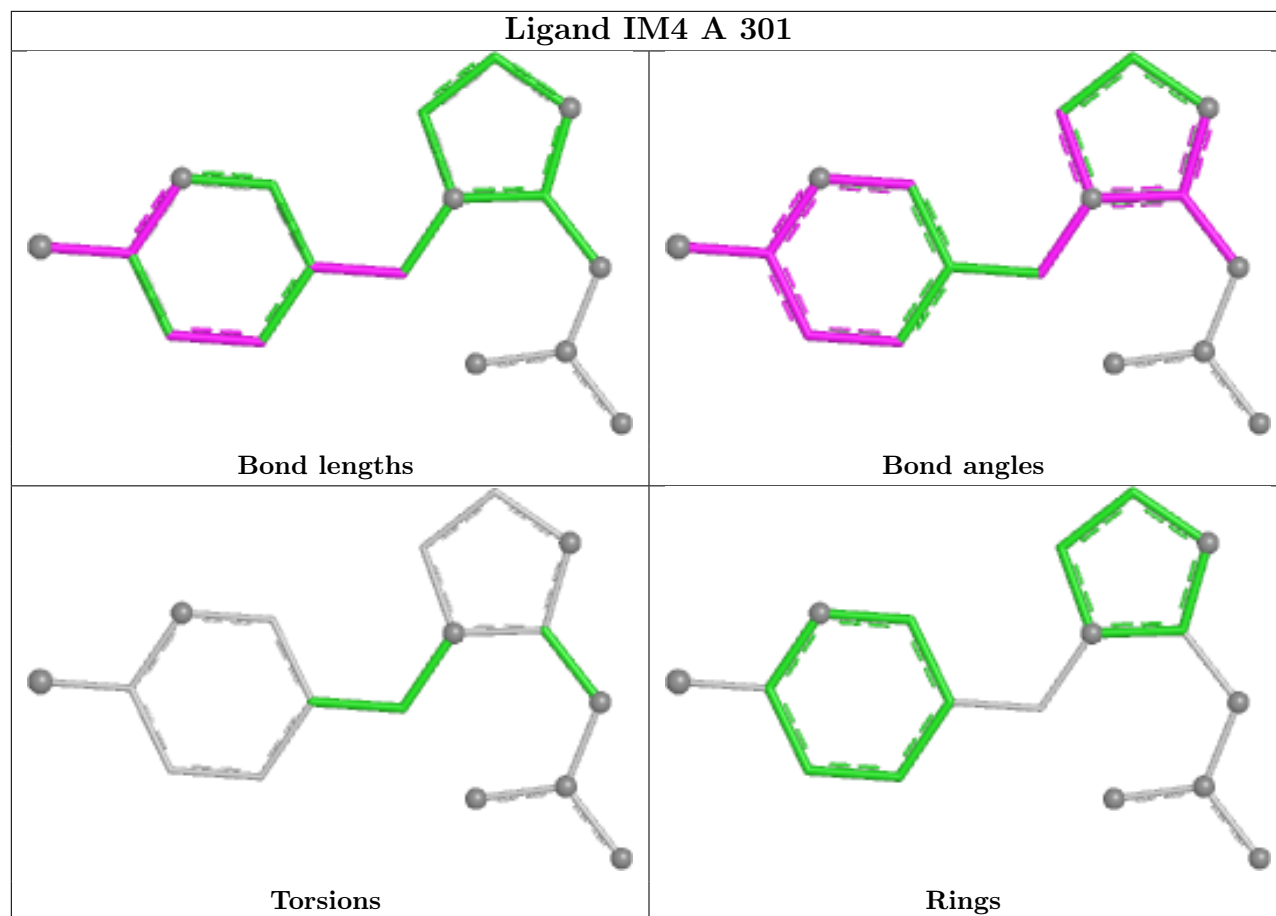
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	IM4	3	0
2	C	303	IM4	2	0
3	D	402	IPA	1	0
3	A	404	IPA	3	0
2	A	301	IM4	4	0
2	D	304	IM4	5	0

