



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 6FER / pdb_00006fer
Title : Crystal Structure of human DDR2 kinase in complex with 2-[4,5-difluoro-2-oxo-1'-(1H-pyrazolo[3,4-b]pyridine-5-carbonyl)spiro[indole-3,4'-piperidine]-1-yl]-N-(2,2,2-trifluoroethyl)acetamide
Authors : Stihle, M.; Richter, H.; Benz, J.; Kuhn, B.; Rudolph, M.G.
Deposited on : 2018-01-03
Resolution : 2.87 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

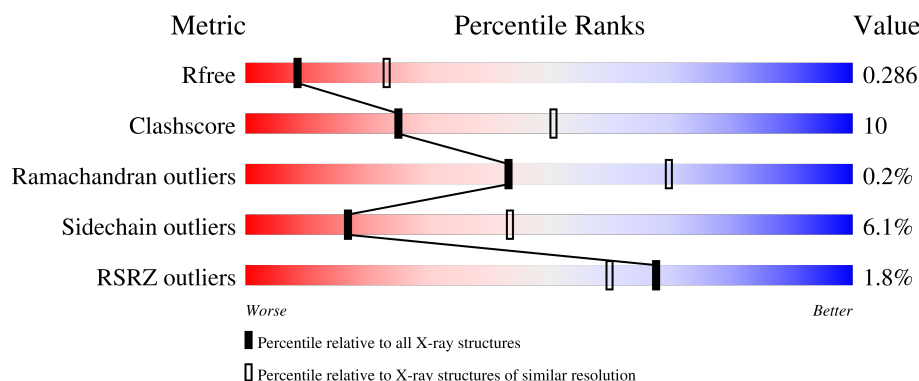
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	309	
1	B	309	
1	C	309	
1	D	309	

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Mol	Chain	Length	Quality of chain
1	E	309	 % 63% 25% 12%
1	F	309	 % 67% 20% 11%
1	G	309	 % 67% 19% 12%
1	H	309	 % 63% 23% 12%
1	I	309	 7% 58% 27% 14%
1	J	309	 % 70% 17% 12%
1	K	309	 6% 60% 26% 13%
1	L	309	 % 56% 31% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27069 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 Discoidin domain-containing receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2200	1408	375	401	16			
1	B	279	Total	C	N	O	S	0	0	0
			2261	1442	387	416	16			
1	C	272	Total	C	N	O	S	0	0	0
			2209	1413	376	404	16			
1	D	280	Total	C	N	O	S	0	0	0
			2268	1447	388	417	16			
1	E	273	Total	C	N	O	S	0	0	0
			2223	1422	380	405	16			
1	F	275	Total	C	N	O	S	0	0	0
			2233	1427	381	409	16			
1	G	273	Total	C	N	O	S	0	0	0
			2220	1419	380	405	16			
1	H	272	Total	C	N	O	S	0	0	0
			2214	1417	379	402	16			
1	I	267	Total	C	N	O	S	0	0	0
			2177	1394	371	396	16			
1	J	272	Total	C	N	O	S	0	0	0
			2214	1417	379	402	16			
1	K	268	Total	C	N	O	S	0	0	0
			2184	1398	372	398	16			
1	L	273	Total	C	N	O	S	0	0	0
			2222	1421	381	404	16			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	903	HIS	-	expression tag	UNP Q16832
A	904	HIS	-	expression tag	UNP Q16832
A	905	HIS	-	expression tag	UNP Q16832
A	906	HIS	-	expression tag	UNP Q16832
A	907	HIS	-	expression tag	UNP Q16832

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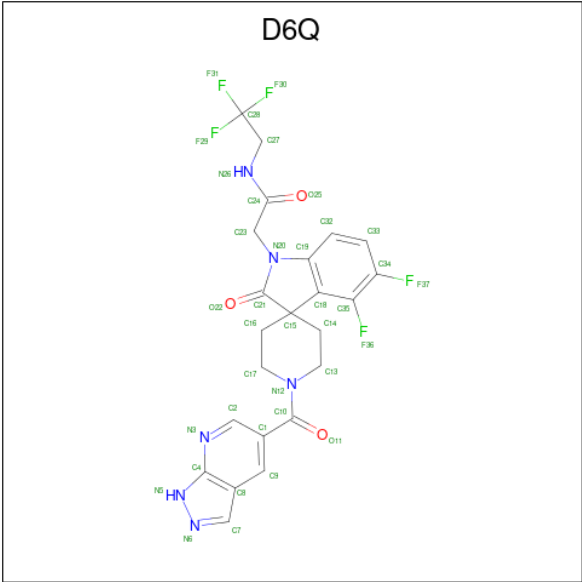
Chain	Residue	Modelled	Actual	Comment	Reference
A	908	HIS	-	expression tag	UNP Q16832
B	903	HIS	-	expression tag	UNP Q16832
B	904	HIS	-	expression tag	UNP Q16832
B	905	HIS	-	expression tag	UNP Q16832
B	906	HIS	-	expression tag	UNP Q16832
B	907	HIS	-	expression tag	UNP Q16832
B	908	HIS	-	expression tag	UNP Q16832
C	903	HIS	-	expression tag	UNP Q16832
C	904	HIS	-	expression tag	UNP Q16832
C	905	HIS	-	expression tag	UNP Q16832
C	906	HIS	-	expression tag	UNP Q16832
C	907	HIS	-	expression tag	UNP Q16832
C	908	HIS	-	expression tag	UNP Q16832
D	903	HIS	-	expression tag	UNP Q16832
D	904	HIS	-	expression tag	UNP Q16832
D	905	HIS	-	expression tag	UNP Q16832
D	906	HIS	-	expression tag	UNP Q16832
D	907	HIS	-	expression tag	UNP Q16832
D	908	HIS	-	expression tag	UNP Q16832
E	903	HIS	-	expression tag	UNP Q16832
E	904	HIS	-	expression tag	UNP Q16832
E	905	HIS	-	expression tag	UNP Q16832
E	906	HIS	-	expression tag	UNP Q16832
E	907	HIS	-	expression tag	UNP Q16832
E	908	HIS	-	expression tag	UNP Q16832
F	903	HIS	-	expression tag	UNP Q16832
F	904	HIS	-	expression tag	UNP Q16832
F	905	HIS	-	expression tag	UNP Q16832
F	906	HIS	-	expression tag	UNP Q16832
F	907	HIS	-	expression tag	UNP Q16832
F	908	HIS	-	expression tag	UNP Q16832
G	903	HIS	-	expression tag	UNP Q16832
G	904	HIS	-	expression tag	UNP Q16832
G	905	HIS	-	expression tag	UNP Q16832
G	906	HIS	-	expression tag	UNP Q16832
G	907	HIS	-	expression tag	UNP Q16832
G	908	HIS	-	expression tag	UNP Q16832
H	903	HIS	-	expression tag	UNP Q16832
H	904	HIS	-	expression tag	UNP Q16832
H	905	HIS	-	expression tag	UNP Q16832
H	906	HIS	-	expression tag	UNP Q16832
H	907	HIS	-	expression tag	UNP Q16832

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Chain	Residue	Modelled	Actual	Comment	Reference
H	908	HIS	-	expression tag	UNP Q16832
I	903	HIS	-	expression tag	UNP Q16832
I	904	HIS	-	expression tag	UNP Q16832
I	905	HIS	-	expression tag	UNP Q16832
I	906	HIS	-	expression tag	UNP Q16832
I	907	HIS	-	expression tag	UNP Q16832
I	908	HIS	-	expression tag	UNP Q16832
J	903	HIS	-	expression tag	UNP Q16832
J	904	HIS	-	expression tag	UNP Q16832
J	905	HIS	-	expression tag	UNP Q16832
J	906	HIS	-	expression tag	UNP Q16832
J	907	HIS	-	expression tag	UNP Q16832
J	908	HIS	-	expression tag	UNP Q16832
K	903	HIS	-	expression tag	UNP Q16832
K	904	HIS	-	expression tag	UNP Q16832
K	905	HIS	-	expression tag	UNP Q16832
K	906	HIS	-	expression tag	UNP Q16832
K	907	HIS	-	expression tag	UNP Q16832
K	908	HIS	-	expression tag	UNP Q16832
L	903	HIS	-	expression tag	UNP Q16832
L	904	HIS	-	expression tag	UNP Q16832
L	905	HIS	-	expression tag	UNP Q16832
L	906	HIS	-	expression tag	UNP Q16832
L	907	HIS	-	expression tag	UNP Q16832
L	908	HIS	-	expression tag	UNP Q16832

- Molecule 2 is 2-[4,5-bis(fluoranyl)-2-oxidanylidene-1'-(1 {H}-pyrazolo[3,4-b]pyridin-5-ylcarbonyl)spiro[indole-3,4'-piperidine]-1-yl]- {N}-[2,2,2-tris(fluoranyl)ethyl]ethanamide (CCD ID: D6Q) (formula: C₂₃H₁₉F₅N₆O₃).

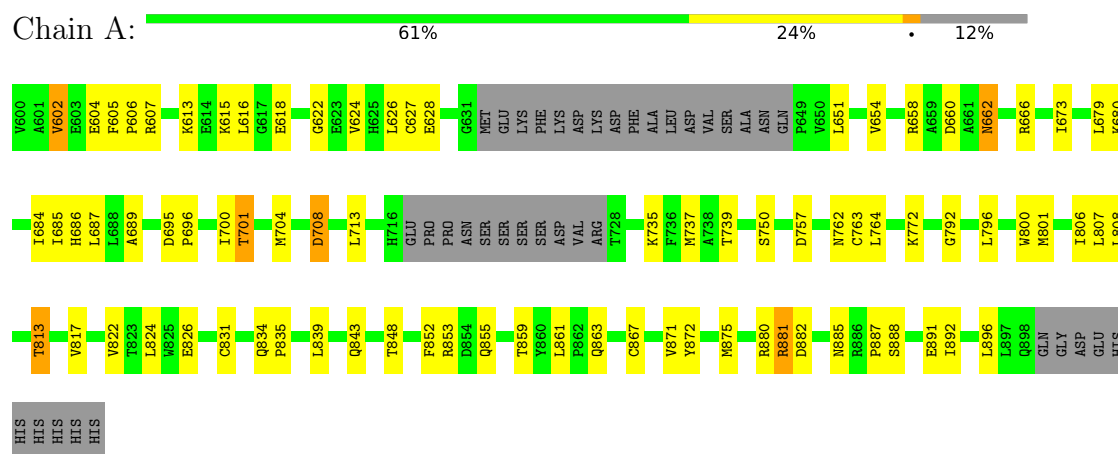


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	B	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	C	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	D	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	E	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	F	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	G	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	H	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	I	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	J	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	K	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	L	1	Total	C	F	N	O	0	0
			37	23	5	6	3		

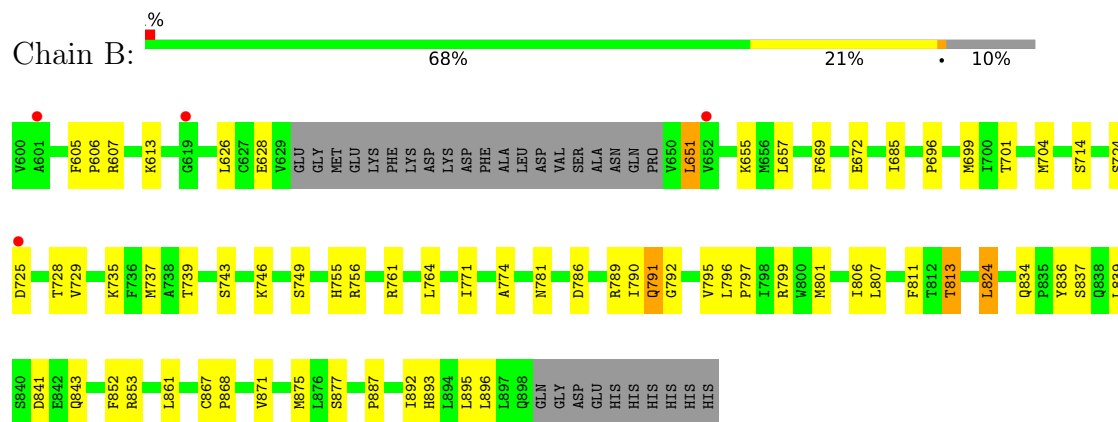
3 Residue-property plots [i](#)

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.

