



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 04:13 PM EDT

PDB ID : 7LPS
Title : Crystal structure of DDB1-CRBN-ALV1 complex bound to Helios (IKZF2 ZF2)
Authors : Nowak, R.P.; Fischer, E.S.
Deposited on : 2021-02-12
Resolution : 3.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

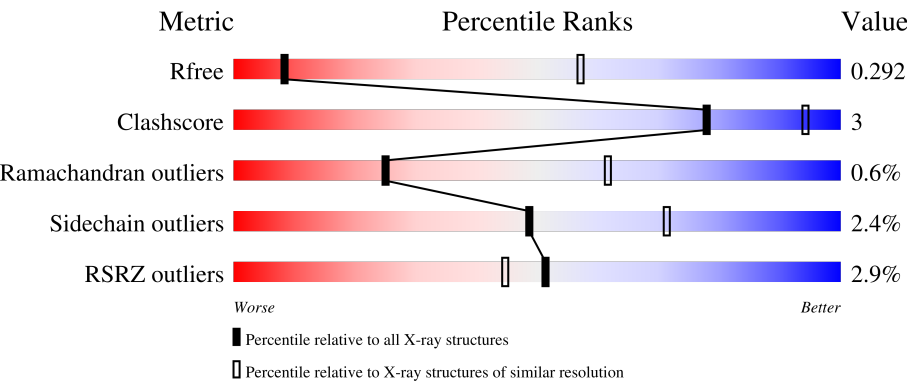
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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 <=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	1140	<div><div>%</div><div>63%5%31%</div></div>
1	D	1140	<div><div>8%</div><div>63%5%31%</div></div>
1	G	1140	<div><div>%</div><div>62%6%32%</div></div>
1	J	1140	<div><div>%</div><div>63%5%32%</div></div>
2	B	390	<div><div></div><div>86%11%..</div></div>

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Mol	Chain	Length	Quality of chain
2	E	390	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>85%</div><div>12%</div><div>..</div></div></div>
2	H	390	<div><div><div></div><div></div><div></div></div><div>85%</div><div>12%</div><div>..</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 37550 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6066	3857	1014	1161	34			
1	D	781	Total	C	N	O	S	0	0	0
			6066	3857	1014	1161	34			
1	G	779	Total	C	N	O	S	0	0	0
			6051	3848	1011	1158	34			
1	J	779	Total	C	N	O	S	0	0	0
			6051	3848	1011	1158	34			

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			
2	E	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			
2	H	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			
2	K	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			

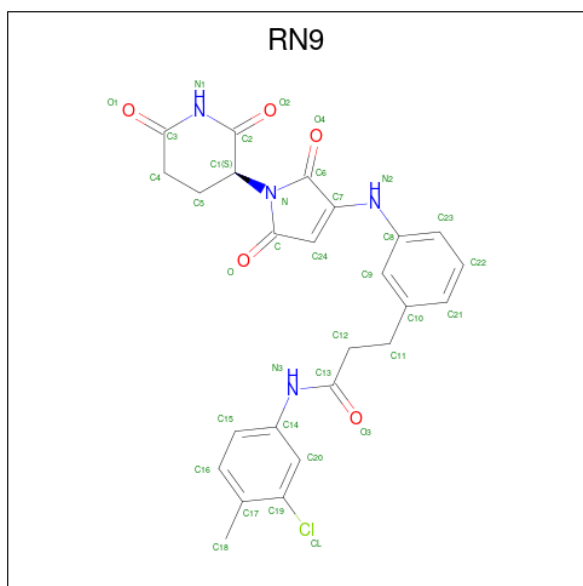
- Molecule 3 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	S	0	0	0
			226	139	47	38	2			
3	F	28	Total	C	N	O	S	0	0	0
			222	137	46	37	2			
3	I	29	Total	C	N	O	S	0	0	0
			226	139	47	38	2			
3	L	28	Total	C	N	O	S	0	0	0
			222	137	46	37	2			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 3-[3-[[1-[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]-2,5-bis(oxidanylidene)pyrrol-3-yl]amino]phenyl]- {N}-(3-chloranyl-4-methyl-phenyl)propanamide (three-letter code: RN9) (formula: C₂₅H₂₃ClN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	0
			35	25	1	4	5		
5	E	1	Total	C	Cl	N	O	0	0
			35	25	1	4	5		

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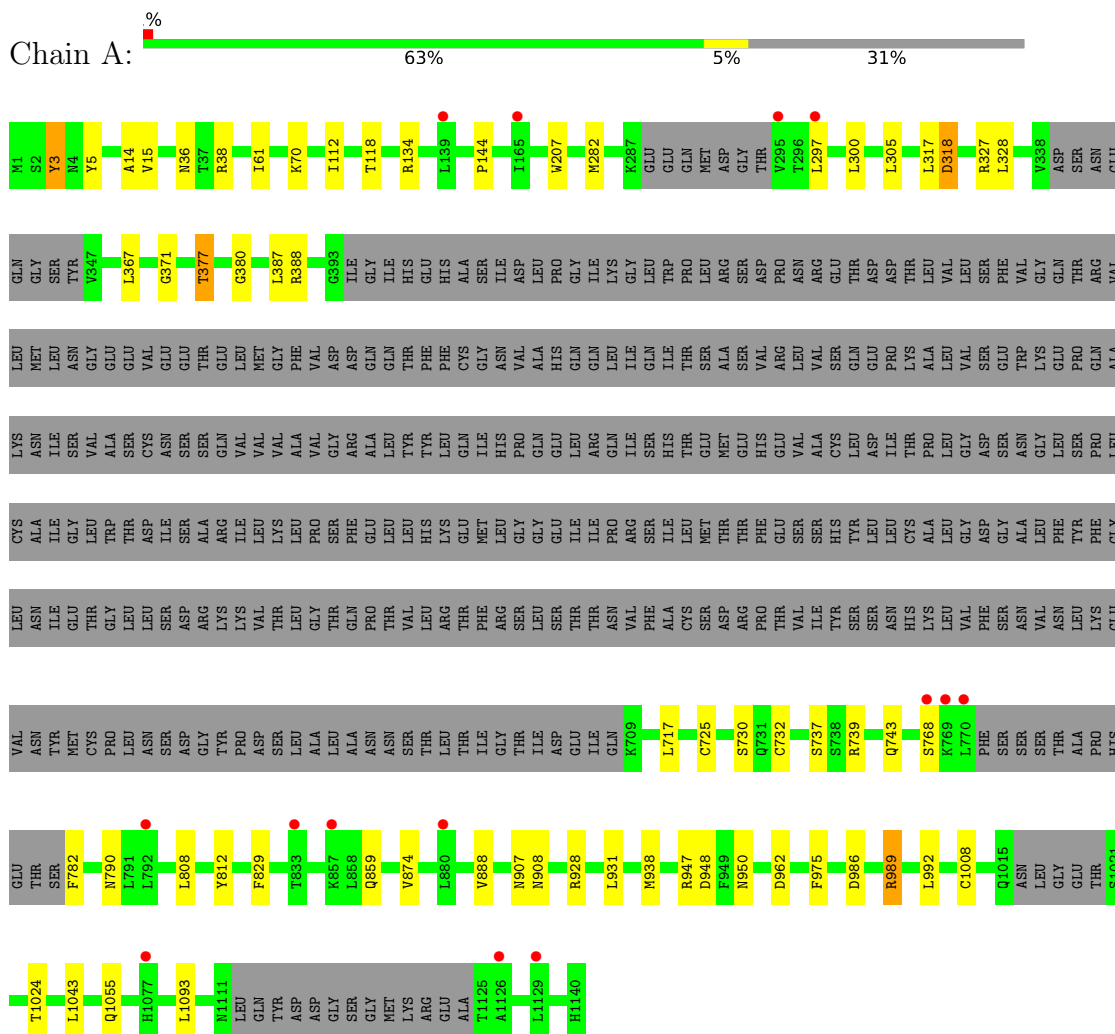
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	Cl	N	O	0	0
			35	25	1	4	5		
5	K	1	Total	C	Cl	N	O	0	0
			35	25	1	4	5		

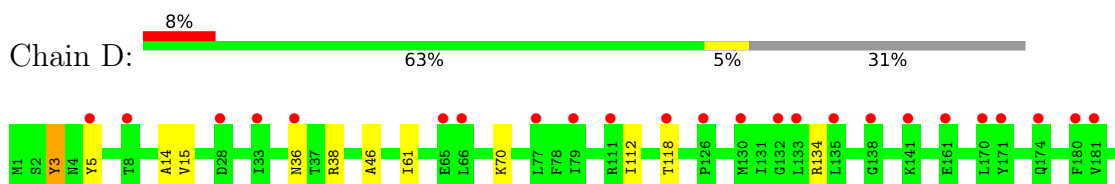
3 Residue-property plots

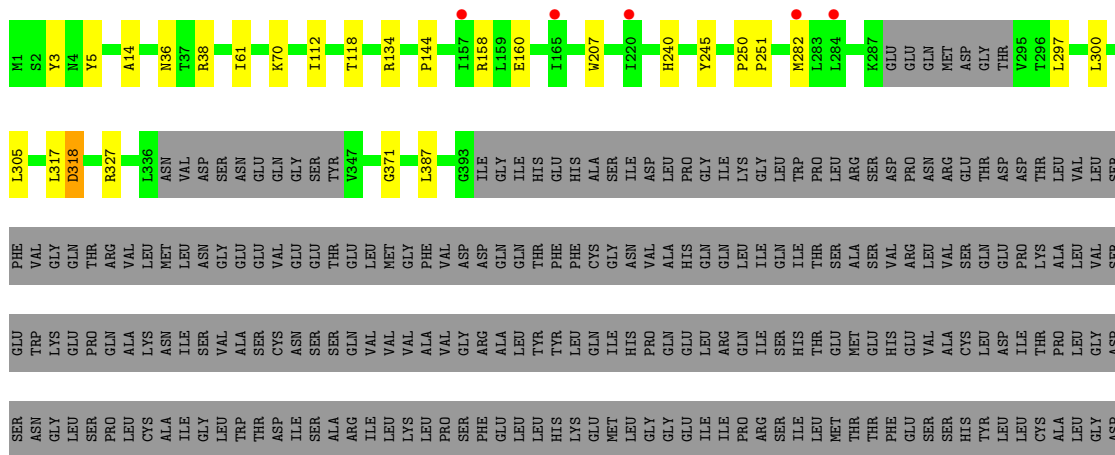
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