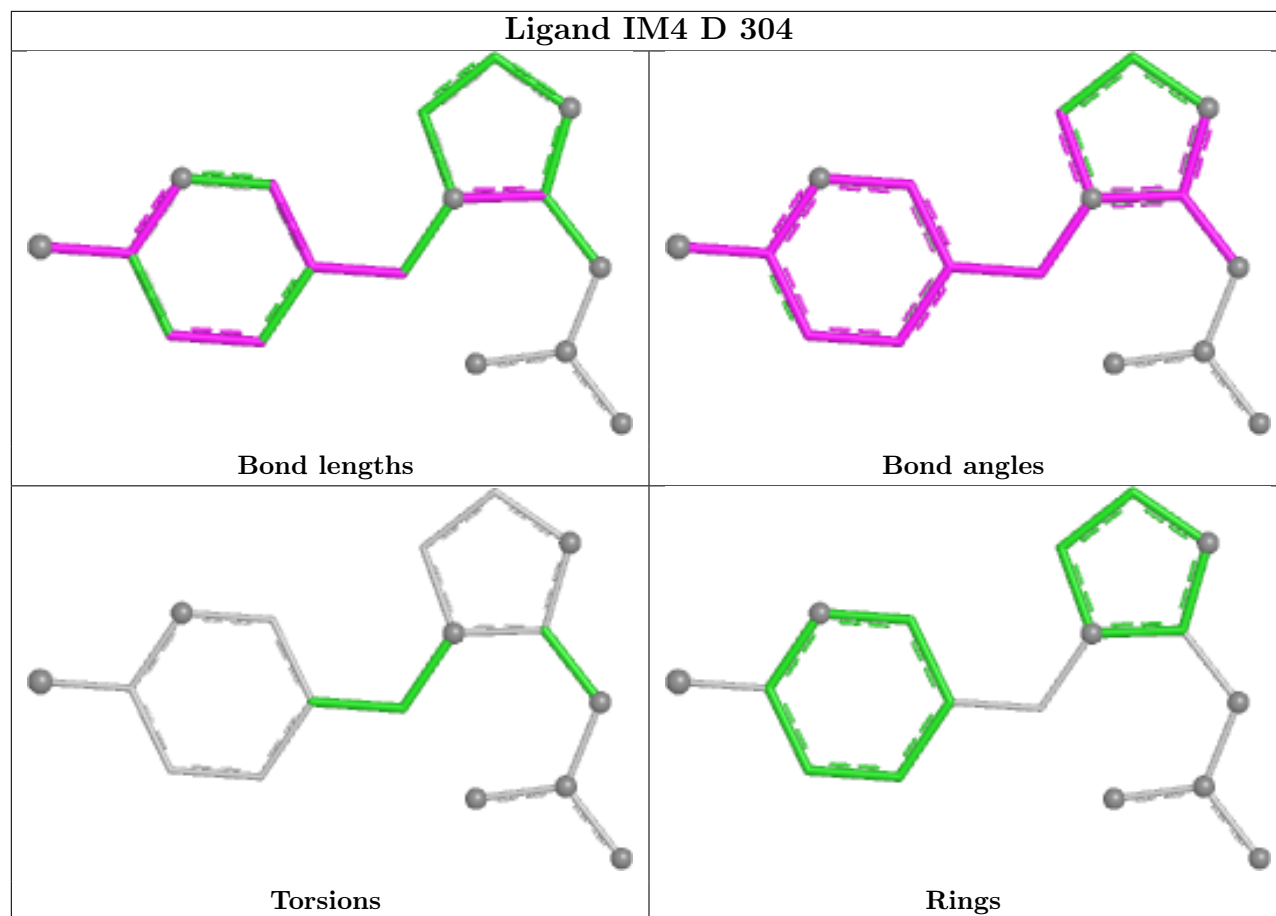
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 IM4 C 303







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	211/227 (92%)	-0.10	7 (3%)	49	45	14, 37, 58, 84	1 (0%)
1	B	212/227 (93%)	-0.17	4 (1%)	66	63	13, 35, 66, 88	1 (0%)
1	C	208/227 (91%)	-0.17	5 (2%)	59	56	24, 35, 56, 84	0
1	D	212/227 (93%)	0.02	8 (3%)	44	40	27, 36, 59, 88	0
1	E	211/227 (92%)	-0.15	5 (2%)	59	56	16, 36, 63, 84	1 (0%)
All	All	1054/1135 (92%)	-0.12	29 (2%)	55	51	13, 36, 62, 88	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	MET	4.9
1	B	19	MET	4.2
1	C	17	SER	4.0
1	E	189	SER	4.0
1	A	19	MET	3.7
1	E	-3	ASP	3.6
1	E	190	CYS	3.4
1	B	18	PRO	3.3
1	D	-3	ASP	3.1
1	B	7	MET	3.0
1	B	17	SER	3.0
1	A	-2	ASP	2.9
1	D	16	ARG	2.9
1	D	18	PRO	2.8
1	E	208	ARG	2.7
1	A	18	PRO	2.6
1	A	0	LEU	2.6
1	C	15	ASN	2.5
1	D	93	TYR	2.3
1	A	208	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1	HIS	2.3
1	D	17	SER	2.2
1	C	208	ARG	2.2
1	A	14	PHE	2.2
1	D	208	ARG	2.2
1	A	17	SER	2.1
1	C	93	TYR	2.1
1	D	1	HIS	2.1
1	E	14	PHE	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](#)