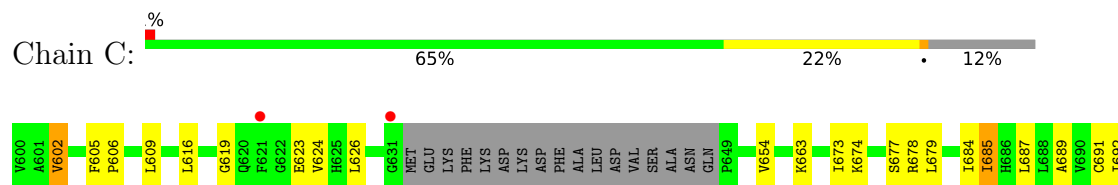
• Molecule 1: Discoidin domain-containing receptor 2

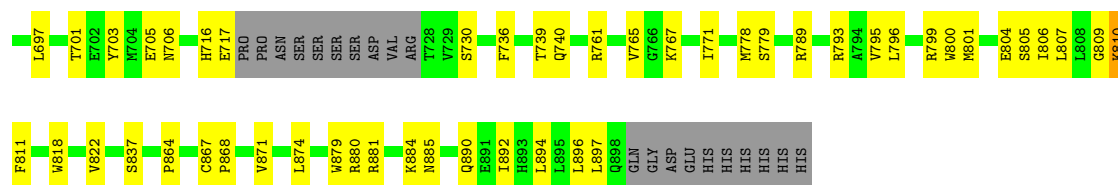


• Molecule 1: Discoidin domain-containing receptor 2



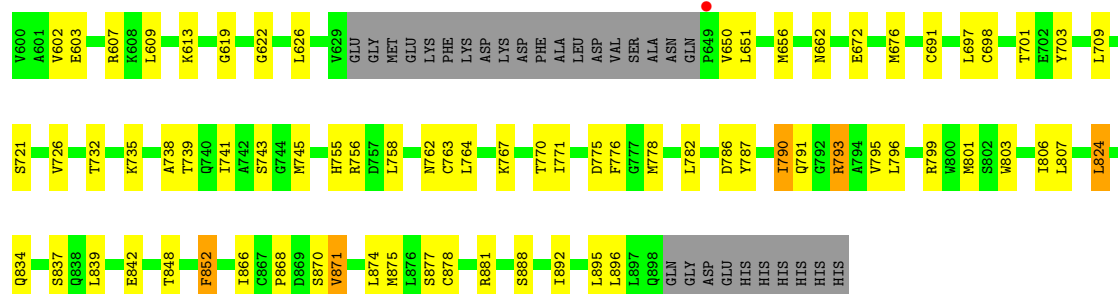
• Molecule 1: Discoidin domain-containing receptor 2





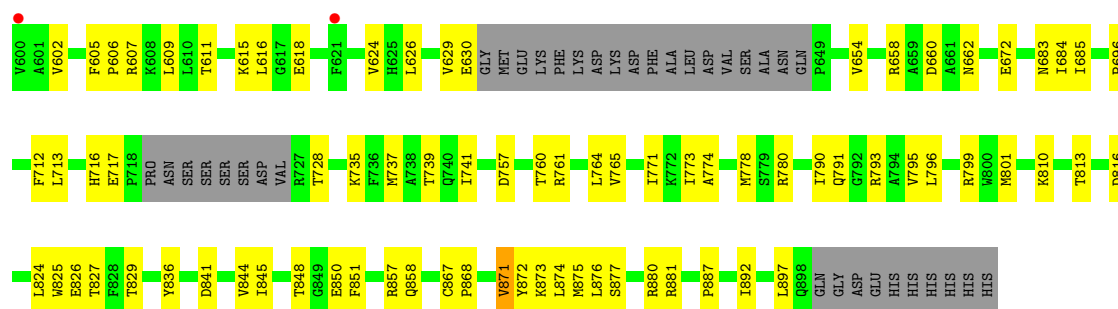
• Molecule 1: Discoidin domain-containing receptor 2

Chain D: 67% 22% 9%



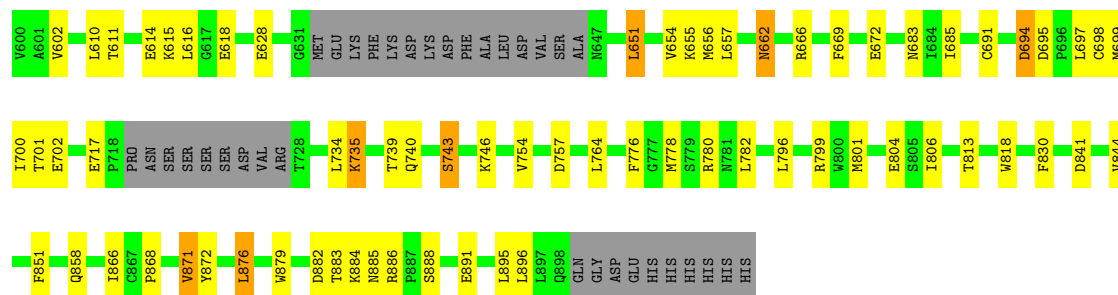
• Molecule 1: Discoidin domain-containing receptor 2

Chain E: 63% 25% 12%



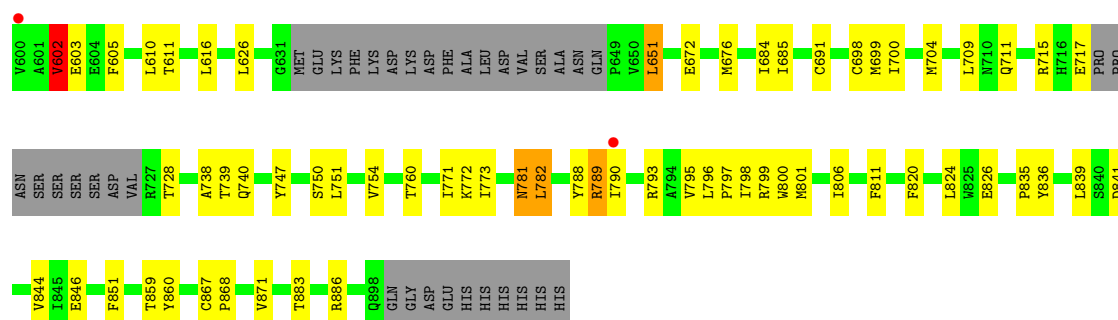
• Molecule 1: Discoidin domain-containing receptor 2

Chain F: 67% 20% 11%



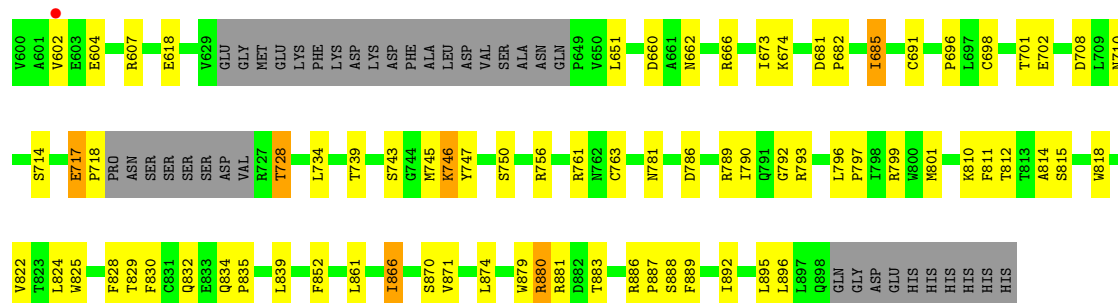
• Molecule 1: Discoidin domain-containing receptor 2

Chain G: 67% 19% 12%



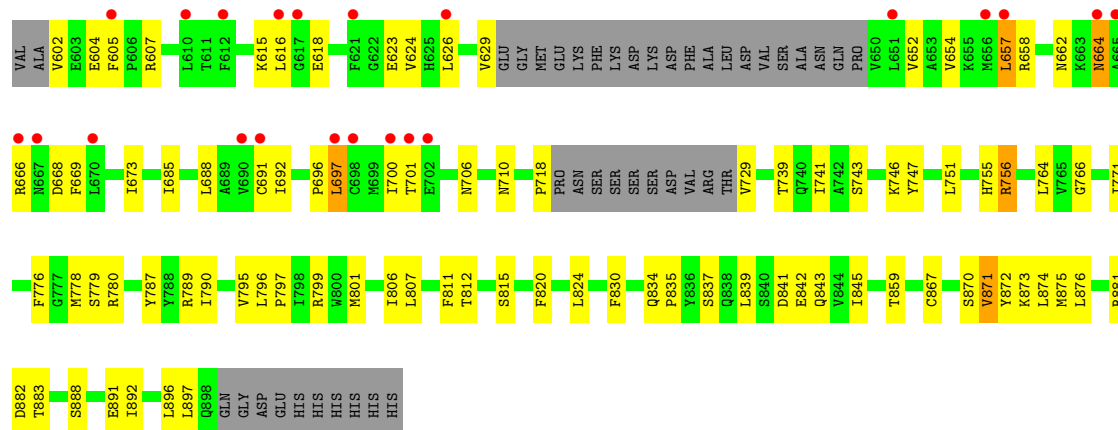
• Molecule 1: Discoidin domain-containing receptor 2

Chain H: 63% 23% 12%



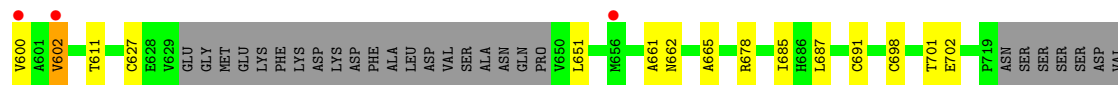
• Molecule 1: Discoidin domain-containing receptor 2

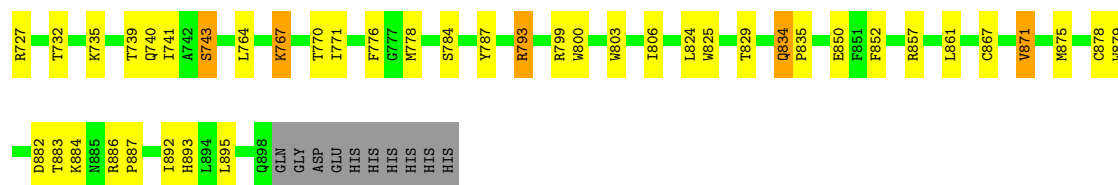
Chain I: 7% 58% 27% 14%



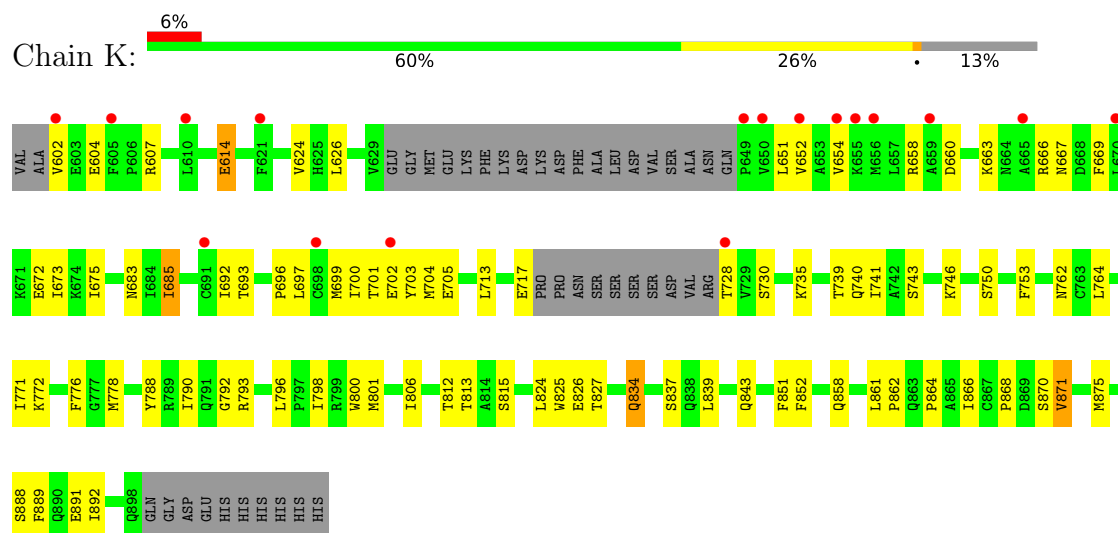
• Molecule 1: Discoidin domain-containing receptor 2

Chain J: 70% 17% 12%

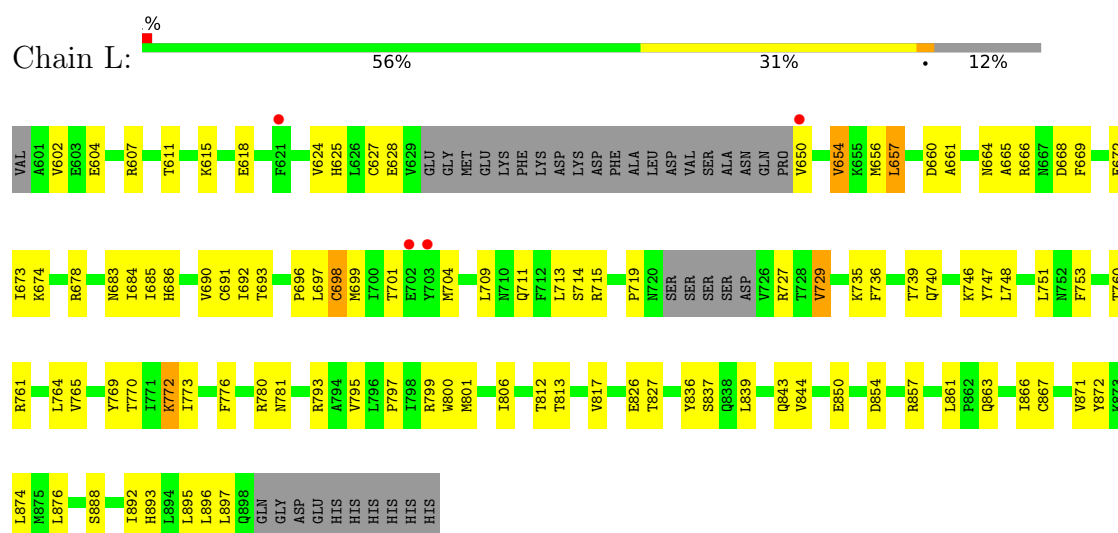




• Molecule 1: Discoidin domain-containing receptor 2



• Molecule 1: Discoidin domain-containing receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.91Å 155.79Å 355.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.87 47.96 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.96-2.87) 99.8 (47.96-2.87)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.11_2558	Depositor
R, R_{free}	0.200 , 0.287 0.202 , 0.286	Depositor DCC
R_{free} test set	4489 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27069	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: D6Q

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	0.34	0/2247	0.55	0/3034
1	B	0.42	1/2310 (0.0%)	0.65	2/3123 (0.1%)
1	C	0.33	0/2256	0.57	0/3046
1	D	0.40	0/2318	0.64	2/3134 (0.1%)
1	E	0.41	0/2271	0.65	0/3067
1	F	0.39	0/2281	0.62	1/3082 (0.0%)
1	G	0.41	1/2267 (0.0%)	0.62	0/3060
1	H	0.40	0/2262	0.66	0/3055
1	I	0.39	0/2224	0.59	0/3003
1	J	0.37	0/2262	0.62	0/3056
1	K	0.33	0/2231	0.55	0/3012
1	L	0.37	0/2270	0.58	0/3067
All	All	0.38	2/27199 (0.0%)	0.61	5/36739 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	792	GLY	CA-C	-5.18	1.46	1.51
1	G	782	LEU	CA-C	-5.01	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	791	GLN	N-CA-C	10.87	123.12	111.28
1	B	790	ILE	N-CA-C	-7.93	99.25	109.80
1	D	866	ILE	CA-C-N	5.36	129.06	121.61
1	D	866	ILE	C-N-CA	5.36	129.06	121.61
1	F	651	LEU	N-CA-C	5.31	117.89	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2191	52	0
1	B	2261	0	2247	39	0
1	C	2209	0	2197	43	0
1	D	2268	0	2255	41	0
1	E	2223	0	2214	44	0
1	F	2233	0	2217	38	0
1	G	2220	0	2210	38	0
1	H	2214	0	2208	50	0
1	I	2177	0	2166	54	0
1	J	2214	0	2207	35	0
1	K	2184	0	2174	50	0
1	L	2222	0	2213	61	0
2	A	37	0	0	1	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
2	D	37	0	0	1	0
2	E	37	0	0	1	0
2	F	37	0	0	1	0
2	G	37	0	0	0	0
2	H	37	0	0	0	0
2	I	37	0	0	2	0
2	J	37	0	0	1	0
2	K	37	0	0	1	0
2	L	37	0	0	0	0
All	All	27069	0	26499	521	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 10.