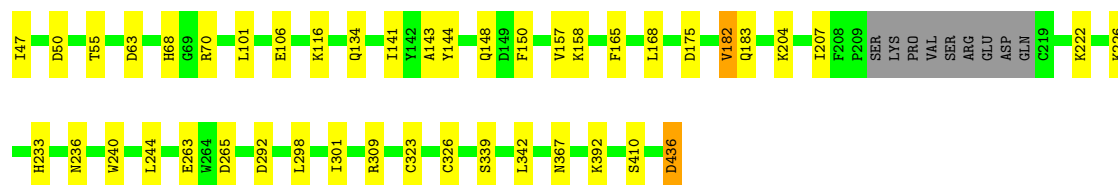
- Molecule 1: DNA damage-binding protein 1



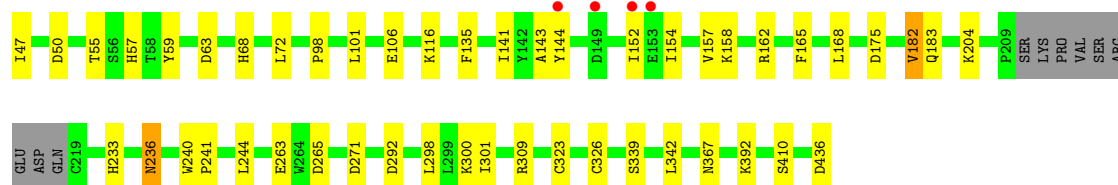
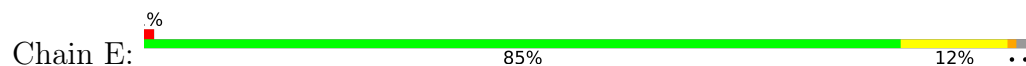
- Molecule 1: DNA damage-binding protein 1



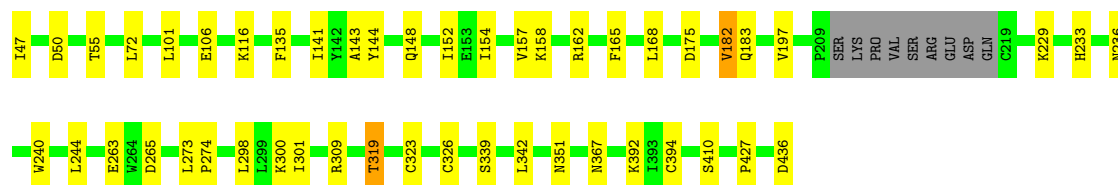
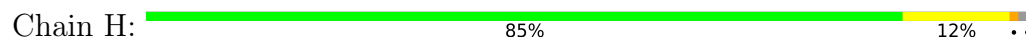




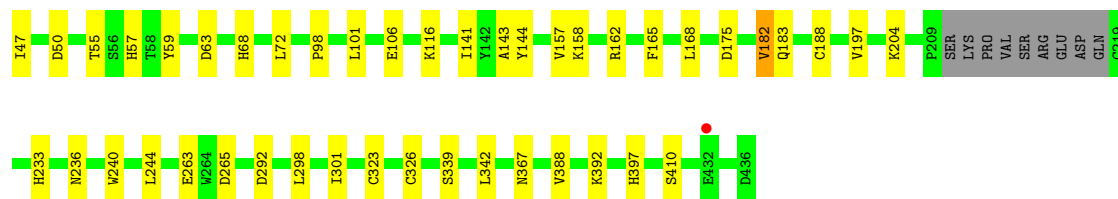
- Molecule 2: Protein cereblon



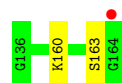
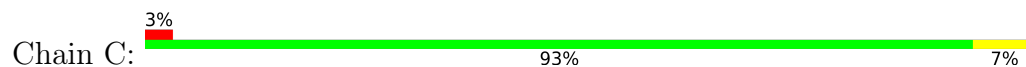
- Molecule 2: Protein cereblon



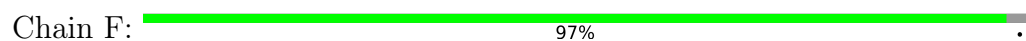
- Molecule 2: Protein cereblon



- Molecule 3: Zinc finger protein Helios



- Molecule 3: Zinc finger protein Helios



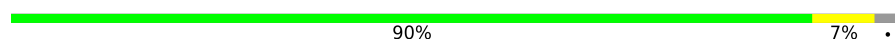


- Molecule 3: Zinc finger protein Helios

Chain I:  93% 7%



- Molecule 3: Zinc finger protein Helios

Chain L:  90% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.80Å 117.29Å 196.71Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	150.57 – 3.78 150.57 – 3.78	Depositor EDS
% Data completeness (in resolution range)	97.6 (150.57-3.78) 97.6 (150.57-3.78)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.78Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (11-DEC-2020)	Depositor
R, R_{free}	0.289 , 0.303 0.275 , 0.292	Depositor DCC
R_{free} test set	3410 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	105.6	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	37550	wwPDB-VP
Average B, all atoms (Å ²)	124.0	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 46.27 % 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 1.1724e-04. 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: RN9, ZN

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	0.23	0/6173	0.42	0/8361
1	D	0.22	0/6173	0.43	0/8361
1	G	0.22	0/6158	0.42	0/8340
1	J	0.22	0/6158	0.42	0/8340
2	B	0.22	0/3141	0.42	0/4264
2	E	0.22	0/3141	0.42	0/4264
2	H	0.21	0/3141	0.42	0/4264
2	K	0.21	0/3141	0.41	0/4264
3	C	0.19	0/231	0.42	0/307
3	F	0.20	0/227	0.39	0/302
3	I	0.20	0/231	0.40	0/307
3	L	0.19	0/227	0.38	0/302
All	All	0.22	0/38142	0.42	0/51676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6066	0	5984	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6066	0	5984	39	0
1	G	6051	0	5969	37	0
1	J	6051	0	5969	40	0
2	B	3068	0	3036	27	0
2	E	3068	0	3036	27	0
2	H	3068	0	3038	22	0
2	K	3068	0	3036	22	0
3	C	226	0	217	1	0
3	F	222	0	214	0	0
3	I	226	0	217	1	0
3	L	222	0	214	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	35	0	0	1	0
5	E	35	0	0	0	0
5	H	35	0	0	1	0
5	K	35	0	0	0	0
All	All	37550	0	36914	218	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 3.