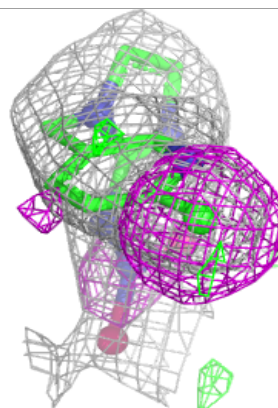
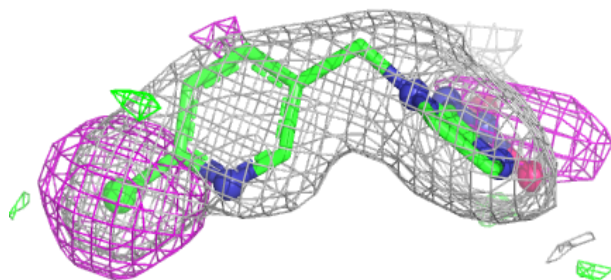
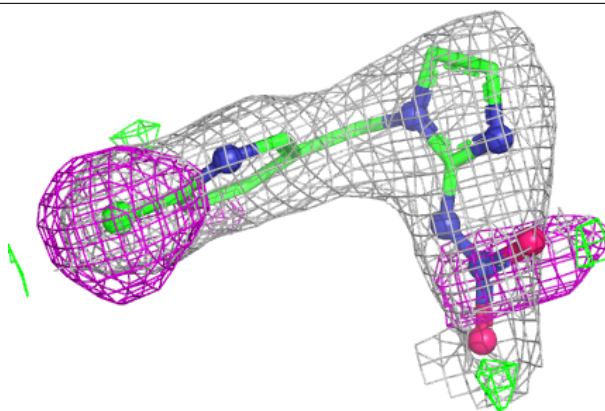
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IM4	A	301	17/17	0.83	0.16	13,35,47,47	0
2	IM4	C	303	17/17	0.83	0.14	7,32,39,43	0
2	IM4	D	304	17/17	0.86	0.16	28,45,58,62	0
2	IM4	B	302	17/17	0.87	0.13	16,34,47,50	0
3	IPA	A	404	4/4	0.87	0.21	56,56,56,56	0
3	IPA	D	402	4/4	0.91	0.16	43,44,45,45	0
3	IPA	C	401	4/4	0.95	0.10	38,38,39,40	0

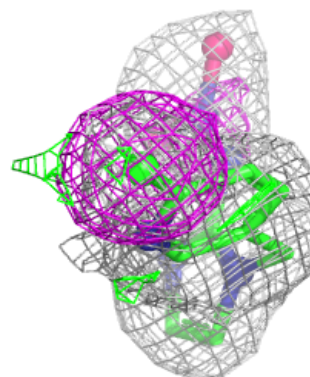
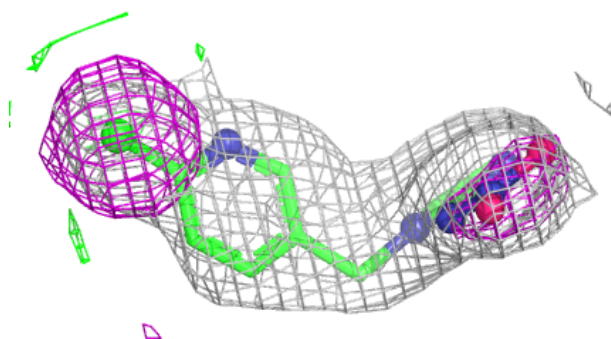
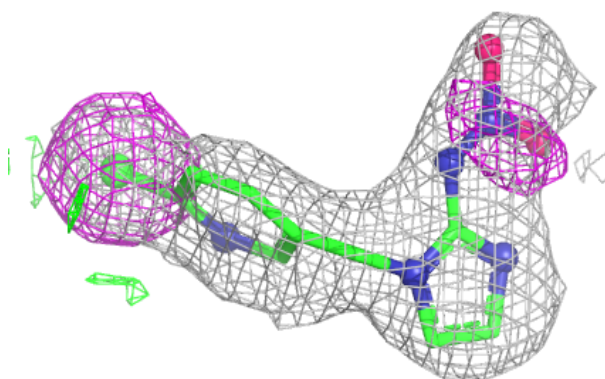
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IM4 A 301:

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

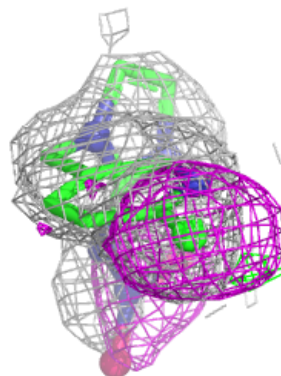
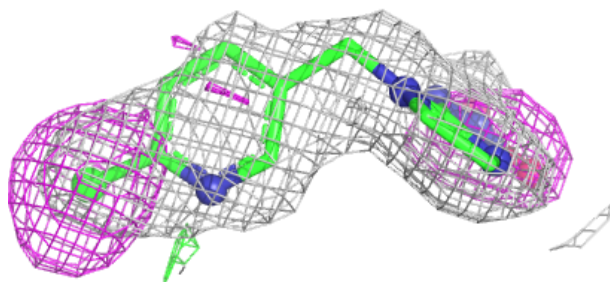
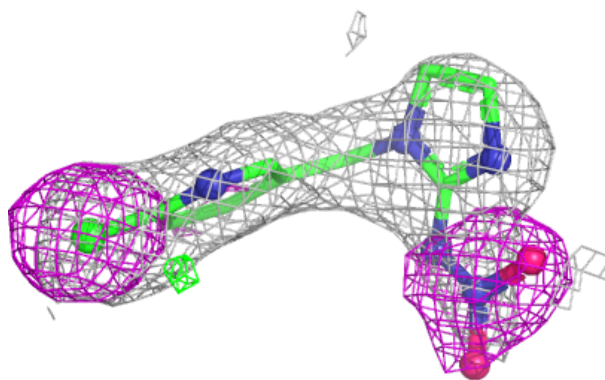
**Electron density around IM4 C 303:**

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

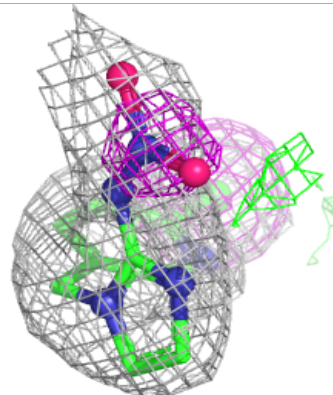
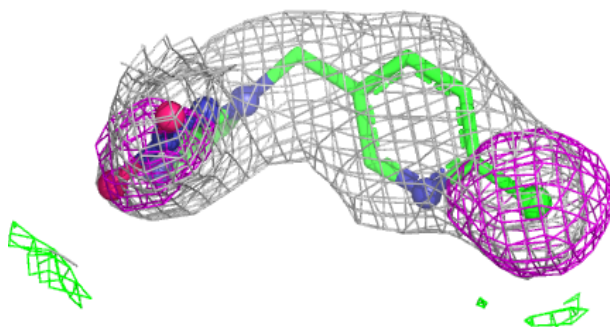
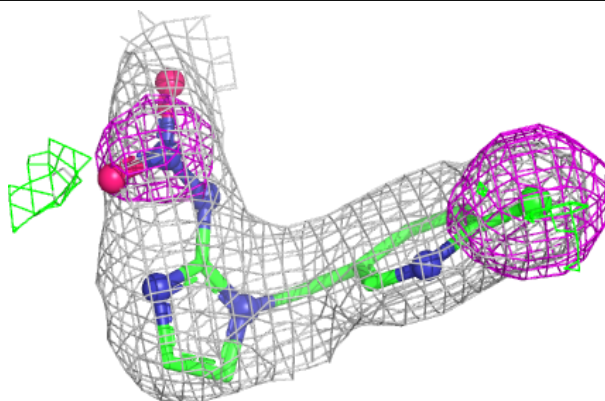


Electron density around IM4 D 304:

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

**Electron density around IM4 B 302:**

$2mF_o-DF_c$ (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.