All (521) 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:D:691:CYS:HB2	1:D:698:CYS:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:LEU:HG	1:A:875:MET:HE2	1.60	0.83
1:K:692:ILE:HG22	1:K:697:LEU:HD22	1.63	0.79
1:I:834:GLN:HG2	1:I:835:PRO:HD2	1.65	0.79
1:H:739:THR:HG22	1:H:896:LEU:HB3	1.68	0.76
1:C:806:ILE:HG22	1:C:807:LEU:HD23	1.70	0.74
1:A:800:TRP:NE1	1:A:826:GLU:OE2	2.21	0.73
1:C:692:ILE:HA	1:C:697:LEU:HD22	1.70	0.73
1:A:807:LEU:HB3	1:K:692:ILE:HD12	1.70	0.72
1:A:689:ALA:HB3	1:A:700:ILE:HD12	1.72	0.72
1:L:692:ILE:HA	1:L:697:LEU:HD22	1.71	0.72
1:E:607:ARG:NH1	1:E:696:PRO:O	2.24	0.71
1:E:685:ILE:HD11	1:E:764:LEU:HD12	1.73	0.70
1:I:664:ASN:O	1:I:668:ASP:HB2	1.91	0.70
1:G:672:GLU:HG2	1:G:699:MET:HE1	1.73	0.70
1:I:607:ARG:HH11	1:I:691:CYS:HB3	1.56	0.70
1:F:628:GLU:HA	1:F:651:LEU:HD23	1.72	0.69
1:I:739:THR:HG22	1:I:896:LEU:HB3	1.73	0.69
1:B:626:LEU:HD11	1:B:651:LEU:HD12	1.75	0.69
1:H:874:LEU:HD11	1:H:892:ILE:HG12	1.73	0.69
1:L:800:TRP:NE1	1:L:826:GLU:OE2	2.22	0.68
1:A:602:VAL:HG11	1:A:687:LEU:HD23	1.75	0.68
1:L:661:ALA:HB1	1:L:665:ALA:HB3	1.76	0.67
1:F:662:ASN:OD1	1:F:662:ASN:N	2.25	0.67
1:J:600:VAL:HG21	1:J:678:ARG:HE	1.60	0.67
1:C:605:PHE:CD1	1:C:606:PRO:HD2	2.29	0.67
1:G:691:CYS:HB2	1:G:698:CYS:HB2	1.76	0.67
1:D:735:LYS:O	1:D:739:THR:HG23	1.94	0.66
1:B:791:GLN:HE22	1:H:789:ARG:HH22	1.44	0.66
1:F:735:LYS:O	1:F:739:THR:HG23	1.96	0.66
1:K:741:ILE:HG13	1:K:771:ILE:HG21	1.77	0.66
1:E:824:LEU:HG	1:E:875:MET:HE2	1.78	0.66
1:J:793:ARG:NH1	1:J:806:ILE:O	2.25	0.66
1:L:748:LEU:HD22	1:L:753:PHE:HD2	1.61	0.65
1:A:867:CYS:SG	1:A:871:VAL:HG23	2.37	0.65
1:L:839:LEU:HD22	1:L:843:GLN:HB3	1.78	0.65
1:K:685:ILE:HD11	1:K:764:LEU:HD12	1.77	0.65
1:D:739:THR:HG22	1:D:896:LEU:HB3	1.78	0.65
1:D:786:ASP:OD1	1:D:834:GLN:NE2	2.26	0.65
1:E:713:LEU:HD21	1:E:737:MET:HE1	1.79	0.65
1:F:796:LEU:HD13	1:F:801:MET:HE1	1.79	0.64
1:L:664:ASN:O	1:L:668:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:TRP:HA	1:C:822:VAL:HG21	1.79	0.64
1:H:852:PHE:O	1:H:881:ARG:NH1	2.30	0.64
1:C:874:LEU:HD21	1:C:892:ILE:HG23	1.78	0.64
1:F:685:ILE:HD11	1:F:764:LEU:HD12	1.79	0.64
1:K:663:LYS:O	1:K:667:ASN:ND2	2.31	0.64
1:G:626:LEU:HD11	1:G:651:LEU:HD12	1.79	0.64
1:C:616:LEU:HD21	1:C:626:LEU:HB2	1.80	0.64
1:G:867:CYS:SG	1:G:871:VAL:HG23	2.38	0.63
1:B:672:GLU:HG2	1:B:699:MET:HE1	1.79	0.63
1:B:613:LYS:HD2	1:B:628:GLU:HB2	1.81	0.62
1:B:685:ILE:HD11	1:B:764:LEU:HD12	1.81	0.62
1:A:685:ILE:HD11	1:A:764:LEU:HD12	1.80	0.62
1:H:660:ASP:HB2	1:L:795:VAL:HG11	1.81	0.61
1:J:600:VAL:HG11	1:J:678:ARG:HG2	1.81	0.61
1:E:735:LYS:O	1:E:739:THR:HG23	2.00	0.60
1:I:618:GLU:O	1:I:779:SER:HB2	2.02	0.60
1:A:792:GLY:HA3	1:K:666:ARG:HD2	1.83	0.60
1:B:806:ILE:HG22	1:B:807:LEU:HD23	1.83	0.60
1:H:790:ILE:HD12	1:H:796:LEU:HD12	1.84	0.60
1:L:836:TYR:H	1:L:861:LEU:HD21	1.66	0.60
1:B:824:LEU:HB3	1:B:875:MET:HE2	1.82	0.60
1:I:692:ILE:HA	1:I:697:LEU:HD22	1.84	0.60
1:L:874:LEU:HD11	1:L:892:ILE:HG12	1.84	0.60
1:G:704:MET:SD	1:G:772:LYS:HD2	2.42	0.59
1:I:806:ILE:HG22	1:I:807:LEU:HD23	1.83	0.59
1:D:745:MET:HE2	1:D:758:LEU:HD22	1.84	0.59
1:G:793:ARG:NH1	1:G:806:ILE:O	2.35	0.59
1:B:735:LYS:O	1:B:739:THR:HG23	2.03	0.59
1:C:691:CYS:O	1:C:697:LEU:HA	2.03	0.59
1:B:756:ARG:HG2	1:B:811:PHE:CD1	2.38	0.59
1:F:694:ASP:OD1	1:F:694:ASP:N	2.36	0.59
1:E:874:LEU:HD21	1:E:892:ILE:HG23	1.85	0.58
1:H:799:ARG:NH2	1:H:839:LEU:O	2.36	0.58
1:A:852:PHE:CE2	1:K:604:GLU:HB2	2.38	0.58
1:D:806:ILE:HG22	1:D:807:LEU:HD23	1.85	0.58
1:L:657:LEU:HD21	1:L:666:ARG:HG3	1.86	0.58
1:B:685:ILE:HG13	1:B:774:ALA:HB2	1.86	0.57
1:J:735:LYS:O	1:J:739:THR:HG23	2.04	0.57
1:B:839:LEU:HD22	1:B:843:GLN:HB3	1.87	0.57
1:A:679:LEU:HD13	1:A:684:ILE:HG21	1.86	0.57
1:J:743:SER:HB2	1:J:893:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:LEU:HD13	1:C:684:ILE:HG21	1.87	0.57
1:D:738:ALA:HB1	1:D:824:LEU:HD12	1.86	0.57
1:A:839:LEU:HD22	1:A:843:GLN:HB3	1.87	0.57
1:C:793:ARG:NH1	1:C:806:ILE:O	2.30	0.57
1:E:872:TYR:CE2	1:E:876:LEU:HD11	2.40	0.57
1:E:874:LEU:O	1:E:877:SER:OG	2.20	0.57
1:K:793:ARG:NH1	1:K:806:ILE:O	2.33	0.57
1:C:890:GLN:N	1:C:890:GLN:OE1	2.34	0.57
1:J:662:ASN:HB2	1:J:665:ALA:H	1.70	0.57
1:L:672:GLU:HG2	1:L:699:MET:HE1	1.86	0.57
1:L:685:ILE:HG12	1:L:773:ILE:O	2.05	0.57
1:A:807:LEU:HD13	1:K:692:ILE:HG13	1.87	0.57
1:E:850:GLU:OE1	1:E:857:ARG:HB2	2.04	0.57
1:A:666:ARG:NH2	1:A:695:ASP:OD2	2.38	0.56
1:F:683:ASN:HD21	1:F:740:GLN:HG2	1.70	0.56
1:L:813:THR:O	1:L:817:VAL:HG23	2.05	0.56
1:A:880:ARG:NH1	1:A:885:ASN:O	2.38	0.56
1:D:791:GLN:NE2	1:E:791:GLN:OE1	2.38	0.56
1:G:605:PHE:HE1	1:G:610:LEU:HG	1.68	0.56
1:L:735:LYS:O	1:L:739:THR:HG23	2.05	0.56
1:E:611:THR:HG23	1:H:728:THR:HB	1.86	0.56
1:J:867:CYS:SG	1:J:871:VAL:HG22	2.46	0.56
1:L:867:CYS:SG	1:L:871:VAL:HG23	2.45	0.56
1:D:626:LEU:HD11	1:D:651:LEU:HB3	1.88	0.56
1:H:685:ILE:HD12	1:H:701:THR:HG21	1.86	0.56
1:L:674:LYS:HB3	1:L:678:ARG:HH12	1.71	0.56
1:C:674:LYS:HB3	1:C:678:ARG:HH12	1.71	0.56
1:H:861:LEU:HD12	1:H:879:TRP:CH2	2.41	0.55
1:K:607:ARG:NH2	1:K:696:PRO:HD2	2.21	0.55
1:H:708:ASP:HA	1:H:763:CYS:O	2.07	0.55
1:K:800:TRP:NE1	1:K:826:GLU:OE2	2.32	0.55
1:A:713:LEU:HD21	1:A:737:MET:HE1	1.86	0.55
1:F:691:CYS:HB2	1:F:698:CYS:HB2	1.89	0.55
1:I:741:ILE:HG13	1:I:771:ILE:HG21	1.89	0.55
1:F:666:ARG:NH2	1:F:695:ASP:OD2	2.30	0.55
1:B:728:THR:HG22	1:B:729:VAL:O	2.07	0.55
1:D:824:LEU:HD23	1:D:875:MET:HE2	1.87	0.55
1:I:657:LEU:HD21	1:I:666:ARG:HG3	1.89	0.55
1:K:607:ARG:NH1	1:K:696:PRO:O	2.39	0.55
1:A:853:ARG:O	1:A:855:GLN:HG3	2.07	0.55
1:B:868:PRO:HD2	1:B:871:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:796:LEU:HB3	1:I:801:MET:SD	2.47	0.55
1:E:660:ASP:HB2	1:I:795:VAL:HG11	1.90	0.54
1:K:624:VAL:HA	1:K:654:VAL:O	2.07	0.54
1:F:796:LEU:HB3	1:F:801:MET:SD	2.47	0.54
1:G:738:ALA:HB1	1:G:824:LEU:HD11	1.90	0.54
1:J:685:ILE:HD11	1:J:764:LEU:HD12	1.88	0.54
1:I:685:ILE:HD12	1:I:701:THR:HG21	1.89	0.54
1:A:685:ILE:HG23	1:A:701:THR:HG21	1.89	0.54
1:F:888:SER:OG	1:F:891:GLU:HG3	2.08	0.54
1:F:782:LEU:HD12	1:F:782:LEU:O	2.08	0.54
1:B:605:PHE:CD1	1:B:606:PRO:HD2	2.43	0.54
1:D:676:MET:HE2	2:D:1001:D6Q:C32	2.38	0.54
1:D:787:TYR:HB3	1:D:795:VAL:HG22	1.89	0.53
1:A:622:GLY:HA2	1:A:658:ARG:HG3	1.90	0.53
1:C:739:THR:HG22	1:C:896:LEU:HB3	1.91	0.53
1:I:685:ILE:HD11	1:I:764:LEU:HD12	1.90	0.53
1:D:852:PHE:CE2	1:I:604:GLU:HB2	2.43	0.53
1:H:710:ASN:O	1:H:714:SER:OG	2.20	0.53
1:H:781:ASN:ND2	1:L:618:GLU:OE2	2.35	0.53
1:K:614:GLU:HG3	1:K:626:LEU:HD23	1.90	0.53
1:D:739:THR:HG22	1:D:896:LEU:CB	2.39	0.53
1:F:656:MET:HG2	1:F:698:CYS:SG	2.49	0.53
1:F:801:MET:HE2	1:F:806:ILE:HG12	1.91	0.53
1:I:623:GLU:HG2	1:I:658:ARG:HH21	1.74	0.53
1:I:799:ARG:NH1	1:I:841:ASP:OD1	2.42	0.53
1:A:686:HIS:O	1:A:701:THR:HG23	2.09	0.52
1:C:606:PRO:HG2	1:C:609:LEU:HD12	1.89	0.52
1:J:778:MET:HG2	1:J:787:TYR:CE2	2.45	0.52
1:B:887:PRO:HB2	1:B:892:ILE:HG13	1.89	0.52
1:H:743:SER:HA	1:H:746:LYS:HD3	1.92	0.52
1:A:604:GLU:HB2	1:H:852:PHE:CE2	2.44	0.52
1:B:704:MET:HG3	1:B:764:LEU:HB3	1.92	0.52
1:H:825:TRP:O	1:H:829:THR:HG23	2.09	0.52
1:G:797:PRO:O	1:G:801:MET:HG3	2.10	0.52
1:A:615:LYS:NZ	1:A:618:GLU:OE2	2.42	0.52
1:B:867:CYS:SG	1:B:871:VAL:HG23	2.50	0.52
1:B:836:TYR:CE1	1:B:861:LEU:HD21	2.45	0.52
1:I:743:SER:O	1:I:746:LYS:HG2	2.09	0.51
1:K:626:LEU:HD12	1:K:652:VAL:O	2.10	0.51
1:A:618:GLU:OE1	1:B:781:ASN:HB3	2.10	0.51
1:I:872:TYR:CE2	1:I:876:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:LEU:HD21	1:D:776:PHE:HZ	1.75	0.51
1:I:839:LEU:HD22	1:I:843:GLN:HB3	1.90	0.51
1:A:666:ARG:HD2	1:H:792:GLY:HA3	1.92	0.51
1:A:852:PHE:CD2	1:K:604:GLU:HB2	2.45	0.51
1:H:743:SER:O	1:H:746:LYS:HG2	2.10	0.51
1:I:867:CYS:SG	1:I:871:VAL:HG22	2.50	0.51
1:D:875:MET:O	1:D:878:CYS:N	2.44	0.51
1:G:868:PRO:HD2	1:G:871:VAL:CG2	2.41	0.51
1:I:888:SER:OG	1:I:891:GLU:HG3	2.11	0.51
1:K:824:LEU:HG	1:K:875:MET:HE2	1.92	0.51
1:L:739:THR:HG22	1:L:896:LEU:HB2	1.93	0.51
1:B:755:HIS:O	1:B:756:ARG:HB2	2.10	0.51
1:K:672:GLU:HG2	1:K:699:MET:HE1	1.92	0.51
1:C:796:LEU:HD13	1:C:801:MET:HE1	1.91	0.51
1:G:781:ASN:OD1	1:G:781:ASN:N	2.42	0.51
1:H:887:PRO:HB2	1:H:892:ILE:HG13	1.91	0.51
1:G:740:GLN:NE2	1:G:771:ILE:H	2.09	0.50
1:J:824:LEU:HG	1:J:875:MET:HE2	1.93	0.50
1:L:760:THR:OG1	1:L:826:GLU:OE1	2.28	0.50
1:A:822:VAL:HG13	1:A:861:LEU:HD11	1.92	0.50
1:D:791:GLN:HE22	1:E:791:GLN:HB3	1.75	0.50
1:A:735:LYS:HE3	1:A:896:LEU:O	2.11	0.50
1:E:868:PRO:HD2	1:E:871:VAL:HG21	1.91	0.50
1:F:739:THR:HG22	1:F:896:LEU:CB	2.42	0.50
1:I:626:LEU:HD12	1:I:652:VAL:O	2.11	0.50
1:I:789:ARG:HB2	1:I:795:VAL:HG12	1.94	0.50
1:C:864:PRO:HB2	1:C:867:CYS:HB2	1.93	0.50
1:L:797:PRO:O	1:L:801:MET:HG3	2.12	0.50
1:D:868:PRO:HD2	1:D:871:VAL:HG21	1.94	0.50
1:G:711:GLN:O	1:G:715:ARG:HG3	2.12	0.50
1:C:602:VAL:HG11	1:C:687:LEU:HD23	1.94	0.50
1:I:706:ASN:ND2	1:I:766:GLY:O	2.45	0.50
1:I:778:MET:HG2	1:I:787:TYR:CE1	2.46	0.50
1:A:613:LYS:HD2	1:A:628:GLU:HB2	1.93	0.49
1:A:660:ASP:HB2	1:B:789:ARG:HB3	1.93	0.49
1:A:739:THR:HG22	1:A:896:LEU:HB3	1.94	0.49
1:F:739:THR:HG22	1:F:896:LEU:HB3	1.94	0.49
1:L:747:TYR:CZ	1:L:751:LEU:HD11	2.47	0.49
1:C:624:VAL:HA	1:C:654:VAL:O	2.13	0.49
1:K:735:LYS:O	1:K:739:THR:HG23	2.12	0.49
1:D:755:HIS:O	1:D:756:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:867:CYS:SG	1:E:871:VAL:HG23	2.52	0.49
1:E:757:ASP:OD1	1:E:761:ARG:NH2	2.44	0.49
1:B:852:PHE:CE2	1:L:604:GLU:HB2	2.48	0.49
1:G:836:TYR:HB3	1:G:839:LEU:HD12	1.95	0.49
1:I:701:THR:OG1	2:I:1001:D6Q:F37	2.21	0.49
1:K:796:LEU:HB3	1:K:801:MET:SD	2.53	0.49
1:H:739:THR:HG22	1:H:896:LEU:CB	2.41	0.49
1:I:604:GLU:CD	1:I:692:ILE:H	2.21	0.49
1:I:756:ARG:HG2	1:I:811:PHE:CD2	2.48	0.49
1:I:776:PHE:CE2	2:I:1001:D6Q:C10	2.96	0.49
1:J:691:CYS:HB2	1:J:698:CYS:HB2	1.95	0.49
1:C:868:PRO:HD2	1:C:871:VAL:HG21	1.95	0.49
1:E:606:PRO:HG2	1:E:609:LEU:HD12	1.95	0.49
1:L:691:CYS:O	1:L:697:LEU:HA	2.13	0.49
1:B:607:ARG:NH1	1:B:696:PRO:O	2.46	0.48
1:C:685:ILE:HD12	1:C:701:THR:HG21	1.94	0.48
1:D:852:PHE:CD1	1:D:852:PHE:C	2.90	0.48
1:G:851:PHE:HE1	1:G:860:TYR:CE1	2.31	0.48
1:H:717:GLU:HA	1:H:718:PRO:HD2	1.56	0.48
1:K:675:ILE:HD13	1:K:753:PHE:HE1	1.78	0.48
1:L:607:ARG:HH11	1:L:691:CYS:HB3	1.78	0.48
1:D:793:ARG:NH1	1:D:806:ILE:O	2.45	0.48
1:F:883:THR:HG22	1:F:886:ARG:CZ	2.43	0.48
1:L:624:VAL:HA	1:L:654:VAL:O	2.14	0.48
1:B:786:ASP:OD1	1:B:834:GLN:NE2	2.31	0.48
1:C:716:HIS:O	1:C:717:GLU:HB2	2.13	0.48
1:E:683:ASN:O	1:E:684:ILE:HD13	2.14	0.48
1:B:739:THR:HG22	1:B:896:LEU:HB3	1.96	0.48
1:F:868:PRO:HD2	1:F:871:VAL:HG21	1.95	0.48
1:G:616:LEU:HD21	1:G:626:LEU:HB2	1.96	0.48
1:G:883:THR:HA	1:G:886:ARG:HG3	1.95	0.48
1:J:825:TRP:O	1:J:829:THR:HG23	2.13	0.48
1:L:611:THR:O	1:L:627:CYS:HA	2.14	0.48
1:I:624:VAL:HG13	1:I:654:VAL:O	2.14	0.48
1:J:685:ILE:HD12	1:J:701:THR:HG21	1.96	0.48
1:K:604:GLU:OE2	1:K:693:THR:HG23	2.13	0.48
1:E:615:LYS:NZ	1:E:618:GLU:OE2	2.37	0.48
1:F:615:LYS:HD3	1:F:618:GLU:HG3	1.96	0.48
1:J:685:ILE:HD11	1:J:764:LEU:CD1	2.44	0.48
1:K:701:THR:HG22	1:K:702:GLU:O	2.14	0.48
1:G:797:PRO:HD2	1:G:801:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:790:ILE:HB	1:E:793:ARG:HB2	1.95	0.47
1:I:820:PHE:CE2	1:I:824:LEU:HD22	2.49	0.47
1:J:661:ALA:HB1	1:J:665:ALA:HB3	1.96	0.47
1:G:684:ILE:HD13	1:G:773:ILE:HB	1.95	0.47
1:K:743:SER:O	1:K:746:LYS:HG2	2.13	0.47
1:A:607:ARG:NH1	1:A:696:PRO:O	2.47	0.47
1:B:799:ARG:NH1	1:B:841:ASP:OD1	2.43	0.47
1:E:624:VAL:HA	1:E:654:VAL:O	2.14	0.47
1:H:797:PRO:O	1:H:801:MET:HG3	2.13	0.47
1:C:801:MET:HE2	1:C:806:ILE:HG13	1.96	0.47
1:G:709:LEU:HD23	1:G:760:THR:HG22	1.97	0.47
1:H:607:ARG:HH11	1:H:691:CYS:HB3	1.79	0.47
1:J:767:LYS:HB2	1:J:767:LYS:HE2	1.62	0.47
1:C:789:ARG:HB3	1:C:795:VAL:HG12	1.96	0.47
1:H:604:GLU:HB2	1:K:852:PHE:CE2	2.50	0.47
1:A:666:ARG:HH22	1:A:695:ASP:CG	2.23	0.47
1:C:874:LEU:HD11	1:C:892:ILE:HG12	1.95	0.47
1:E:799:ARG:NH1	1:E:841:ASP:OD1	2.39	0.47
1:H:681:ASP:HB2	1:H:747:TYR:CD2	2.49	0.47
1:H:861:LEU:HD12	1:H:879:TRP:CZ2	2.49	0.47
1:J:741:ILE:HG13	1:J:771:ILE:HG21	1.97	0.47
1:J:887:PRO:HB2	1:J:892:ILE:HG13	1.97	0.47
1:B:789:ARG:HB2	1:B:795:VAL:HG12	1.97	0.47
1:C:740:GLN:NE2	1:C:771:ILE:H	2.13	0.47
1:I:797:PRO:O	1:I:801:MET:HG3	2.15	0.47
1:C:767:LYS:HE3	1:C:767:LYS:HB2	1.60	0.47
1:K:669:PHE:CE1	1:K:699:MET:HE2	2.50	0.47
1:A:887:PRO:HB2	1:A:892:ILE:HG13	1.96	0.47
1:E:796:LEU:HB3	1:E:801:MET:SD	2.55	0.47