All (218) 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:A:70:LYS:HB2	2:E:63:ASP:HB3	1.55	0.88
2:B:68:HIS:CD2	1:D:197:LEU:HD13	2.12	0.85
1:J:739:ARG:NH1	1:J:790:ASN:HD21	1.83	0.76
1:D:14:ALA:HB1	1:D:327:ARG:HD2	1.71	0.70
1:A:14:ALA:HB1	1:A:327:ARG:HD2	1.74	0.69
1:G:14:ALA:HB1	1:G:327:ARG:HD2	1.73	0.69
1:J:231:ILE:HD13	1:J:240:HIS:CD2	2.28	0.68
2:K:57:HIS:HD1	2:K:59:TYR:HH	1.42	0.67
2:B:68:HIS:NE2	1:D:197:LEU:HD13	2.11	0.66
2:B:148:GLN:HB3	1:J:47:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:143:ALA:HB3	2:K:158:LYS:HB2	1.79	0.65
1:J:948:ASP:HB2	1:J:992:LEU:HB2	1.78	0.64
1:A:986:ASP:HA	1:A:989:ARG:HD3	1.79	0.64
2:H:143:ALA:HB3	2:H:158:LYS:HB2	1.80	0.64
1:A:144:PRO:HB3	2:E:68:HIS:CE1	2.33	0.63
2:E:57:HIS:HD1	2:E:59:TYR:HH	1.44	0.63
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.81	0.62
1:D:317:LEU:O	1:D:318:ASP:HB2	1.99	0.62
1:J:986:ASP:HA	1:J:989:ARG:HD3	1.81	0.62
1:G:785:GLU:HB2	2:H:229:LYS:NZ	2.14	0.62
1:J:317:LEU:O	1:J:318:ASP:HB2	1.99	0.62
2:E:143:ALA:HB3	2:E:158:LYS:HB2	1.81	0.61
2:E:309:ARG:HE	2:E:436:ASP:CG	2.04	0.61
1:A:317:LEU:O	1:A:318:ASP:HB2	2.00	0.61
1:D:739:ARG:NH1	1:D:790:ASN:HD21	1.97	0.61
1:G:317:LEU:O	1:G:318:ASP:HB2	2.00	0.60
1:J:63:VAL:HB	1:J:80:LEU:HB3	1.83	0.60
1:G:158:ARG:NE	1:J:158:ARG:HE	2.00	0.60
1:D:725:CYS:HG	1:D:829:PHE:HE1	1.50	0.58
2:K:298:LEU:HD12	2:K:301:ILE:HD12	1.86	0.58
1:G:986:ASP:HA	1:G:989:ARG:HD3	1.86	0.57
1:J:14:ALA:HB1	1:J:327:ARG:HD2	1.86	0.57
2:H:298:LEU:HD12	2:H:301:ILE:HD12	1.86	0.57
2:B:63:ASP:HB3	1:D:70:LYS:NZ	2.20	0.57
1:D:888:VAL:HG23	1:D:907:ASN:HD21	1.70	0.56
1:G:1055:GLN:HG2	1:G:1093:LEU:HD23	1.87	0.56
2:E:298:LEU:HD12	2:E:301:ILE:HD12	1.87	0.56
2:B:298:LEU:HD12	2:B:301:ILE:HD12	1.86	0.56
1:J:1055:GLN:HG2	1:J:1093:LEU:HD23	1.88	0.56
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	1.88	0.56
2:E:152:ILE:HD12	2:E:154:ILE:HD11	1.87	0.56
2:B:68:HIS:CD2	1:D:197:LEU:CD1	2.88	0.56
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.88	0.55
1:G:158:ARG:HE	1:J:158:ARG:NE	2.05	0.55
1:J:931:LEU:HD12	1:J:947:ARG:HB3	1.88	0.55
1:G:948:ASP:HB2	1:G:992:LEU:HB2	1.88	0.55
1:G:158:ARG:HE	1:J:158:ARG:HE	1.54	0.55
1:A:888:VAL:HG23	1:A:907:ASN:HD21	1.71	0.55
1:A:730:SER:HG	1:A:732:CYS:HG	1.53	0.54
1:G:888:VAL:HG23	1:G:907:ASN:HD21	1.72	0.54
1:D:931:LEU:HD12	1:D:947:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:785:GLU:HB2	2:H:229:LYS:HZ3	1.70	0.54
1:G:931:LEU:HD12	1:G:947:ARG:HB3	1.89	0.54
1:D:948:ASP:HB2	1:D:992:LEU:HB2	1.88	0.54
1:G:387:LEU:HG	1:G:717:LEU:HD11	1.89	0.54
1:G:118:THR:HB	1:G:134:ARG:HH22	1.73	0.54
1:A:931:LEU:HD12	1:A:947:ARG:HB3	1.90	0.53
1:A:739:ARG:NH1	1:A:790:ASN:HD21	2.07	0.53
1:J:952:ASN:HD22	1:J:1080:ARG:HH22	1.57	0.53
1:D:1055:GLN:HG2	1:D:1093:LEU:HD23	1.91	0.53
1:A:118:THR:HB	1:A:134:ARG:HH22	1.74	0.52
1:A:297:LEU:HD21	1:A:300:LEU:HD21	1.91	0.52
1:A:377:THR:HG23	1:A:388:ARG:HB2	1.91	0.52
2:B:70:ARG:HE	1:D:198:ARG:HB2	1.74	0.52
1:J:118:THR:HB	1:J:134:ARG:HH22	1.73	0.52
1:A:928:ARG:NH1	1:A:975:PHE:CE2	2.77	0.52
1:D:928:ARG:NH1	1:D:975:PHE:CE2	2.78	0.52
1:D:297:LEU:HD21	1:D:300:LEU:HD21	1.91	0.52
1:G:297:LEU:HD21	1:G:300:LEU:HD21	1.92	0.52
1:D:118:THR:HB	1:D:134:ARG:HH22	1.75	0.52
1:G:928:ARG:NH1	1:G:975:PHE:CE2	2.78	0.51
1:G:998:PHE:HB2	1:G:1088:PHE:CD1	2.45	0.51
1:G:928:ARG:HB3	1:G:950:ASN:O	2.11	0.51
1:D:928:ARG:HB3	1:D:950:ASN:O	2.11	0.51
1:G:158:ARG:HE	1:J:158:ARG:CD	2.24	0.51
1:J:905:HIS:ND1	1:J:907:ASN:ND2	2.58	0.51
1:A:144:PRO:CB	2:E:68:HIS:CE1	2.94	0.51
1:A:928:ARG:HB3	1:A:950:ASN:O	2.11	0.51
1:J:297:LEU:HD21	1:J:300:LEU:HD21	1.93	0.51
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.93	0.50
1:G:796:GLN:HE21	1:G:797:HIS:CE1	2.29	0.50
2:K:57:HIS:CE1	2:K:98:PRO:HG3	2.46	0.50
2:E:55:THR:HG21	2:E:342:LEU:HB2	1.94	0.50
1:A:743:GLN:HB3	1:A:782:PHE:HB3	1.93	0.50
2:B:68:HIS:CG	1:D:197:LEU:HD13	2.47	0.50
1:J:952:ASN:OD1	1:J:970:ASN:HB3	2.11	0.50
2:H:309:ARG:HE	2:H:436:ASP:CG	2.14	0.50
2:B:168:LEU:HD11	2:B:183:GLN:HB2	1.94	0.50
2:E:57:HIS:CE1	2:E:98:PRO:HG3	2.47	0.50
1:G:70:LYS:HB2	2:K:63:ASP:HB3	1.94	0.50
1:J:739:ARG:NH1	1:J:790:ASN:ND2	2.58	0.50
1:D:282:MET:HB2	1:D:305:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:55:THR:HG21	2:K:342:LEU:HB2	1.94	0.50
1:J:741:GLU:HG2	1:J:751:ALA:HA	1.93	0.49
2:B:150:PHE:HA	1:J:350:MET:HE3	1.94	0.49
2:K:168:LEU:HD11	2:K:183:GLN:HB2	1.94	0.49
1:G:282:MET:HB2	1:G:305:LEU:HD11	1.93	0.49
2:B:55:THR:HG21	2:B:342:LEU:HB2	1.94	0.49
2:E:265:ASP:HB2	2:E:339:SER:HB2	1.95	0.49
2:B:240:TRP:HB3	2:B:244:LEU:HD23	1.95	0.49
1:J:282:MET:HB2	1:J:305:LEU:HD11	1.93	0.49
2:H:168:LEU:HD11	2:H:183:GLN:HB2	1.94	0.49
1:J:953:TRP:HB2	1:J:970:ASN:HB2	1.93	0.49
2:K:265:ASP:HB2	2:K:339:SER:HB2	1.94	0.49
1:A:725:CYS:SG	1:A:829:PHE:CE1	3.06	0.49
2:B:68:HIS:CE1	1:D:197:LEU:HD13	2.47	0.49
2:E:168:LEU:HD11	2:E:183:GLN:HB2	1.94	0.49
2:K:101:LEU:HD13	2:K:106:GLU:HB3	1.93	0.49
2:H:165:PHE:HB2	2:H:182:VAL:HG13	1.95	0.49
2:B:367:ASN:HA	2:B:392:LYS:HD2	1.95	0.48
2:E:367:ASN:HA	2:E:392:LYS:HD2	1.95	0.48
2:H:265:ASP:HB2	2:H:339:SER:HB2	1.94	0.48
2:H:367:ASN:HA	2:H:392:LYS:HD2	1.95	0.48
2:B:309:ARG:HE	2:B:436:ASP:CG	2.16	0.48
2:H:240:TRP:HB3	2:H:244:LEU:HD23	1.95	0.48
1:A:725:CYS:HG	1:A:829:PHE:HE1	1.60	0.48
2:B:265:ASP:HB2	2:B:339:SER:HB2	1.95	0.48
1:D:743:GLN:HB3	1:D:782:PHE:HB3	1.93	0.48
2:H:55:THR:HG21	2:H:342:LEU:HB2	1.94	0.48
1:J:5:TYR:HB2	1:J:1043:LEU:HD11	1.96	0.48
2:K:240:TRP:HB3	2:K:244:LEU:HD23	1.95	0.48
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.96	0.48
1:J:231:ILE:CD1	1:J:240:HIS:CD2	2.95	0.48
1:G:160:GLU:HG3	1:J:160:GLU:HB2	1.96	0.48
1:D:725:CYS:SG	1:D:829:PHE:CE1	3.07	0.48
1:D:377:THR:HG23	1:D:388:ARG:HB2	1.94	0.47
1:G:743:GLN:HB3	1:G:782:PHE:HB3	1.96	0.47
1:G:813:ALA:HA	1:G:833:THR:HG22	1.96	0.47
1:D:5:TYR:HB2	1:D:1043:LEU:HD11	1.96	0.47
2:E:240:TRP:HB3	2:E:244:LEU:HD23	1.97	0.47
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.97	0.47
2:H:101:LEU:HD13	2:H:106:GLU:HB3	1.95	0.47
2:K:367:ASN:HA	2:K:392:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:165:PHE:HB2	2:K:182:VAL:HG13	1.97	0.47
1:D:15:VAL:O	1:D:327:ARG:HG2	2.15	0.47
1:G:1024:THR:HG21	1:G:1139:ILE:HG21	1.96	0.47
2:E:141:ILE:HG23	2:E:157:VAL:HG13	1.98	0.46
2:K:141:ILE:HG23	2:K:157:VAL:HG13	1.97	0.46
2:K:388:VAL:HG13	2:K:397:HIS:HD2	1.80	0.46
1:G:5:TYR:HB2	1:G:1043:LEU:HD11	1.95	0.46
2:K:388:VAL:HG13	2:K:397:HIS:CD2	2.50	0.46
1:A:144:PRO:CB	2:E:68:HIS:HE1	2.29	0.46
2:B:101:LEU:HD13	2:B:106:GLU:HB3	1.97	0.46
2:H:323:CYS:HB3	2:H:326:CYS:HB2	1.97	0.46
3:L:141:HIS:CD2	3:L:148:SER:HA	2.51	0.46
1:A:725:CYS:SG	1:A:829:PHE:HE1	2.39	0.45
1:G:240:HIS:NE2	1:G:245:TYR:HE2	2.14	0.45
1:D:725:CYS:SG	1:D:829:PHE:HE1	2.39	0.45
2:K:323:CYS:HB3	2:K:326:CYS:HB2	1.98	0.45
1:A:768:SER:HA	1:A:808:LEU:HD22	1.98	0.45
1:J:768:SER:HA	1:J:808:LEU:HD22	1.99	0.45
1:J:1024:THR:HG21	1:J:1139:ILE:HG21	1.98	0.45
2:B:47:ILE:N	2:B:410:SER:HG	2.15	0.45
1:D:768:SER:HA	1:D:808:LEU:HD22	1.99	0.45
2:E:323:CYS:HB3	2:E:326:CYS:HB2	1.99	0.45
2:H:141:ILE:HG23	2:H:157:VAL:HG13	1.98	0.45
1:J:739:ARG:HH12	1:J:790:ASN:HD21	1.62	0.45
2:K:47:ILE:N	2:K:410:SER:HG	2.15	0.45
2:B:141:ILE:HG23	2:B:157:VAL:HG13	1.98	0.45
2:E:47:ILE:N	2:E:410:SER:HG	2.15	0.45
1:G:768:SER:HA	1:G:808:LEU:HD22	1.98	0.45
1:D:387:LEU:HG	1:D:717:LEU:HD11	1.98	0.44
2:H:72:LEU:HD21	2:H:162:ARG:HD3	2.00	0.44
5:B:502:RN9:C24	5:B:502:RN9:C9	2.95	0.44
1:A:118:THR:HG22	1:A:118:THR:O	2.18	0.44
2:H:319:THR:HG23	2:H:427:PRO:HD3	2.00	0.44
5:H:502:RN9:C9	5:H:502:RN9:C24	2.96	0.44
1:A:986:ASP:HA	1:A:989:ARG:CD	2.47	0.44
2:B:63:ASP:CB	1:D:70:LYS:NZ	2.81	0.44
2:B:165:PHE:HB2	2:B:182:VAL:HG13	2.00	0.44
1:G:158:ARG:CZ	1:J:158:ARG:HE	2.31	0.44
2:H:47:ILE:N	2:H:410:SER:HG	2.15	0.44
2:B:63:ASP:HB3	1:D:70:LYS:HZ2	1.84	0.43
1:A:15:VAL:O	1:A:327:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:141:HIS:HD2	3:L:148:SER:HA	1.83	0.43
3:C:160:LYS:O	3:C:163:SER:OG	2.31	0.43
1:G:250:PRO:HA	1:G:251:PRO:HD3	1.92	0.43
2:B:323:CYS:HB3	2:B:326:CYS:HB2	1.99	0.43
1:D:217:SER:O	2:E:204:LYS:HD2	2.18	0.43
2:E:135:PHE:CE2	2:E:300:LYS:HE2	2.54	0.43
2:K:233:HIS:O	2:K:236:ASN:OD1	2.37	0.43
2:H:273:LEU:HA	2:H:274:PRO:HD3	1.95	0.43
1:J:118:THR:HG22	1:J:118:THR:O	2.19	0.43
2:K:72:LEU:HD21	2:K:162:ARG:HD3	2.01	0.43
1:G:144:PRO:HB3	2:K:68:HIS:CE1	2.54	0.43
1:D:812:TYR:CZ	2:E:241:PRO:HB3	2.54	0.42
1:G:118:THR:O	1:G:118:THR:HG22	2.19	0.42
2:B:233:HIS:O	2:B:236:ASN:OD1	2.37	0.42
1:J:272:LEU:HD22	1:J:280:LEU:HD11	2.02	0.42
1:G:986:ASP:HA	1:G:989:ARG:CD	2.49	0.42
2:H:233:HIS:O	2:H:236:ASN:OD1	2.36	0.42
1:J:1080:ARG:CZ	2:K:188:CYS:SG	3.07	0.42
2:E:165:PHE:HB2	2:E:182:VAL:HG13	2.02	0.42
1:J:118:THR:HG23	2:K:204:LYS:HA	2.01	0.42
1:A:328:LEU:O	1:A:380:GLY:HA2	2.20	0.41
1:G:987:GLU:HA	1:G:990:GLN:HE21	1.85	0.41
1:G:953:TRP:HB2	1:G:970:ASN:HB2	2.02	0.41
2:E:233:HIS:O	2:E:236:ASN:OD1	2.37	0.41
2:H:135:PHE:CE2	2:H:300:LYS:HE2	2.55	0.41
3:I:159:ILE:HA	3:I:162:HIS:HD2	1.84	0.41
1:J:928:ARG:HB3	1:J:950:ASN:O	2.20	0.41
1:D:118:THR:HG22	1:D:118:THR:O	2.18	0.41
2:E:135:PHE:HE2	2:E:300:LYS:HE2	1.86	0.41
1:J:986:ASP:HA	1:J:989:ARG:CD	2.48	0.41
1:D:910:MET:SD	2:E:309:ARG:NH2	2.91	0.41
2:E:72:LEU:HD21	2:E:162:ARG:HD3	2.02	0.41
2:B:222:LYS:HG2	2:B:226:LYS:HE3	2.03	0.41
2:E:101:LEU:HD13	2:E:106:GLU:HB3	2.03	0.41
2:H:152:ILE:HG13	2:H:154:ILE:HD11	2.03	0.41
1:J:789:HIS:NE2	1:J:812:TYR:CD1	2.89	0.41
1:D:328:LEU:O	1:D:380:GLY:HA2	2.21	0.40
1:D:46:ALA:HB1	2:H:148:GLN:HB2	2.04	0.40
1:A:118:THR:HG23	2:B:204:LYS:HA	2.02	0.40
1:D:359:ILE:HG23	1:D:377:THR:OG1	2.21	0.40
1:D:953:TRP:HB2	1:D:970:ASN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ARG:HE	1:J:158:ARG:HD2	1.87	0.40
1:J:843:PRO:HG2	1:J:869:ALA:HB2	2.03	0.40
1:D:928:ARG:NE	1:D:950:ASN:HB3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	767/1140 (67%)	727 (95%)	35 (5%)	5 (1%)	22	59
1	D	767/1140 (67%)	729 (95%)	33 (4%)	5 (1%)	22	59
1	G	765/1140 (67%)	734 (96%)	26 (3%)	5 (1%)	22	59
1	J	765/1140 (67%)	736 (96%)	24 (3%)	5 (1%)	22	59
2	B	377/390 (97%)	364 (97%)	11 (3%)	2 (0%)	29	65
2	E	377/390 (97%)	363 (96%)	12 (3%)	2 (0%)	29	65
2	H	377/390 (97%)	362 (96%)	13 (3%)	2 (0%)	29	65
2	K	377/390 (97%)	365 (97%)	10 (3%)	2 (0%)	29	65
3	C	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
3	F	26/29 (90%)	24 (92%)	2 (8%)	0	100	100
3	I	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
3	L	26/29 (90%)	24 (92%)	2 (8%)	0	100	100
All	All	4678/6236 (75%)	4478 (96%)	172 (4%)	28 (1%)	25	61