1:F:701:THR:HG22	1:F:702:GLU:O	2.15	0.47
1:J:834:GLN:HG3	1:J:835:PRO:HD2	1.96	0.47
1:L:607:ARG:NH2	1:L:696:PRO:HD2	2.30	0.47
1:L:711:GLN:HB3	1:L:715:ARG:HE	1.79	0.47
1:G:684:ILE:CD1	1:G:773:ILE:HB	2.45	0.46
1:H:814:ALA:HB1	1:H:886:ARG:HH11	1.80	0.46
1:I:841:ASP:O	1:I:845:ILE:HG12	2.15	0.46
1:L:761:ARG:HB2	1:L:780:ARG:HH22	1.80	0.46
1:C:736:PHE:O	1:C:740:GLN:HG3	2.16	0.46
1:E:741:ILE:HG13	1:E:771:ILE:HG21	1.97	0.46
1:C:805:SER:O	1:C:809:GLY:HA2	2.15	0.46
1:J:850:GLU:OE1	1:J:857:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:850:GLU:OE1	1:L:857:ARG:HB2	2.16	0.46
1:L:895:LEU:HD23	1:L:895:LEU:HA	1.63	0.46
1:B:801:MET:HE3	1:B:811:PHE:HE1	1.80	0.46
1:L:747:TYR:CE2	1:L:751:LEU:HD11	2.51	0.46
1:A:796:LEU:HD13	1:A:801:MET:HE1	1.96	0.46
1:D:790:ILE:HB	1:D:793:ARG:HG3	1.98	0.46
1:H:822:VAL:HG22	1:H:861:LEU:HD11	1.96	0.46
1:E:616:LEU:HD12	1:E:624:VAL:HG12	1.97	0.46
1:G:799:ARG:HB3	1:G:835:PRO:HG2	1.98	0.46
1:A:881:ARG:HG3	1:A:882:ASP:N	2.30	0.46
1:F:872:TYR:CZ	1:F:876:LEU:HD21	2.51	0.46
1:G:782:LEU:HD23	1:G:782:LEU:O	2.16	0.46
1:H:607:ARG:NH2	1:H:696:PRO:HD2	2.31	0.46
1:L:669:PHE:O	1:L:673:ILE:HG13	2.16	0.46
1:J:861:LEU:HD12	1:J:879:TRP:CZ2	2.50	0.46
1:J:883:THR:HG22	1:J:886:ARG:CZ	2.46	0.46
1:K:626:LEU:HD11	1:K:651:LEU:HD12	1.98	0.46
1:A:888:SER:OG	1:A:891:GLU:HG3	2.16	0.46
1:G:790:ILE:HB	1:G:793:ARG:HB2	1.98	0.46
1:G:796:LEU:HB3	1:G:801:MET:SD	2.55	0.45
1:G:798:ILE:HD12	1:G:844:VAL:CG1	2.46	0.45
1:H:756:ARG:HG2	1:H:811:PHE:CD1	2.52	0.45
1:J:861:LEU:HD12	1:J:879:TRP:CH2	2.50	0.45
1:K:669:PHE:O	1:K:673:ILE:HG13	2.16	0.45
1:D:656:MET:HG2	1:D:698:CYS:SG	2.57	0.45
1:E:868:PRO:HD2	1:E:871:VAL:CG2	2.46	0.45
1:H:818:TRP:CE3	1:H:879:TRP:HA	2.51	0.45
1:L:748:LEU:HD22	1:L:753:PHE:CD2	2.46	0.45
1:C:868:PRO:HD2	1:C:871:VAL:CG2	2.46	0.45
1:L:761:ARG:HB2	1:L:780:ARG:NH2	2.31	0.45
1:D:613:LYS:HB3	1:D:613:LYS:HE3	1.76	0.45
1:H:666:ARG:HE	1:K:792:GLY:HA3	1.82	0.45
1:H:887:PRO:HG2	1:H:892:ILE:HD11	1.99	0.45
1:L:893:HIS:NE2	1:L:897:LEU:HD11	2.32	0.45
1:D:778:MET:HG2	1:D:787:TYR:CE1	2.52	0.45
1:A:708:ASP:HA	1:A:763:CYS:O	2.17	0.45
1:K:868:PRO:HD2	1:K:871:VAL:HG21	1.99	0.45
1:I:729:VAL:HB	1:I:830:PHE:HE2	1.82	0.45
1:J:799:ARG:HB2	1:J:800:TRP:CZ3	2.52	0.45
1:J:803:TRP:CZ3	1:J:852:PHE:CD1	3.05	0.45
1:B:737:MET:SD	1:B:771:ILE:HD11	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:609:LEU:HD22	1:E:630:GLU:HB2	1.99	0.45
1:G:717:GLU:O	1:G:717:GLU:HG3	2.17	0.45
1:I:874:LEU:HD21	1:I:892:ILE:HG23	1.99	0.45
1:A:704:MET:HG3	1:A:764:LEU:HB3	1.99	0.45
1:F:655:LYS:HD3	1:F:699:MET:HE3	1.98	0.45
1:F:672:GLU:HG2	1:F:699:MET:HE1	1.99	0.45
1:F:851:PHE:CD1	1:F:858:GLN:HG3	2.51	0.45
1:H:834:GLN:HG2	1:H:835:PRO:HD2	1.98	0.45
1:I:657:LEU:HB2	1:I:669:PHE:CE1	2.52	0.45
1:L:739:THR:HG22	1:L:896:LEU:CB	2.47	0.45
1:H:734:LEU:HD13	1:H:828:PHE:HA	1.99	0.44
1:K:796:LEU:HD13	1:K:801:MET:HE1	1.99	0.44
1:K:868:PRO:O	1:K:871:VAL:HG23	2.16	0.44
1:A:605:PHE:CD1	1:A:606:PRO:HD2	2.52	0.44
1:A:616:LEU:HD21	1:A:626:LEU:HB2	1.98	0.44
1:A:801:MET:HE2	1:A:806:ILE:HG13	1.98	0.44
1:D:764:LEU:HD21	1:D:776:PHE:CZ	2.51	0.44
1:H:618:GLU:CD	1:L:781:ASN:HD22	2.24	0.44
1:B:657:LEU:HB2	1:B:669:PHE:CD1	2.52	0.44
1:B:796:LEU:HB3	1:B:801:MET:SD	2.57	0.44
1:B:853:ARG:HH21	1:L:693:THR:HG21	1.82	0.44
1:A:863:GLN:HA	1:A:872:TYR:CE1	2.53	0.44
1:C:894:LEU:HA	1:C:894:LEU:HD23	1.71	0.44
1:H:718:PRO:HB3	1:H:830:PHE:CE1	2.52	0.44
1:L:713:LEU:HD11	1:L:827:THR:HG23	1.99	0.44
1:G:691:CYS:HB2	1:G:698:CYS:CB	2.45	0.44
1:H:789:ARG:HD2	1:L:660:ASP:HA	1.98	0.44
1:C:880:ARG:HD2	1:C:885:ASN:O	2.18	0.44
1:D:741:ILE:HG13	1:D:771:ILE:HG21	1.99	0.44
1:F:799:ARG:NH1	1:F:841:ASP:OD1	2.50	0.44
1:I:605:PHE:HZ	1:I:629:VAL:HG13	1.83	0.44
1:J:878:CYS:O	1:J:886:ARG:HD3	2.17	0.44
1:C:706:ASN:HB2	1:C:765:VAL:HG12	1.99	0.44
1:H:701:THR:HG22	1:H:702:GLU:N	2.33	0.44
1:E:684:ILE:HD13	1:E:773:ILE:HB	2.00	0.44
1:G:676:MET:HB3	1:G:676:MET:HE3	1.62	0.44
1:C:884:LYS:HG3	1:C:885:ASN:OD1	2.18	0.44
1:A:704:MET:SD	1:A:772:LYS:HD2	2.58	0.43
1:F:669:PHE:CE2	1:F:697:LEU:HB2	2.53	0.43
1:K:834:GLN:O	1:K:837:SER:HB3	2.18	0.43
1:D:607:ARG:HE	1:D:607:ARG:HB2	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:607:ARG:HH11	1:H:691:CYS:CB	2.31	0.43
1:I:605:PHE:CZ	1:I:629:VAL:HG13	2.53	0.43
1:A:624:VAL:HG11	2:A:1001:D6Q:O11	2.18	0.43
1:D:767:LYS:O	1:D:770:THR:HG23	2.18	0.43
1:E:813:THR:HA	1:E:816:ASP:HB2	1.99	0.43
1:H:825:TRP:CD1	1:H:861:LEU:HB3	2.53	0.43
1:J:776:PHE:HE1	2:J:1001:D6Q:O11	2.02	0.43
1:K:713:LEU:HD11	1:K:827:THR:HG23	2.00	0.43
1:C:703:TYR:CZ	1:C:705:GLU:HA	2.53	0.43
1:I:615:LYS:HE3	1:I:615:LYS:HB2	1.77	0.43
1:E:851:PHE:CD1	1:E:858:GLN:HB2	2.53	0.43
1:K:825:TRP:CG	1:K:861:LEU:HD13	2.53	0.43
1:L:625:HIS:ND1	1:L:656:MET:HE3	2.34	0.43
1:F:743:SER:O	1:F:746:LYS:HG2	2.19	0.43
1:G:789:ARG:HB3	1:G:795:VAL:HG12	2.00	0.43
1:H:681:ASP:CG	1:H:682:PRO:HD2	2.44	0.43
1:L:729:VAL:HG13	1:L:769:TYR:HE2	1.84	0.43
1:A:813:THR:O	1:A:817:VAL:HG23	2.19	0.43
1:C:619:GLY:HA2	1:C:779:SER:HB2	2.01	0.43
1:E:887:PRO:HB2	1:E:892:ILE:HG13	2.01	0.43
1:K:889:PHE:HA	1:K:892:ILE:HD12	2.01	0.43
1:L:690:VAL:HB	1:L:692:ILE:HG23	2.01	0.43
1:A:624:VAL:HA	1:A:654:VAL:O	2.18	0.43
1:D:626:LEU:HD13	1:D:703:TYR:CD1	2.54	0.43
1:L:876:LEU:HD23	1:L:876:LEU:HA	1.77	0.43
1:F:858:GLN:OE1	1:F:858:GLN:N	2.51	0.43
1:I:824:LEU:HG	1:I:875:MET:HE2	2.01	0.43
1:K:704:MET:HE2	1:K:772:LYS:HD2	2.01	0.43
1:E:810:LYS:HG3	1:E:810:LYS:O	2.19	0.42
1:L:628:GLU:HG3	1:L:650:VAL:O	2.19	0.42
1:L:863:GLN:HB2	1:L:872:TYR:CD2	2.54	0.42
1:A:871:VAL:O	1:A:875:MET:HG3	2.19	0.42
1:F:884:LYS:HG3	1:F:885:ASN:OD1	2.19	0.42
1:A:662:ASN:OD1	1:A:662:ASN:N	2.48	0.42
1:C:801:MET:HB3	1:C:806:ILE:HG13	2.02	0.42
1:K:683:ASN:OD1	1:K:740:GLN:HB3	2.19	0.42
1:C:804:GLU:HG3	1:C:810:LYS:HG2	2.02	0.42
1:D:803:TRP:HA	1:D:848:THR:HG23	2.01	0.42
1:B:655:LYS:HE2	1:B:669:PHE:CE1	2.54	0.42
1:E:760:THR:HG23	1:E:826:GLU:OE1	2.19	0.42
1:E:765:VAL:HG22	1:E:771:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:654:VAL:HG22	1:F:700:ILE:HG23	2.02	0.42
1:F:818:TRP:CE3	1:F:879:TRP:HA	2.54	0.42
1:I:616:LEU:HB2	1:I:624:VAL:HG12	2.02	0.42
1:I:688:LEU:HB2	1:I:700:ILE:HG22	2.00	0.42
1:K:673:ILE:HG12	1:K:699:MET:SD	2.60	0.42
1:C:663:LYS:HB3	1:C:663:LYS:HE2	1.84	0.42
1:D:796:LEU:HD13	1:D:801:MET:HE1	2.00	0.42
1:D:871:VAL:O	1:D:874:LEU:HB3	2.19	0.42
1:E:712:PHE:O	1:E:716:HIS:HD2	2.02	0.42
1:E:761:ARG:HB2	1:E:780:ARG:NH2	2.35	0.42
1:E:897:LEU:HD23	1:E:897:LEU:HA	1.85	0.42
1:G:747:TYR:CZ	1:G:751:LEU:HD11	2.53	0.42
1:C:605:PHE:HB2	1:C:689:ALA:HB1	2.02	0.42
1:H:781:ASN:HB3	1:L:615:LYS:NZ	2.35	0.42
1:E:774:ALA:HB1	2:E:1001:D6Q:O22	2.19	0.42
1:F:804:GLU:CD	1:F:804:GLU:H	2.28	0.42
1:H:745:MET:HB3	1:H:889:PHE:CD2	2.55	0.42
1:I:657:LEU:CD2	1:I:666:ARG:HG3	2.48	0.42
1:J:685:ILE:HD13	1:J:685:ILE:HA	1.93	0.42
1:L:683:ASN:OD1	1:L:740:GLN:NE2	2.48	0.42
1:L:704:MET:HE2	1:L:772:LYS:HB2	2.01	0.42
1:C:801:MET:HE2	1:C:806:ILE:CG1	2.50	0.42
1:L:684:ILE:HD13	1:L:773:ILE:HB	2.02	0.42
1:C:818:TRP:CD2	1:C:879:TRP:HD1	2.38	0.42
1:E:605:PHE:CD1	1:E:606:PRO:HD2	2.55	0.42
1:F:882:ASP:OD2	1:F:884:LYS:HE3	2.19	0.42
1:H:812:THR:O	1:H:815:SER:N	2.53	0.42
1:J:882:ASP:OD2	1:J:884:LYS:HE3	2.19	0.42
1:K:776:PHE:HE1	2:K:1001:D6Q:C10	2.33	0.42
1:K:788:TYR:HB3	1:K:798:ILE:HD13	2.02	0.42
1:A:757:ASP:O	1:A:762:ASN:ND2	2.41	0.41
1:D:875:MET:O	1:D:878:CYS:HB2	2.20	0.41
1:F:616:LEU:HD23	1:F:616:LEU:HA	1.86	0.41
1:G:788:TYR:CD1	1:G:841:ASP:HB3	2.55	0.41
1:H:799:ARG:HD3	1:H:835:PRO:O	2.20	0.41
1:K:762:ASN:OD1	1:K:776:PHE:HD2	2.02	0.41
1:L:736:PHE:O	1:L:740:GLN:HG3	2.20	0.41
1:B:801:MET:HE3	1:B:811:PHE:CE1	2.54	0.41
1:D:709:LEU:N	1:D:763:CYS:O	2.47	0.41
1:E:761:ARG:HB2	1:E:780:ARG:HH22	1.85	0.41
1:G:800:TRP:NE1	1:G:826:GLU:OE2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:778:MET:SD	1:I:795:VAL:HG23	2.61	0.41
1:I:780:ARG:H	1:I:780:ARG:HG3	1.60	0.41
1:I:812:THR:O	1:I:815:SER:OG	2.33	0.41
1:A:806:ILE:HG22	1:A:807:LEU:HD23	2.02	0.41
1:C:897:LEU:HA	1:C:897:LEU:HD23	1.78	0.41
1:E:616:LEU:HD21	1:E:626:LEU:HB2	2.02	0.41
1:E:825:TRP:CZ2	1:E:829:THR:HG21	2.55	0.41
1:K:851:PHE:CE1	1:K:858:GLN:HG3	2.55	0.41
1:L:793:ARG:NH1	1:L:806:ILE:O	2.53	0.41
1:B:839:LEU:HD23	1:B:839:LEU:HA	1.64	0.41
1:C:674:LYS:O	1:C:677:SER:OG	2.29	0.41
1:H:880:ARG:N	1:H:880:ARG:HD2	2.34	0.41
1:K:663:LYS:HE3	1:K:663:LYS:HB2	1.86	0.41
1:F:683:ASN:ND2	1:F:740:GLN:HG2	2.35	0.41
1:G:801:MET:HE3	1:G:811:PHE:CE1	2.55	0.41
1:I:755:HIS:O	1:I:756:ARG:HB2	2.20	0.41
1:D:619:GLY:N	1:D:622:GLY:O	2.41	0.41
1:F:734:LEU:HD11	1:F:830:PHE:CZ	2.56	0.41
1:I:870:SER:O	1:I:873:LYS:HB3	2.21	0.41
1:I:897:LEU:HD23	1:I:897:LEU:HA	1.89	0.41
1:K:626:LEU:HD13	1:K:703:TYR:CD1	2.56	0.41
1:L:709:LEU:HD23	1:L:760:THR:HG22	2.01	0.41
1:A:807:LEU:O	1:A:808:LEU:HD23	2.21	0.41
1:J:740:GLN:OE1	1:J:770:THR:HA	2.21	0.41
1:L:685:ILE:HD13	1:L:685:ILE:HA	1.85	0.41
1:L:740:GLN:OE1	1:L:770:THR:HA	2.20	0.41
1:A:834:GLN:HG3	1:A:835:PRO:HD2	2.01	0.41
1:G:602:VAL:HB	1:G:603:GLU:H	1.63	0.41
1:K:658:ARG:HB3	1:K:660:ASP:OD1	2.21	0.41
1:L:799:ARG:HB2	1:L:800:TRP:CZ3	2.55	0.41
1:A:735:LYS:O	1:A:739:THR:HG23	2.21	0.41
1:B:685:ILE:HG23	1:B:701:THR:HG21	2.03	0.41
1:B:749:SER:OG	1:B:813:THR:HG21	2.20	0.41
1:C:805:SER:HB2	1:C:811:PHE:CE2	2.56	0.41
1:H:866:ILE:H	1:H:866:ILE:HG12	1.63	0.41
1:I:616:LEU:HD11	1:I:626:LEU:HB2	2.03	0.41
1:I:881:ARG:HD3	1:I:882:ASP:N	2.36	0.41
1:K:839:LEU:HB3	1:K:843:GLN:HB2	2.03	0.41
1:L:764:LEU:HD21	1:L:776:PHE:HZ	1.86	0.41
1:B:797:PRO:O	1:B:801:MET:HG3	2.21	0.41
1:E:877:SER:HA	1:E:880:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:776:PHE:CE2	2:F:1001:D6Q:C10	3.04	0.41
1:G:685:ILE:HD13	1:G:685:ILE:HA	1.85	0.41
1:J:611:THR:O	1:J:627:CYS:HA	2.21	0.41
1:K:888:SER:OG	1:K:891:GLU:HG3	2.21	0.41
1:B:746:LYS:HE2	1:B:893:HIS:ND1	2.36	0.40
1:I:607:ARG:NH2	1:I:696:PRO:HD2	2.36	0.40
1:J:895:LEU:HA	1:J:895:LEU:HD23	1.80	0.40
1:L:654:VAL:HG12	1:L:698:CYS:HB3	2.03	0.40
1:L:686:HIS:O	1:L:701:THR:HG23	2.20	0.40
1:D:852:PHE:HD1	1:D:852:PHE:O	2.04	0.40
1:E:713:LEU:HD11	1:E:827:THR:HG23	2.03	0.40
1:F:610:LEU:HD13	1:F:654:VAL:HG21	2.02	0.40
1:G:820:PHE:CZ	1:G:824:LEU:HD13	2.57	0.40
1:H:681:ASP:HB2	1:H:747:TYR:CG	2.56	0.40
1:J:701:THR:HG22	1:J:702:GLU:N	2.36	0.40
1:J:727:ARG:HD2	1:J:727:ARG:HA	1.81	0.40
1:K:717:GLU:O	1:K:728:THR:HG23	2.22	0.40
1:D:762:ASN:OD1	1:D:775:ASP:HA	2.22	0.40
1:D:799:ARG:NH2	1:D:839:LEU:O	2.53	0.40
1:D:888:SER:O	1:D:892:ILE:HG13	2.22	0.40
1:G:626:LEU:HD11	1:G:651:LEU:HB2	2.03	0.40
1:H:786:ASP:O	1:H:797:PRO:HA	2.22	0.40
1:I:747:TYR:CE1	1:I:751:LEU:HD11	2.57	0.40
1:J:687:LEU:HD12	1:J:687:LEU:HA	1.93	0.40
1:D:691:CYS:O	1:D:697:LEU:HA	2.20	0.40
1:I:718:PRO:HD3	1:I:830:PHE:CD1	2.56	0.40
1:K:862:PRO:O	1:K:864:PRO:HD3	2.22	0.40
1:L:684:ILE:HG22	1:L:685:ILE:N	2.37	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	265/309 (86%)	257 (97%)	8 (3%)	0	100	100
1	B	275/309 (89%)	264 (96%)	11 (4%)	0	100	100
1	C	266/309 (86%)	259 (97%)	7 (3%)	0	100	100
1	D	276/309 (89%)	268 (97%)	8 (3%)	0	100	100
1	E	267/309 (86%)	254 (95%)	13 (5%)	0	100	100
1	F	269/309 (87%)	260 (97%)	8 (3%)	1 (0%)	30	56
1	G	267/309 (86%)	253 (95%)	13 (5%)	1 (0%)	30	56
1	H	266/309 (86%)	258 (97%)	8 (3%)	0	100	100
1	I	261/309 (84%)	249 (95%)	10 (4%)	2 (1%)	16	41
1	J	266/309 (86%)	254 (96%)	11 (4%)	1 (0%)	30	56
1	K	262/309 (85%)	252 (96%)	10 (4%)	0	100	100
1	L	267/309 (86%)	253 (95%)	12 (4%)	2 (1%)	18	44
All	All	3207/3708 (86%)	3081 (96%)	119 (4%)	7 (0%)	43	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	719	PRO
1	F	757	ASP
1	I	756	ARG
1	I	662	ASN
1	L	854	ASP
1	J	602	VAL
1	G	602	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	243/278 (87%)	229 (94%)	14 (6%)	18	46
1	B	252/278 (91%)	241 (96%)	11 (4%)	25	56
1	C	244/278 (88%)	233 (96%)	11 (4%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	253/278 (91%)	230 (91%)	23 (9%)	9	26
1	E	246/278 (88%)	230 (94%)	16 (6%)	15	41
1	F	247/278 (89%)	229 (93%)	18 (7%)	13	35
1	G	245/278 (88%)	233 (95%)	12 (5%)	22	51
1	H	245/278 (88%)	222 (91%)	23 (9%)	8	24
1	I	241/278 (87%)	229 (95%)	12 (5%)	22	51
1	J	245/278 (88%)	236 (96%)	9 (4%)	30	62
1	K	242/278 (87%)	226 (93%)	16 (7%)	15	40
1	L	246/278 (88%)	231 (94%)	15 (6%)	17	43
All	All	2949/3336 (88%)	2769 (94%)	180 (6%)	17	43

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	VAL
1	A	627	CYS
1	A	651	LEU
1	A	662	ASN
1	A	673	ILE
1	A	680	LYS
1	A	701	THR
1	A	708	ASP
1	A	750	SER
1	A	813	THR
1	A	831	CYS
1	A	848	THR
1	A	859	THR
1	A	881	ARG
1	B	651	LEU
1	B	714	SER
1	B	724	SER
1	B	725	ASP
1	B	743	SER
1	B	761	ARG
1	B	813	THR
1	B	824	LEU
1	B	837	SER
1	B	877	SER
1	B	895	LEU

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Mol	Chain	Res	Type
1	C	602	VAL
1	C	623	GLU
1	C	673	ILE
1	C	685	ILE
1	C	730	SER
1	C	761	ARG
1	C	778	MET
1	C	799	ARG
1	C	810	LYS
1	C	837	SER
1	C	881	ARG
1	D	602	VAL
1	D	603	GLU
1	D	609	LEU
1	D	650	VAL
1	D	662	ASN
1	D	672	GLU
1	D	701	THR
1	D	721	SER
1	D	726	VAL
1	D	732	THR
1	D	743	SER
1	D	782	LEU
1	D	790	ILE
1	D	793	ARG
1	D	824	LEU
1	D	837	SER
1	D	842	GLU
1	D	852	PHE
1	D	870	SER
1	D	871	VAL
1	D	877	SER
1	D	881	ARG
1	D	895	LEU
1	E	602	VAL
1	E	629	VAL
1	E	658	ARG
1	E	662	ASN
1	E	672	GLU
1	E	717	GLU
1	E	728	THR
1	E	778	MET