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	ASP

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Mol	Chain	Res	Type
2	B	50	ASP
1	D	318	ASP
2	E	50	ASP
1	G	318	ASP
2	H	50	ASP
1	J	318	ASP
2	K	50	ASP
1	A	3	TYR
1	D	3	TYR
1	G	3	TYR
1	G	36	ASN
1	J	3	TYR
1	J	36	ASN
1	A	36	ASN
2	B	116	LYS
1	D	36	ASN
2	E	116	LYS
2	H	116	LYS
1	J	371	GLY
2	K	116	LYS
1	A	371	GLY
1	D	371	GLY
1	G	371	GLY
1	G	61	ILE
1	A	61	ILE
1	D	61	ILE
1	J	61	ILE

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	664/999 (66%)	648 (98%)	16 (2%)	49	71
1	D	664/999 (66%)	645 (97%)	19 (3%)	42	67
1	G	662/999 (66%)	646 (98%)	16 (2%)	49	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	662/999 (66%)	645 (97%)	17 (3%)	46	70
2	B	344/354 (97%)	336 (98%)	8 (2%)	50	72
2	E	344/354 (97%)	337 (98%)	7 (2%)	55	75
2	H	344/354 (97%)	336 (98%)	8 (2%)	50	72
2	K	344/354 (97%)	338 (98%)	6 (2%)	60	79
3	C	24/24 (100%)	24 (100%)	0	100	100
3	F	24/24 (100%)	24 (100%)	0	100	100
3	I	24/24 (100%)	24 (100%)	0	100	100
3	L	24/24 (100%)	24 (100%)	0	100	100
All	All	4124/5508 (75%)	4027 (98%)	97 (2%)	49	71