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Mol	Chain	Res	Type
1	E	795	VAL
1	E	836	TYR
1	E	844	VAL
1	E	845	ILE
1	E	848	THR
1	E	871	VAL
1	E	873	LYS
1	E	881	ARG
1	F	602	VAL
1	F	611	THR
1	F	614	GLU
1	F	657	LEU
1	F	662	ASN
1	F	694	ASP
1	F	717	GLU
1	F	735	LYS
1	F	743	SER
1	F	754	VAL
1	F	778	MET
1	F	780	ARG
1	F	813	THR
1	F	844	VAL
1	F	866	ILE
1	F	871	VAL
1	F	876	LEU
1	F	895	LEU
1	G	602	VAL
1	G	611	THR
1	G	651	LEU
1	G	700	ILE
1	G	728	THR
1	G	739	THR
1	G	750	SER
1	G	754	VAL
1	G	781	ASN
1	G	789	ARG
1	G	846	GLU
1	G	859	THR
1	H	602	VAL
1	H	651	LEU
1	H	662	ASN
1	H	673	ILE

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Mol	Chain	Res	Type
1	H	674	LYS
1	H	685	ILE
1	H	698	CYS
1	H	717	GLU
1	H	728	THR
1	H	746	LYS
1	H	750	SER
1	H	761	ARG
1	H	793	ARG
1	H	810	LYS
1	H	824	LEU
1	H	832	GLN
1	H	866	ILE
1	H	870	SER
1	H	871	VAL
1	H	880	ARG
1	H	883	THR
1	H	888	SER
1	H	895	LEU
1	I	602	VAL
1	I	657	LEU
1	I	664	ASN
1	I	673	ILE
1	I	697	LEU
1	I	710	ASN
1	I	790	ILE
1	I	837	SER
1	I	842	GLU
1	I	859	THR
1	I	871	VAL
1	I	883	THR
1	J	602	VAL
1	J	651	LEU
1	J	732	THR
1	J	743	SER
1	J	767	LYS
1	J	784	SER
1	J	793	ARG
1	J	834	GLN
1	J	871	VAL
1	K	602	VAL
1	K	614	GLU

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Mol	Chain	Res	Type
1	K	685	ILE
1	K	700	ILE
1	K	705	GLU
1	K	730	SER
1	K	750	SER
1	K	778	MET
1	K	790	ILE
1	K	812	THR
1	K	813	THR
1	K	815	SER
1	K	834	GLN
1	K	866	ILE
1	K	870	SER
1	K	871	VAL
1	L	602	VAL
1	L	654	VAL
1	L	657	LEU
1	L	698	CYS
1	L	714	SER
1	L	727	ARG
1	L	729	VAL
1	L	746	LYS
1	L	765	VAL
1	L	772	LYS
1	L	812	THR
1	L	837	SER
1	L	844	VAL
1	L	866	ILE
1	L	888	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	843	GLN
1	B	710	ASN
1	B	791	GLN
1	C	662	ASN
1	D	710	ASN
1	D	791	GLN
1	D	855	GLN
1	D	885	ASN
1	E	686	HIS

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Mol	Chain	Res	Type
1	E	706	ASN
1	E	716	HIS
1	E	733	ASN
1	E	791	GLN
1	F	686	HIS
1	F	716	HIS
1	H	683	ASN
1	H	733	ASN
1	H	893	HIS
1	I	664	ASN
1	I	667	ASN
1	I	706	ASN
1	I	710	ASN
1	K	733	ASN
1	L	838	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	D6Q	I	1001	-	41,41,41	1.92	11 (26%)	58,63,63	2.46	18 (31%)
2	D6Q	G	1001	-	41,41,41	1.99	9 (21%)	58,63,63	1.79	12 (20%)
2	D6Q	E	1001	-	41,41,41	2.02	8 (19%)	58,63,63	2.20	16 (27%)
2	D6Q	B	1001	-	41,41,41	2.48	11 (26%)	58,63,63	1.72	14 (24%)
2	D6Q	A	1001	-	41,41,41	1.87	15 (36%)	58,63,63	2.02	16 (27%)
2	D6Q	J	1001	-	41,41,41	1.90	9 (21%)	58,63,63	2.17	18 (31%)
2	D6Q	C	1001	-	41,41,41	1.93	9 (21%)	58,63,63	2.07	15 (25%)
2	D6Q	H	1001	-	41,41,41	2.04	8 (19%)	58,63,63	1.87	13 (22%)
2	D6Q	L	1001	-	41,41,41	2.02	12 (29%)	58,63,63	2.18	19 (32%)
2	D6Q	F	1001	-	41,41,41	2.14	12 (29%)	58,63,63	2.13	16 (27%)
2	D6Q	K	1001	-	41,41,41	2.24	9 (21%)	58,63,63	2.05	16 (27%)
2	D6Q	D	1001	-	41,41,41	1.85	7 (17%)	58,63,63	2.06	15 (25%)

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	D6Q	I	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	G	1001	-	-	4/18/50/50	0/5/5/5
2	D6Q	E	1001	-	-	4/18/50/50	0/5/5/5
2	D6Q	B	1001	-	-	1/18/50/50	0/5/5/5
2	D6Q	A	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	J	1001	-	-	7/18/50/50	0/5/5/5
2	D6Q	C	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	H	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	L	1001	-	-	8/18/50/50	0/5/5/5
2	D6Q	F	1001	-	-	0/18/50/50	0/5/5/5
2	D6Q	K	1001	-	-	1/18/50/50	0/5/5/5
2	D6Q	D	1001	-	-	2/18/50/50	0/5/5/5

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	D6Q	C21-N20	7.66	1.45	1.36
2	K	1001	D6Q	C21-N20	6.67	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	D6Q	C27-C28	6.42	1.60	1.49
2	G	1001	D6Q	C21-N20	6.27	1.43	1.36
2	H	1001	D6Q	C27-C28	6.15	1.59	1.49
2	F	1001	D6Q	C21-N20	6.03	1.43	1.36
2	E	1001	D6Q	C7-N6	5.95	1.36	1.32
2	J	1001	D6Q	C21-N20	5.91	1.43	1.36
2	D	1001	D6Q	C21-N20	5.91	1.43	1.36
2	B	1001	D6Q	C4-N5	5.77	1.39	1.35
2	E	1001	D6Q	C4-N5	5.45	1.39	1.35
2	K	1001	D6Q	C10-N12	5.44	1.46	1.34
2	H	1001	D6Q	C4-N5	5.37	1.39	1.35
2	C	1001	D6Q	C7-N6	5.26	1.35	1.32
2	G	1001	D6Q	C4-N5	5.16	1.39	1.35
2	I	1001	D6Q	C27-C28	5.14	1.58	1.49
2	B	1001	D6Q	C7-N6	5.12	1.35	1.32
2	K	1001	D6Q	C27-C28	4.95	1.57	1.49
2	D	1001	D6Q	C27-C28	4.88	1.57	1.49
2	B	1001	D6Q	C10-N12	4.85	1.45	1.34
2	L	1001	D6Q	C4-N5	4.82	1.39	1.35
2	I	1001	D6Q	C10-N12	4.78	1.44	1.34
2	B	1001	D6Q	C27-C28	4.66	1.57	1.49
2	L	1001	D6Q	C21-N20	4.64	1.41	1.36
2	F	1001	D6Q	C27-C28	4.62	1.57	1.49
2	L	1001	D6Q	C10-N12	4.58	1.44	1.34
2	H	1001	D6Q	C21-N20	4.57	1.41	1.36
2	F	1001	D6Q	C4-N5	4.56	1.38	1.35
2	F	1001	D6Q	C7-N6	4.56	1.35	1.32
2	G	1001	D6Q	C27-C28	4.53	1.57	1.49
2	H	1001	D6Q	C7-N6	4.49	1.35	1.32
2	K	1001	D6Q	C4-N5	4.39	1.38	1.35
2	F	1001	D6Q	C10-N12	4.32	1.43	1.34
2	A	1001	D6Q	C21-N20	4.23	1.41	1.36
2	K	1001	D6Q	C7-N6	4.22	1.35	1.32
2	A	1001	D6Q	C4-N5	4.21	1.38	1.35
2	E	1001	D6Q	C27-C28	4.12	1.56	1.49
2	E	1001	D6Q	C15-C18	-4.04	1.46	1.52
2	J	1001	D6Q	C10-N12	4.03	1.43	1.34
2	H	1001	D6Q	C10-N12	4.03	1.43	1.34
2	E	1001	D6Q	C21-N20	3.98	1.41	1.36
2	L	1001	D6Q	C2-C1	3.96	1.45	1.39
2	C	1001	D6Q	C21-N20	3.80	1.40	1.36
2	I	1001	D6Q	C24-N26	3.76	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	D6Q	C18-C35	-3.76	1.34	1.39
2	D	1001	D6Q	C7-N6	3.63	1.34	1.32
2	J	1001	D6Q	C27-C28	3.63	1.55	1.49
2	D	1001	D6Q	C10-N12	3.61	1.42	1.34
2	B	1001	D6Q	C23-C24	3.52	1.58	1.52
2	D	1001	D6Q	C24-N26	3.44	1.41	1.33
2	C	1001	D6Q	C24-N26	3.37	1.41	1.33
2	B	1001	D6Q	F36-C35	-3.36	1.30	1.34
2	J	1001	D6Q	C15-C21	-3.33	1.49	1.53
2	J	1001	D6Q	C4-N5	3.33	1.37	1.35
2	K	1001	D6Q	C2-C1	3.31	1.44	1.39
2	L	1001	D6Q	C7-N6	3.29	1.34	1.32
2	K	1001	D6Q	C24-N26	3.28	1.41	1.33
2	I	1001	D6Q	C15-C18	-3.28	1.47	1.52
2	I	1001	D6Q	C4-N5	3.20	1.37	1.35
2	J	1001	D6Q	C7-N6	3.17	1.34	1.32
2	A	1001	D6Q	C10-N12	3.16	1.41	1.34
2	F	1001	D6Q	C24-N26	3.16	1.40	1.33
2	J	1001	D6Q	C15-C18	-3.15	1.47	1.52
2	G	1001	D6Q	C18-C35	-3.12	1.35	1.39
2	I	1001	D6Q	C21-N20	3.12	1.40	1.36
2	G	1001	D6Q	C10-N12	3.11	1.41	1.34
2	F	1001	D6Q	F36-C35	-3.10	1.30	1.34
2	I	1001	D6Q	C7-N6	2.96	1.34	1.32
2	E	1001	D6Q	C16-C15	-2.94	1.51	1.54
2	L	1001	D6Q	C34-C35	2.91	1.43	1.37
2	A	1001	D6Q	C16-C15	-2.90	1.51	1.54
2	G	1001	D6Q	C7-N6	2.88	1.34	1.32
2	F	1001	D6Q	C1-C10	-2.86	1.45	1.50
2	G	1001	D6Q	C2-C1	2.85	1.43	1.39
2	L	1001	D6Q	C27-C28	2.84	1.54	1.49
2	A	1001	D6Q	C7-N6	2.82	1.34	1.32
2	C	1001	D6Q	C23-C24	2.81	1.57	1.52
2	A	1001	D6Q	C27-C28	2.80	1.54	1.49
2	H	1001	D6Q	C24-N26	2.78	1.40	1.33
2	L	1001	D6Q	F36-C35	-2.78	1.30	1.34
2	K	1001	D6Q	C19-C18	2.76	1.42	1.39
2	B	1001	D6Q	C24-N26	2.71	1.39	1.33
2	I	1001	D6Q	C34-C35	2.70	1.42	1.37
2	A	1001	D6Q	F36-C35	-2.66	1.31	1.34
2	A	1001	D6Q	C17-N12	2.65	1.51	1.47
2	C	1001	D6Q	C4-N5	2.65	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	D6Q	C2-C1	2.64	1.43	1.39
2	E	1001	D6Q	C24-N26	2.62	1.39	1.33
2	J	1001	D6Q	C2-C1	2.62	1.43	1.39
2	A	1001	D6Q	C34-C35	2.62	1.42	1.37
2	G	1001	D6Q	C15-C18	-2.61	1.48	1.52
2	I	1001	D6Q	C14-C15	-2.58	1.51	1.54
2	D	1001	D6Q	C4-N5	2.53	1.37	1.35
2	K	1001	D6Q	C34-C35	2.53	1.42	1.37
2	C	1001	D6Q	C14-C15	-2.52	1.51	1.54
2	A	1001	D6Q	C2-C1	2.50	1.43	1.39
2	L	1001	D6Q	C4-N3	2.41	1.38	1.35
2	L	1001	D6Q	C24-N26	2.40	1.39	1.33
2	F	1001	D6Q	C16-C15	-2.39	1.51	1.54
2	E	1001	D6Q	C32-C19	-2.39	1.35	1.39
2	A	1001	D6Q	C24-N26	2.35	1.39	1.33
2	F	1001	D6Q	C23-C24	2.35	1.56	1.52
2	A	1001	D6Q	C18-C35	-2.29	1.36	1.39
2	C	1001	D6Q	C10-N12	2.29	1.39	1.34
2	I	1001	D6Q	C2-C1	2.27	1.42	1.39
2	L	1001	D6Q	C8-C4	2.26	1.45	1.42
2	B	1001	D6Q	C34-C35	2.22	1.42	1.37
2	H	1001	D6Q	F36-C35	-2.19	1.31	1.34
2	F	1001	D6Q	C4-N3	2.17	1.38	1.35
2	A	1001	D6Q	C15-C18	-2.17	1.49	1.52
2	H	1001	D6Q	C34-C35	2.16	1.41	1.37
2	B	1001	D6Q	C8-C7	2.13	1.44	1.42
2	F	1001	D6Q	C19-C18	2.12	1.42	1.39
2	A	1001	D6Q	C32-C19	-2.12	1.36	1.39
2	J	1001	D6Q	F36-C35	-2.11	1.31	1.34
2	A	1001	D6Q	N5-N6	2.10	1.38	1.36
2	C	1001	D6Q	C16-C15	-2.09	1.52	1.54
2	L	1001	D6Q	C15-C18	-2.08	1.49	1.52
2	I	1001	D6Q	O22-C21	-2.06	1.19	1.22
2	G	1001	D6Q	C4-N3	2.03	1.38	1.35