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	38	ARG
1	A	112	ILE
1	A	207	TRP
1	A	367	LEU
1	A	377	THR
1	A	737	SER
1	A	812	TYR
1	A	859	GLN
1	A	874	VAL
1	A	908	ASN
1	A	938	MET
1	A	962	ASP
1	A	989	ARG
1	A	1008	CYS
1	A	1024	THR
2	B	134	GLN
2	B	144	TYR
2	B	175	ASP
2	B	182	VAL
2	B	207	ILE
2	B	263	GLU
2	B	292	ASP
2	B	436	ASP
1	D	3	TYR

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Mol	Chain	Res	Type
1	D	38	ARG
1	D	112	ILE
1	D	198	ARG
1	D	207	TRP
1	D	367	LEU
1	D	377	THR
1	D	737	SER
1	D	770	LEU
1	D	812	TYR
1	D	859	GLN
1	D	874	VAL
1	D	908	ASN
1	D	938	MET
1	D	962	ASP
1	D	987	GLU
1	D	989	ARG
1	D	1008	CYS
1	D	1024	THR
2	E	144	TYR
2	E	175	ASP
2	E	182	VAL
2	E	236	ASN
2	E	263	GLU
2	E	271	ASP
2	E	292	ASP
1	G	38	ARG
1	G	112	ILE
1	G	207	TRP
1	G	737	SER
1	G	743	GLN
1	G	782	PHE
1	G	812	TYR
1	G	859	GLN
1	G	872	SER
1	G	874	VAL
1	G	938	MET
1	G	979	LYS
1	G	989	ARG
1	G	1008	CYS
1	G	1024	THR
1	G	1071	SER
2	H	144	TYR

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Mol	Chain	Res	Type
2	H	175	ASP
2	H	182	VAL
2	H	197	VAL
2	H	263	GLU
2	H	319	THR
2	H	351	ASN
2	H	394	CYS
1	J	38	ARG
1	J	112	ILE
1	J	141	LYS
1	J	148	ASP
1	J	160	GLU
1	J	207	TRP
1	J	812	TYR
1	J	859	GLN
1	J	872	SER
1	J	874	VAL
1	J	928	ARG
1	J	962	ASP
1	J	979	LYS
1	J	989	ARG
1	J	1008	CYS
1	J	1024	THR
1	J	1071	SER
2	K	144	TYR
2	K	175	ASP
2	K	182	VAL
2	K	197	VAL
2	K	263	GLU
2	K	292	ASP

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	790	ASN
1	A	970	ASN
1	A	990	GLN
2	B	57	HIS
2	B	390	GLN
1	D	790	ASN
1	D	970	ASN
1	D	990	GLN

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Mol	Chain	Res	Type
2	E	68	HIS
2	E	390	GLN
2	E	397	HIS
1	G	392	ASN
1	G	797	HIS
1	G	970	ASN
1	G	990	GLN
2	H	57	HIS
2	H	79	GLN
2	H	325	GLN
1	J	240	HIS
1	J	790	ASN
1	J	907	ASN
2	K	390	GLN
2	K	397	HIS

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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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
5	RN9	H	502	-	38,38,38	1.88	14 (36%)	53,54,54	2.29	11 (20%)
5	RN9	B	502	-	38,38,38	1.91	11 (28%)	53,54,54	2.30	10 (18%)
5	RN9	K	1002	-	38,38,38	1.90	12 (31%)	53,54,54	2.29	11 (20%)
5	RN9	E	1002	-	38,38,38	1.90	12 (31%)	53,54,54	2.18	15 (28%)

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
5	RN9	H	502	-	-	2/17/46/46	0/4/4/4
5	RN9	B	502	-	-	2/17/46/46	0/4/4/4
5	RN9	K	1002	-	-	1/17/46/46	0/4/4/4
5	RN9	E	1002	-	-	6/17/46/46	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	RN9	C13-N3	4.92	1.46	1.35
5	E	1002	RN9	C13-N3	4.79	1.46	1.35
5	H	502	RN9	C13-N3	4.77	1.46	1.35
5	K	1002	RN9	C7-N2	4.57	1.46	1.36
5	K	1002	RN9	C13-N3	4.55	1.45	1.35
5	B	502	RN9	C7-N2	4.53	1.45	1.36
5	E	1002	RN9	C7-N2	4.47	1.45	1.36
5	K	1002	RN9	C3-N1	4.33	1.45	1.37
5	E	1002	RN9	C3-N1	4.28	1.44	1.37
5	H	502	RN9	C7-N2	4.14	1.45	1.36
5	B	502	RN9	C3-N1	4.05	1.44	1.37
5	B	502	RN9	C2-N1	4.04	1.44	1.37
5	H	502	RN9	C2-N1	3.96	1.44	1.37
5	E	1002	RN9	C2-N1	3.91	1.44	1.37
5	H	502	RN9	C3-N1	3.86	1.44	1.37
5	K	1002	RN9	C2-N1	3.51	1.43	1.37
5	K	1002	RN9	C7-C6	3.25	1.54	1.49
5	B	502	RN9	C7-C6	3.00	1.53	1.49
5	H	502	RN9	C7-C6	2.80	1.53	1.49
5	B	502	RN9	C24-C	2.68	1.54	1.44
5	E	1002	RN9	C24-C	2.57	1.53	1.44
5	K	1002	RN9	O3-C13	-2.57	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	RN9	C7-C6	2.55	1.53	1.49
5	H	502	RN9	C24-C	2.53	1.53	1.44
5	H	502	RN9	O3-C13	-2.38	1.18	1.23
5	K	1002	RN9	C24-C	2.38	1.53	1.44
5	E	1002	RN9	C19-CL	2.37	1.79	1.73
5	E	1002	RN9	O3-C13	-2.37	1.18	1.23
5	E	1002	RN9	O1-C3	-2.34	1.18	1.23
5	B	502	RN9	O1-C3	-2.32	1.18	1.23
5	H	502	RN9	O1-C3	-2.31	1.18	1.23
5	E	1002	RN9	O-C	-2.28	1.18	1.23
5	B	502	RN9	O3-C13	-2.27	1.18	1.23
5	B	502	RN9	C8-N2	2.24	1.46	1.41
5	B	502	RN9	O2-C2	-2.22	1.19	1.23
5	H	502	RN9	O2-C2	-2.22	1.19	1.23
5	K	1002	RN9	O-C	-2.22	1.18	1.23
5	H	502	RN9	C14-N3	2.21	1.46	1.41
5	E	1002	RN9	O2-C2	-2.21	1.19	1.23
5	K	1002	RN9	O1-C3	-2.19	1.18	1.23
5	K	1002	RN9	C8-N2	2.17	1.46	1.41
5	K	1002	RN9	O2-C2	-2.16	1.19	1.23
5	H	502	RN9	C19-CL	2.12	1.78	1.73
5	H	502	RN9	O-C	-2.12	1.19	1.23
5	K	1002	RN9	C19-CL	2.11	1.78	1.73
5	H	502	RN9	O4-C6	-2.07	1.18	1.23
5	E	1002	RN9	C8-N2	2.05	1.45	1.41
5	H	502	RN9	C8-N2	2.04	1.45	1.41
5	B	502	RN9	O-C	-2.01	1.19	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	RN9	C6-C7-N2	11.11	124.76	115.68
5	H	502	RN9	C6-C7-N2	10.60	124.35	115.68
5	K	1002	RN9	C6-C7-N2	10.09	123.93	115.68
5	E	1002	RN9	C6-C7-N2	7.52	121.83	115.68
5	E	1002	RN9	C3-N1-C2	-5.87	118.44	126.61
5	K	1002	RN9	C3-N1-C2	-5.72	118.64	126.61
5	H	502	RN9	C3-N1-C2	-5.72	118.64	126.61
5	B	502	RN9	C3-N1-C2	-5.50	118.95	126.61
5	E	1002	RN9	C4-C3-N1	5.05	122.33	116.65
5	K	1002	RN9	C4-C3-N1	4.83	122.08	116.65
5	K	1002	RN9	C2-C1-N	-4.67	104.82	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1002	RN9	C1-C2-N1	4.52	122.33	116.25
5	H	502	RN9	C2-C1-N	-4.51	104.96	109.08
5	B	502	RN9	C1-C2-N1	4.42	122.19	116.25
5	H	502	RN9	C1-C2-N1	4.36	122.12	116.25
5	H	502	RN9	C4-C3-N1	4.35	121.54	116.65
5	B	502	RN9	C4-C3-N1	4.26	121.43	116.65
5	E	1002	RN9	C1-C2-N1	4.18	121.87	116.25
5	E	1002	RN9	C12-C13-N3	4.11	121.84	114.59
5	E	1002	RN9	C2-C1-N	-3.76	105.65	109.08
5	H	502	RN9	C24-C7-N2	-3.56	127.85	135.41
5	B	502	RN9	C24-C7-N2	-3.54	127.89	135.41
5	B	502	RN9	C5-C1-C2	3.49	117.60	111.61
5	B	502	RN9	C5-C1-N	-3.23	106.02	113.85
5	K	1002	RN9	C24-C7-N2	-3.23	128.57	135.41
5	H	502	RN9	C5-C1-C2	3.17	117.07	111.61
5	K	1002	RN9	C5-C1-C2	3.09	116.92	111.61
5	E	1002	RN9	C5-C1-C2	2.97	116.72	111.61
5	B	502	RN9	C7-C6-N	2.96	108.14	105.60
5	E	1002	RN9	C7-C6-N	2.69	107.90	105.60
5	H	502	RN9	C5-C1-N	-2.64	107.45	113.85
5	E	1002	RN9	C20-C19-C17	-2.56	118.91	122.74
5	H	502	RN9	C7-C6-N	2.54	107.78	105.60
5	E	1002	RN9	C16-C17-C19	2.45	121.87	116.43
5	E	1002	RN9	C14-N3-C13	-2.41	123.29	127.50
5	E	1002	RN9	O3-C13-N3	-2.37	119.30	123.63
5	K	1002	RN9	C7-C6-N	2.30	107.57	105.60
5	E	1002	RN9	C18-C17-C19	-2.23	117.44	122.29
5	H	502	RN9	C12-C13-N3	2.22	118.50	114.59
5	E	1002	RN9	C24-C7-N2	-2.21	130.73	135.41
5	K	1002	RN9	C5-C1-N	-2.17	108.58	113.85
5	K	1002	RN9	C15-C14-N3	-2.16	113.14	120.40
5	E	1002	RN9	C5-C1-N	-2.15	108.64	113.85
5	K	1002	RN9	C20-C14-N3	2.15	127.19	120.18
5	H	502	RN9	C20-C19-C17	-2.06	119.65	122.74
5	B	502	RN9	C12-C13-N3	2.06	118.22	114.59
5	B	502	RN9	C20-C19-C17	-2.01	119.72	122.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1002	RN9	C15-C14-N3-C13

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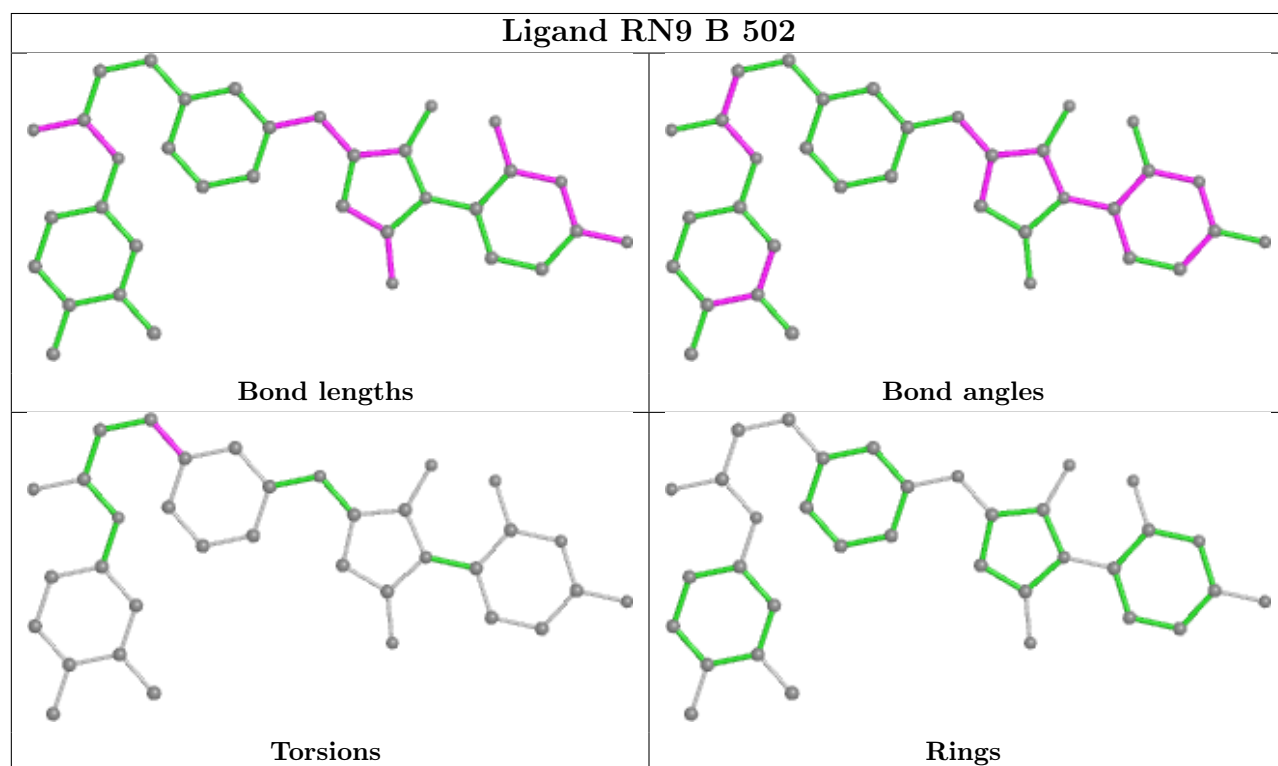
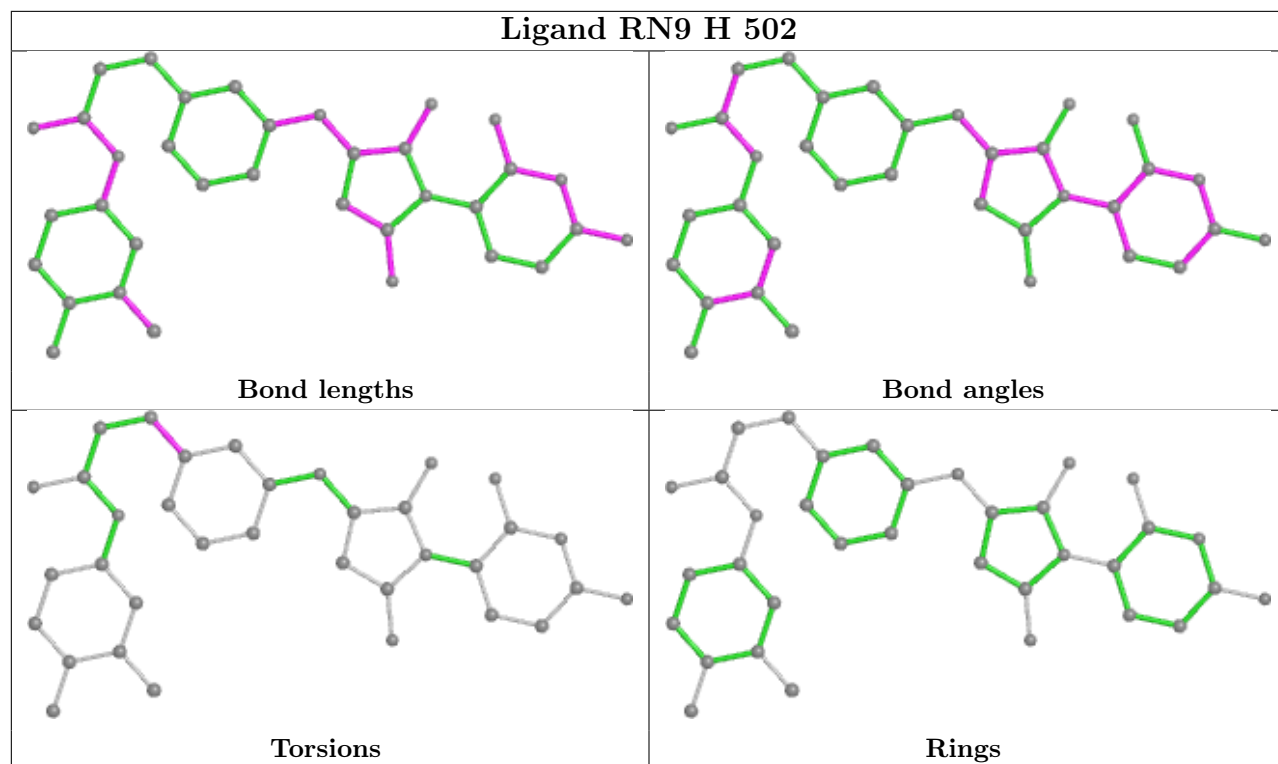
Mol	Chain	Res	Type	Atoms
5	E	1002	RN9	C20-C14-N3-C13
5	E	1002	RN9	C11-C12-C13-O3
5	E	1002	RN9	C11-C12-C13-N3
5	K	1002	RN9	C10-C11-C12-C13
5	E	1002	RN9	C21-C10-C11-C12
5	H	502	RN9	C21-C10-C11-C12
5	H	502	RN9	C9-C10-C11-C12
5	E	1002	RN9	C9-C10-C11-C12
5	B	502	RN9	C9-C10-C11-C12
5	B	502	RN9	C21-C10-C11-C12

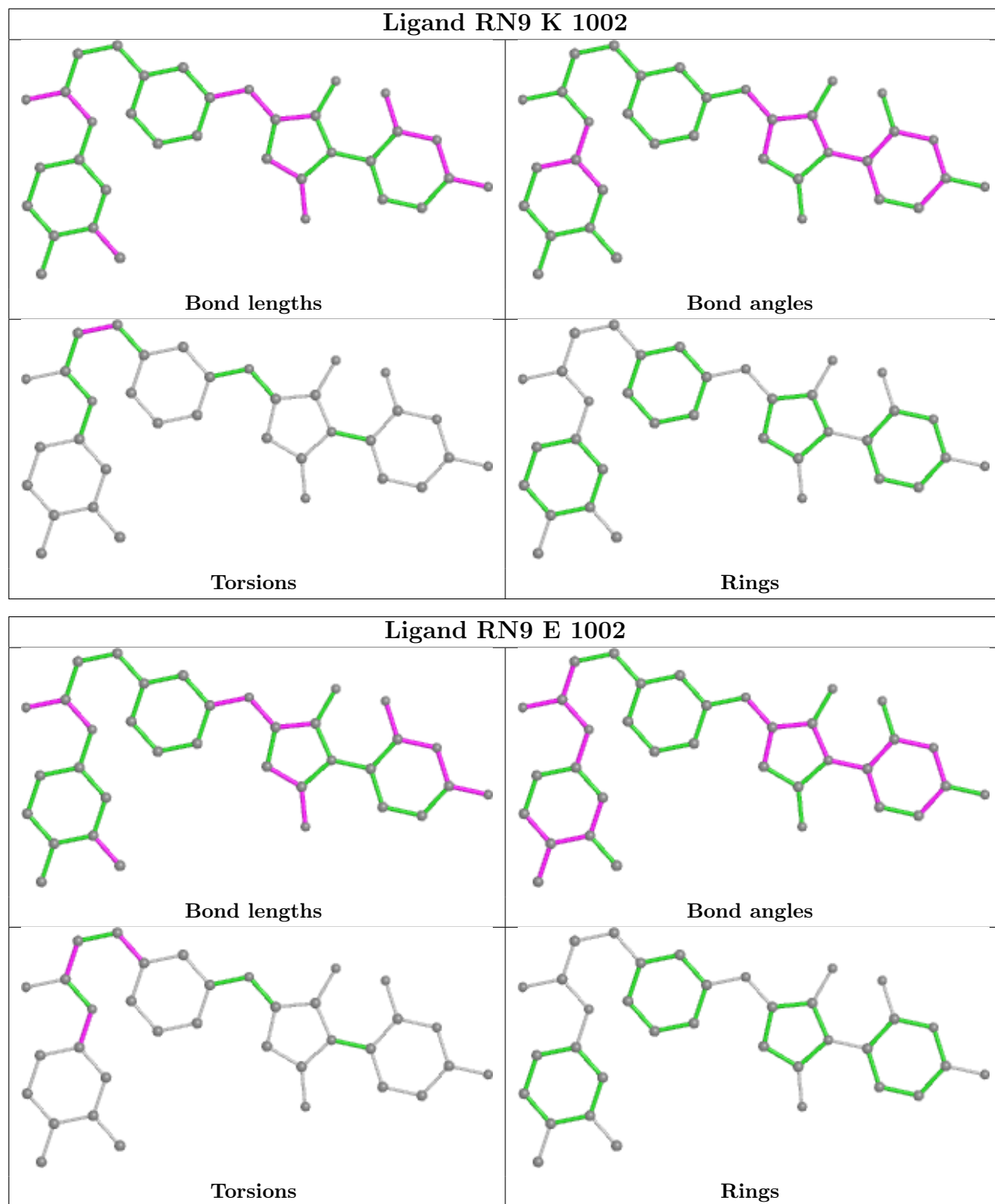
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	502	RN9	1	0
5	B	502	RN9	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	781/1140 (68%)	0.07	14 (1%) 68 65	66, 119, 172, 226	0
1	D	781/1140 (68%)	0.56	95 (12%) 4 4	99, 169, 249, 284	0
1	G	779/1140 (68%)	0.10	14 (1%) 68 65	64, 120, 179, 212	0
1	J	779/1140 (68%)	0.04	7 (0%) 84 82	58, 103, 168, 199	0
2	B	381/390 (97%)	-0.06	0 100 100	73, 106, 168, 199	0
2	E	381/390 (97%)	0.02	4 (1%) 82 80	74, 112, 179, 216	0
2	H	381/390 (97%)	-0.08	0 100 100	58, 100, 160, 220	0
2	K	381/390 (97%)	0.00	1 (0%) 94 94	67, 101, 153, 192	0
3	C	29/29 (100%)	-0.28	1 (3%) 45 40	89, 108, 157, 182	0
3	F	28/29 (96%)	-0.22	0 100 100	82, 116, 161, 197	0
3	I	29/29 (100%)	-0.37	0 100 100	89, 112, 172, 192	0
3	L	28/29 (96%)	-0.25	0 100 100	91, 106, 131, 136	0
All	All	4758/6236 (76%)	0.11	136 (2%) 51 45	58, 117, 195, 284	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	THR	6.0
1	D	317	LEU	5.4
1	D	321	VAL	5.3
1	D	830	ILE	5.2
1	D	247	ALA	5.1
1	D	1127	ASP	5.1
1	D	356	LEU	5.0
1	A	297	LEU	4.6
1	D	246	LEU	4.6
1	D	717	LEU	4.5
1	G	768	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	861	VAL	4.5
1	D	161	GLU	4.3
1	D	855	ASP	4.1
1	D	239	TYR	4.1
1	D	822	GLY	4.0
1	A	768	SER	3.9
1	G	770	LEU	3.8
1	D	393	GLY	3.8
1	D	282	MET	3.8
1	D	237	ILE	3.8
1	D	821	LEU	3.7
1	D	236	SER	3.7
1	D	1094	ILE	3.7
1	D	354	THR	3.7
1	D	370	GLN	3.6
1	D	284	LEU	3.6
1	D	854	SER	3.6
1	D	273	LEU	3.5
1	D	174	GLN	3.4
1	D	1014	MET	3.4
1	D	716	PRO	3.4
1	J	768	SER	3.4
1	D	130	MET	3.4
1	D	65	GLU	3.4
1	D	316	TYR	3.3
1	D	28	ASP	3.2
1	D	318	ASP	3.2
1	D	66	LEU	3.2
1	D	1015	GLN	3.2
1	D	366	ASP	3.1
1	D	850	VAL	3.1
1	D	133	LEU	3.1
1	D	1098	LEU	3.1
1	D	181	VAL	3.1
1	D	77	LEU	3.1
1	D	862	ALA	3.1
1	A	770	LEU	3.0
1	D	8	THR	3.0
1	D	320	GLY	3.0
1	D	190	VAL	2.9
1	J	745	THR	2.9
1	A	295	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	135	LEU	2.8
1	D	802	LEU	2.7
1	D	793	ILE	2.7
1	D	315	THR	2.7
1	D	933	LEU	2.7
1	A	1077	HIS	2.7
1	D	1099	ASP	2.6
1	G	769	LYS	2.6
1	A	139	LEU	2.6
2	E	153	GLU	2.6
1	D	871	TYR	2.6
1	D	1126	ALA	2.6
1	G	165	ILE	2.6
1	D	1092	ASP	2.6
1	D	1000	LEU	2.5
1	D	1011	SER	2.5
1	D	919	ASP	2.5
1	D	180	PHE	2.5
1	G	1079	GLU	2.5
1	D	1054	MET	2.5
1	D	1010	GLY	2.5
1	A	857	LYS	2.5
1	D	269	SER	2.5
1	G	282	MET	2.5
1	D	132	GLY	2.5
1	G	1126	ALA	2.4
1	D	959	ILE	2.4
1	D	141	LYS	2.4
1	D	138	GLY	2.4
1	D	812	TYR	2.4
1	G	833	THR	2.4
1	G	284	LEU	2.4
1	D	1022	THR	2.3
1	A	769	LYS	2.3
1	D	368	GLU	2.3
1	D	322	VAL	2.3
1	D	859	GLN	2.3
1	D	171	TYR	2.3
1	A	1126	ALA	2.3
1	D	5	TYR	2.3
1	D	303	GLU	2.3
3	C	164	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	1140	HIS	2.3
1	D	248	ILE	2.3
1	D	126	PRO	2.2
1	J	855	ASP	2.2
1	J	893	TRP	2.2
1	D	111	ARG	2.2
1	D	79	ILE	2.2
1	D	938	MET	2.2
1	G	857	LYS	2.2
1	D	118	THR	2.2
1	D	923	VAL	2.2
1	D	804	ALA	2.2
1	G	1080	ARG	2.1
1	D	307	GLU	2.1
1	D	829	PHE	2.1
2	E	152	ILE	2.1
2	K	432	GLU	2.1
1	D	308	THR	2.1
1	D	847	ARG	2.1
1	G	220	ILE	2.1
1	D	267	ASN	2.1
2	E	149	ASP	2.1
1	A	165	ILE	2.1
1	A	880	LEU	2.1
1	D	195	VAL	2.1
1	G	1043	LEU	2.1
1	D	33	ILE	2.1
1	D	301	ARG	2.1
2	E	144	TYR	2.1
1	A	1129	LEU	2.1
1	D	272	LEU	2.1
1	A	833	THR	2.0
1	J	720	SER	2.0
1	D	211	ASN	2.0
1	D	36	ASN	2.0
1	D	730	SER	2.0
1	A	792	LEU	2.0
1	D	934	ALA	2.0
1	G	157	ILE	2.0
1	D	170	LEU	2.0
1	J	733	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 monosaccharides in this entry.

6.4 Ligands [i](#)

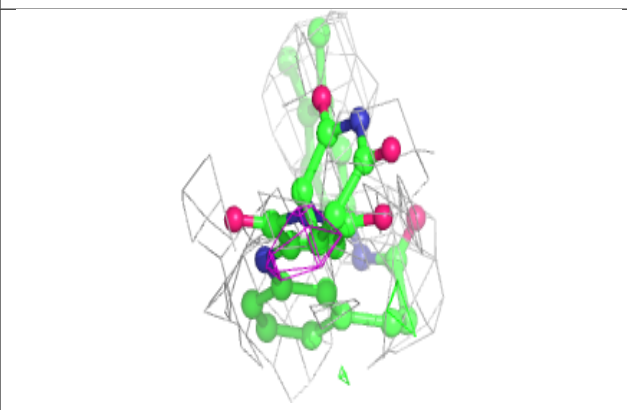
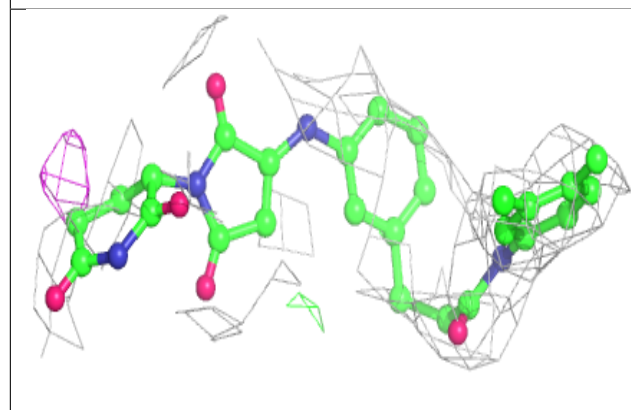
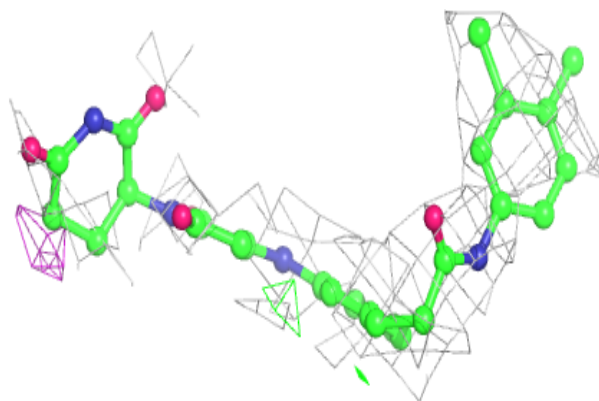
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	RN9	H	502	35/35	0.87	0.28	92,109,127,142	0
5	RN9	B	502	35/35	0.88	0.28	89,105,123,138	0
5	RN9	K	1002	35/35	0.89	0.35	91,107,125,140	0
5	RN9	E	1002	35/35	0.92	0.34	90,122,151,154	0
4	ZN	L	201	1/1	0.97	0.13	83,83,83,83	0
4	ZN	C	201	1/1	0.98	0.18	95,95,95,95	0
4	ZN	F	201	1/1	0.98	0.14	82,82,82,82	0
4	ZN	H	501	1/1	0.98	0.22	75,75,75,75	0
4	ZN	I	201	1/1	0.98	0.18	95,95,95,95	0
4	ZN	K	1001	1/1	0.98	0.20	89,89,89,89	0
4	ZN	E	1001	1/1	0.99	0.19	87,87,87,87	0
4	ZN	B	501	1/1	0.99	0.21	84,84,84,84	0

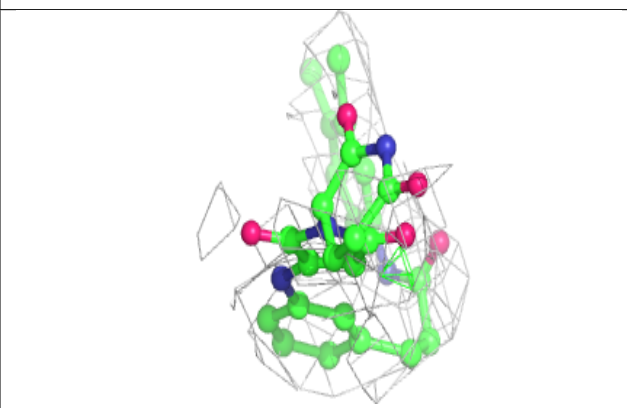
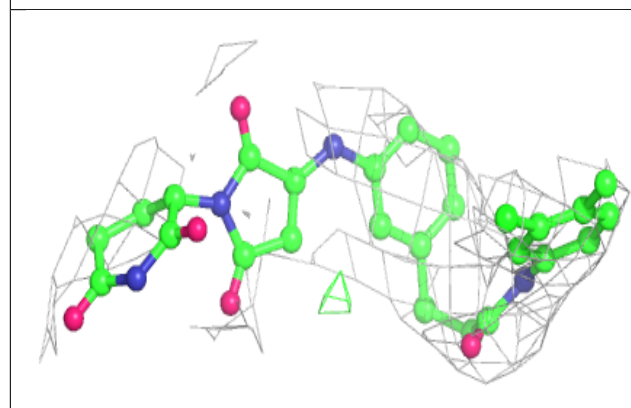
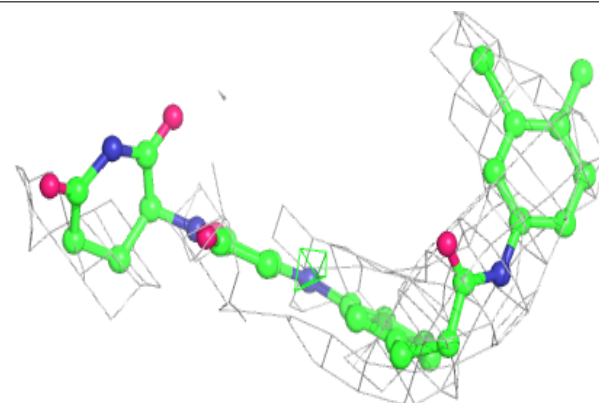
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RN9 H 502:

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

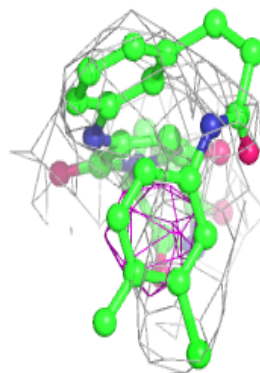
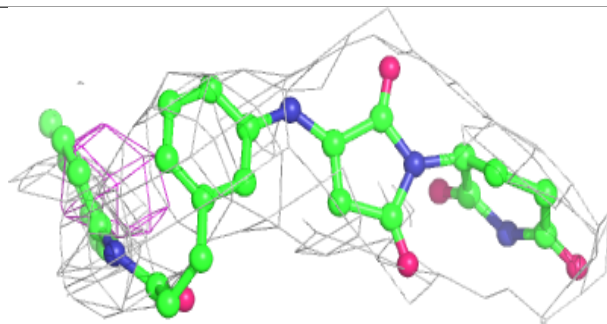
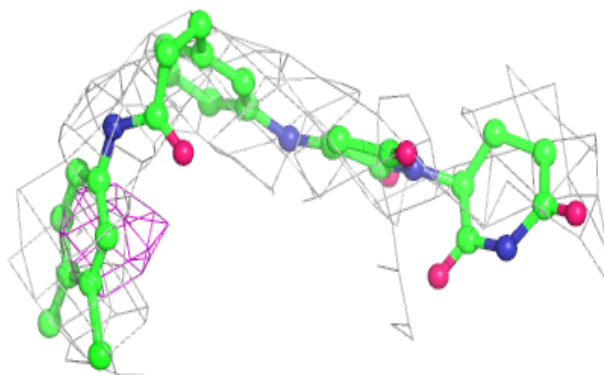
**Electron density around RN9 B 502:**

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

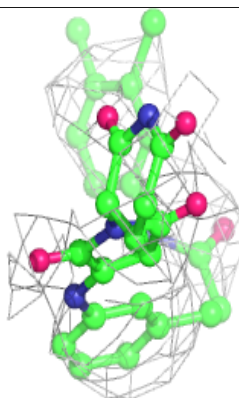
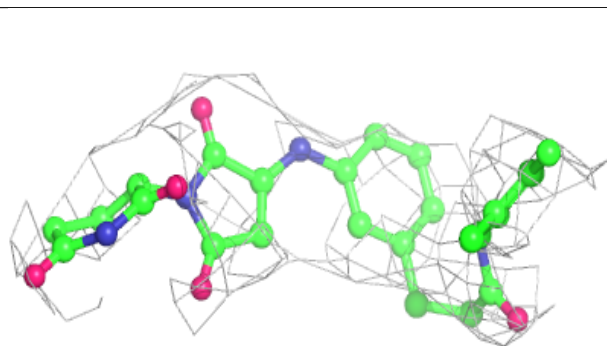
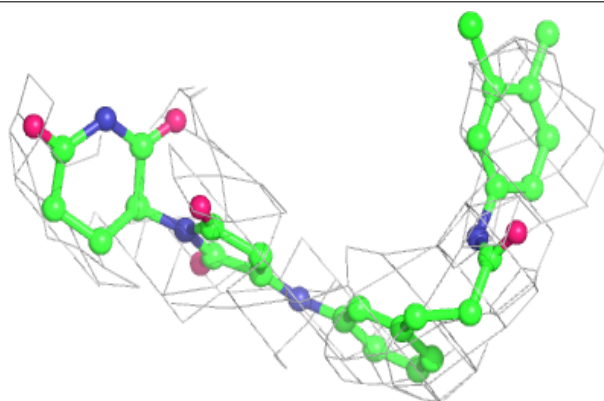


Electron density around RN9 K 1002:

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

**Electron density around RN9 E 1002:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.