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1001	D6Q	C28-C27-N26	8.85	123.29	111.82
2	J	1001	D6Q	C27-N26-C24	-7.69	113.08	123.23
2	D	1001	D6Q	C28-C27-N26	-7.00	102.74	111.82
2	A	1001	D6Q	C28-C27-N26	-6.35	103.59	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	D6Q	O22-C21-C15	6.32	132.22	126.27
2	C	1001	D6Q	C4-N5-N6	-6.28	109.79	111.26
2	C	1001	D6Q	O22-C21-N20	-6.28	119.81	125.85
2	H	1001	D6Q	O22-C21-N20	-6.23	119.86	125.85
2	L	1001	D6Q	C7-N6-N5	5.94	109.12	106.02
2	G	1001	D6Q	C28-C27-N26	-5.88	104.19	111.82
2	F	1001	D6Q	C7-N6-N5	5.85	109.08	106.02
2	A	1001	D6Q	O22-C21-N20	-5.73	120.34	125.85
2	I	1001	D6Q	O22-C21-N20	-5.73	120.35	125.85
2	F	1001	D6Q	O22-C21-N20	-5.56	120.51	125.85
2	C	1001	D6Q	C7-N6-N5	5.55	108.92	106.02
2	I	1001	D6Q	C16-C15-C14	5.45	116.34	109.89
2	K	1001	D6Q	C28-C27-N26	5.42	118.84	111.82
2	A	1001	D6Q	O22-C21-C15	5.39	131.34	126.27
2	F	1001	D6Q	C4-N5-N6	-5.36	110.01	111.26
2	H	1001	D6Q	O22-C21-C15	5.33	131.29	126.27
2	D	1001	D6Q	O22-C21-N20	-5.28	120.77	125.85
2	E	1001	D6Q	C4-N5-N6	-5.23	110.04	111.26
2	C	1001	D6Q	O22-C21-C15	4.99	130.97	126.27
2	J	1001	D6Q	C16-C15-C14	4.97	115.78	109.89
2	E	1001	D6Q	C16-C15-C14	4.93	115.73	109.89
2	L	1001	D6Q	O22-C21-N20	-4.93	121.11	125.85
2	J	1001	D6Q	C7-N6-N5	4.92	108.59	106.02
2	D	1001	D6Q	C7-N6-N5	4.86	108.56	106.02
2	I	1001	D6Q	C7-N6-N5	4.80	108.53	106.02
2	E	1001	D6Q	C15-C21-N20	-4.58	105.75	108.43
2	K	1001	D6Q	O22-C21-N20	-4.57	121.46	125.85
2	B	1001	D6Q	C19-N20-C21	-4.52	108.54	111.16
2	K	1001	D6Q	C7-N6-N5	4.47	108.36	106.02
2	D	1001	D6Q	O22-C21-C15	4.47	130.48	126.27
2	E	1001	D6Q	C7-N6-N5	4.40	108.32	106.02
2	F	1001	D6Q	C8-C7-N6	-4.35	108.52	111.68
2	L	1001	D6Q	C1-C10-N12	4.29	124.03	118.66
2	F	1001	D6Q	O22-C21-C15	4.25	130.27	126.27
2	A	1001	D6Q	C7-N6-N5	4.22	108.23	106.02
2	L	1001	D6Q	C18-C15-C21	-4.19	99.50	101.94
2	B	1001	D6Q	O22-C21-N20	-4.18	121.83	125.85
2	I	1001	D6Q	C19-N20-C21	-4.14	108.76	111.16
2	G	1001	D6Q	C16-C15-C14	4.11	114.77	109.89
2	E	1001	D6Q	O22-C21-N20	-4.01	122.00	125.85
2	I	1001	D6Q	O22-C21-C15	3.99	130.03	126.27
2	K	1001	D6Q	C4-C8-C7	3.95	106.39	104.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1001	D6Q	C8-C4-N5	-3.94	105.50	107.21
2	K	1001	D6Q	C8-C7-N6	-3.93	108.82	111.68
2	G	1001	D6Q	C8-C9-C1	-3.90	115.18	121.32
2	F	1001	D6Q	C19-N20-C21	-3.80	108.96	111.16
2	D	1001	D6Q	C8-C9-C1	-3.78	115.36	121.32
2	F	1001	D6Q	C9-C1-C2	3.73	121.76	117.92
2	K	1001	D6Q	C19-N20-C21	-3.73	109.00	111.16
2	J	1001	D6Q	C8-C7-N6	-3.71	108.98	111.68
2	C	1001	D6Q	C8-C9-C1	-3.71	115.48	121.32
2	I	1001	D6Q	C4-N5-N6	-3.70	110.40	111.26
2	H	1001	D6Q	C18-C15-C21	-3.69	99.79	101.94
2	L	1001	D6Q	C8-C7-N6	-3.67	109.01	111.68
2	G	1001	D6Q	C9-C1-C2	3.64	121.66	117.92
2	B	1001	D6Q	C8-C9-C1	-3.62	115.62	121.32
2	L	1001	D6Q	C4-N5-N6	-3.62	110.42	111.26
2	I	1001	D6Q	C8-C7-N6	-3.54	109.10	111.68
2	E	1001	D6Q	C18-C15-C21	3.52	103.99	101.94
2	E	1001	D6Q	C8-C9-C1	-3.51	115.79	121.32
2	L	1001	D6Q	C8-C4-N5	-3.51	105.69	107.21
2	B	1001	D6Q	C1-C10-N12	3.48	123.01	118.66
2	D	1001	D6Q	C8-C7-N6	-3.48	109.15	111.68
2	L	1001	D6Q	C16-C15-C14	3.47	114.01	109.89
2	C	1001	D6Q	C8-C7-N6	-3.46	109.16	111.68
2	K	1001	D6Q	O22-C21-C15	3.46	129.53	126.27
2	E	1001	D6Q	C14-C15-C18	-3.46	101.10	111.81
2	D	1001	D6Q	C9-C1-C2	3.45	121.47	117.92
2	K	1001	D6Q	C16-C15-C14	3.41	113.93	109.89
2	I	1001	D6Q	C1-C10-N12	3.38	122.88	118.66
2	I	1001	D6Q	C4-C8-C7	3.37	106.08	104.25
2	H	1001	D6Q	C7-N6-N5	3.36	107.78	106.02
2	I	1001	D6Q	C9-C1-C2	3.32	121.34	117.92
2	L	1001	D6Q	C24-C23-N20	-3.31	102.97	112.48
2	L	1001	D6Q	O22-C21-C15	3.29	129.37	126.27
2	C	1001	D6Q	C19-N20-C21	-3.29	109.25	111.16
2	F	1001	D6Q	C4-C8-C7	3.28	106.03	104.25
2	B	1001	D6Q	O22-C21-C15	3.27	129.34	126.27
2	G	1001	D6Q	O22-C21-C15	3.26	129.34	126.27
2	B	1001	D6Q	C7-N6-N5	3.25	107.72	106.02
2	L	1001	D6Q	N5-C4-N3	3.24	128.68	125.83
2	F	1001	D6Q	C27-N26-C24	-3.15	119.07	123.23
2	F	1001	D6Q	N5-C4-N3	3.15	128.60	125.83
2	D	1001	D6Q	C4-N5-N6	-3.13	110.53	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1001	D6Q	F31-C28-F30	-3.10	95.51	106.44
2	A	1001	D6Q	N5-C4-N3	3.09	128.55	125.83
2	H	1001	D6Q	C1-C10-N12	3.09	122.52	118.66
2	A	1001	D6Q	C8-C9-C1	-3.09	116.45	121.32
2	J	1001	D6Q	C1-C10-N12	3.04	122.46	118.66
2	J	1001	D6Q	C24-C23-N20	-3.04	103.75	112.48
2	I	1001	D6Q	C8-C4-N5	-3.03	105.89	107.21
2	E	1001	D6Q	C9-C1-C2	3.02	121.03	117.92
2	L	1001	D6Q	C19-N20-C21	-3.02	109.41	111.16
2	I	1001	D6Q	F29-C28-C27	3.01	119.86	111.87
2	K	1001	D6Q	C24-C23-N20	-3.00	103.85	112.48
2	H	1001	D6Q	C27-N26-C24	-3.00	119.28	123.23
2	D	1001	D6Q	C18-C15-C21	-3.00	100.19	101.94
2	J	1001	D6Q	C18-C19-N20	-2.99	107.63	109.67
2	G	1001	D6Q	O22-C21-N20	-2.98	122.98	125.85
2	I	1001	D6Q	C24-C23-N20	-2.98	103.92	112.48
2	I	1001	D6Q	C8-C9-C1	-2.97	116.64	121.32
2	L	1001	D6Q	O11-C10-N12	-2.96	117.69	122.35
2	G	1001	D6Q	C7-N6-N5	2.94	107.56	106.02
2	E	1001	D6Q	C17-C16-C15	-2.93	108.59	112.74
2	J	1001	D6Q	C4-N5-N6	-2.91	110.58	111.26
2	H	1001	D6Q	N5-C4-N3	2.90	128.38	125.83
2	G	1001	D6Q	C8-C4-N5	-2.88	105.96	107.21
2	K	1001	D6Q	N5-C4-N3	2.87	128.36	125.83
2	B	1001	D6Q	C9-C1-C2	2.87	120.88	117.92
2	K	1001	D6Q	C1-C10-N12	2.87	122.24	118.66
2	E	1001	D6Q	C8-C7-N6	-2.82	109.62	111.68
2	L	1001	D6Q	F29-C28-C27	2.80	119.31	111.87
2	L	1001	D6Q	C4-C8-C7	2.80	105.77	104.25
2	J	1001	D6Q	C8-C9-C1	-2.79	116.93	121.32
2	F	1001	D6Q	C8-C4-N3	-2.76	125.02	126.66
2	C	1001	D6Q	O11-C10-N12	-2.76	118.01	122.35
2	F	1001	D6Q	C8-C9-C1	-2.71	117.05	121.32
2	B	1001	D6Q	C28-C27-N26	-2.71	108.30	111.82
2	H	1001	D6Q	C8-C9-C1	-2.71	117.06	121.32
2	H	1001	D6Q	C8-C4-N3	-2.66	125.08	126.66
2	H	1001	D6Q	C4-N5-N6	-2.65	110.64	111.26
2	F	1001	D6Q	C1-C10-N12	2.65	121.97	118.66
2	H	1001	D6Q	C8-C7-N6	-2.60	109.78	111.68
2	E	1001	D6Q	C27-N26-C24	-2.58	119.82	123.23
2	K	1001	D6Q	C8-C9-C1	-2.58	117.25	121.32
2	L	1001	D6Q	C8-C9-C1	-2.57	117.28	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1001	D6Q	N5-C4-N3	2.56	128.08	125.83
2	J	1001	D6Q	O22-C21-C15	2.56	128.68	126.27
2	L	1001	D6Q	C27-N26-C24	-2.54	119.88	123.23
2	E	1001	D6Q	C16-C17-N12	-2.53	106.09	110.82
2	C	1001	D6Q	C9-C1-C2	2.53	120.53	117.92
2	D	1001	D6Q	C4-C8-C7	2.52	105.62	104.25
2	C	1001	D6Q	C1-C10-N12	2.51	121.80	118.66
2	A	1001	D6Q	C8-C7-N6	-2.48	109.87	111.68
2	A	1001	D6Q	C8-C4-N3	-2.47	125.19	126.66
2	B	1001	D6Q	O25-C24-C23	2.46	125.33	121.02
2	D	1001	D6Q	C8-C4-N5	-2.45	106.15	107.21
2	G	1001	D6Q	C2-C1-C10	-2.43	113.95	121.02
2	A	1001	D6Q	C9-C1-C2	2.39	120.38	117.92
2	C	1001	D6Q	C2-C1-C10	-2.39	114.09	121.02
2	B	1001	D6Q	C8-C7-N6	-2.39	109.94	111.68
2	G	1001	D6Q	C14-C15-C18	-2.38	104.42	111.81
2	G	1001	D6Q	N5-C4-N3	2.38	127.92	125.83
2	K	1001	D6Q	F29-C28-C27	2.38	118.18	111.87
2	J	1001	D6Q	C16-C17-N12	-2.36	106.41	110.82
2	D	1001	D6Q	C1-C10-N12	2.35	121.60	118.66
2	K	1001	D6Q	F31-C28-F30	-2.35	98.16	106.44
2	J	1001	D6Q	C4-C8-C7	2.34	105.52	104.25
2	E	1001	D6Q	C2-C1-C10	-2.34	114.22	121.02
2	A	1001	D6Q	C13-N12-C10	-2.34	115.56	122.79
2	C	1001	D6Q	C9-C1-C10	2.33	125.30	120.13
2	I	1001	D6Q	N5-C4-N3	2.31	127.87	125.83
2	C	1001	D6Q	C13-C14-C15	-2.31	109.46	112.74
2	A	1001	D6Q	C16-C15-C14	2.29	112.60	109.89
2	K	1001	D6Q	C9-C1-C2	2.28	120.26	117.92
2	C	1001	D6Q	C13-N12-C10	-2.27	115.76	122.79
2	A	1001	D6Q	C17-C16-C15	-2.26	109.53	112.74
2	A	1001	D6Q	C19-N20-C21	-2.26	109.85	111.16
2	D	1001	D6Q	C2-C1-C10	-2.22	114.58	121.02
2	A	1001	D6Q	C4-N5-N6	-2.22	110.74	111.26
2	A	1001	D6Q	C8-C4-N5	-2.21	106.25	107.21
2	H	1001	D6Q	C13-C14-C15	-2.20	109.62	112.74
2	B	1001	D6Q	C2-C1-C10	-2.20	114.64	121.02
2	D	1001	D6Q	C2-N3-C4	-2.19	111.89	116.19
2	J	1001	D6Q	O11-C10-N12	-2.17	118.93	122.35
2	F	1001	D6Q	C33-C34-C35	-2.17	119.26	121.18
2	F	1001	D6Q	C2-C1-C10	-2.15	114.77	121.02
2	H	1001	D6Q	O11-C10-N12	-2.14	118.98	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	D6Q	C28-C27-N26	-2.13	109.06	111.82
2	I	1001	D6Q	C23-N20-C19	2.12	128.42	125.18
2	J	1001	D6Q	F31-C28-C27	-2.12	106.25	111.87
2	J	1001	D6Q	O22-C21-N20	-2.08	123.85	125.85
2	B	1001	D6Q	N5-C4-N3	2.07	127.65	125.83
2	G	1001	D6Q	C19-N20-C21	-2.06	109.96	111.16
2	E	1001	D6Q	C14-C13-N12	-2.05	106.99	110.82
2	L	1001	D6Q	C2-N3-C4	-2.05	112.17	116.19
2	C	1001	D6Q	C1-C2-N3	2.05	126.61	123.59
2	A	1001	D6Q	C24-C23-N20	-2.04	106.63	112.48
2	J	1001	D6Q	C8-C4-N5	-2.03	106.33	107.21
2	L	1001	D6Q	C18-C19-N20	-2.02	108.29	109.67
2	B	1001	D6Q	C8-C4-N3	-2.02	125.46	126.66
2	I	1001	D6Q	C15-C21-N20	2.02	109.61	108.43
2	B	1001	D6Q	C4-N5-N6	-2.01	110.79	111.26
2	D	1001	D6Q	C19-N20-C21	-2.01	110.00	111.16

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	D6Q	N26-C27-C28-F29
2	C	1001	D6Q	N26-C27-C28-F30
2	C	1001	D6Q	N26-C27-C28-F31
2	H	1001	D6Q	N26-C27-C28-F29
2	H	1001	D6Q	N26-C27-C28-F30
2	H	1001	D6Q	N26-C27-C28-F31
2	I	1001	D6Q	N26-C27-C28-F29
2	I	1001	D6Q	N26-C27-C28-F30
2	I	1001	D6Q	N26-C27-C28-F31
2	L	1001	D6Q	N26-C27-C28-F29
2	L	1001	D6Q	N26-C27-C28-F30
2	L	1001	D6Q	N26-C27-C28-F31
2	J	1001	D6Q	O11-C10-N12-C17
2	J	1001	D6Q	C1-C10-N12-C17
2	L	1001	D6Q	C2-C1-C10-O11
2	E	1001	D6Q	O11-C10-N12-C17
2	L	1001	D6Q	C2-C1-C10-N12
2	E	1001	D6Q	N26-C27-C28-F31
2	G	1001	D6Q	N26-C27-C28-F31
2	L	1001	D6Q	O11-C10-N12-C17
2	J	1001	D6Q	C2-C1-C10-O11

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Mol	Chain	Res	Type	Atoms
2	J	1001	D6Q	C2-C1-C10-N12
2	E	1001	D6Q	N26-C27-C28-F30
2	G	1001	D6Q	O11-C10-N12-C17
2	J	1001	D6Q	O11-C10-N12-C13
2	D	1001	D6Q	C28-C27-N26-C24
2	J	1001	D6Q	C28-C27-N26-C24
2	A	1001	D6Q	N26-C27-C28-F30
2	E	1001	D6Q	N26-C27-C28-F29
2	A	1001	D6Q	O11-C10-N12-C17
2	D	1001	D6Q	O11-C10-N12-C13
2	J	1001	D6Q	N26-C27-C28-F30
2	B	1001	D6Q	O11-C10-N12-C13
2	L	1001	D6Q	C1-C10-N12-C17
2	G	1001	D6Q	N26-C27-C28-F30
2	K	1001	D6Q	N26-C27-C28-F30
2	A	1001	D6Q	N26-C27-C28-F31
2	G	1001	D6Q	N26-C27-C28-F29
2	L	1001	D6Q	C9-C1-C10-O11

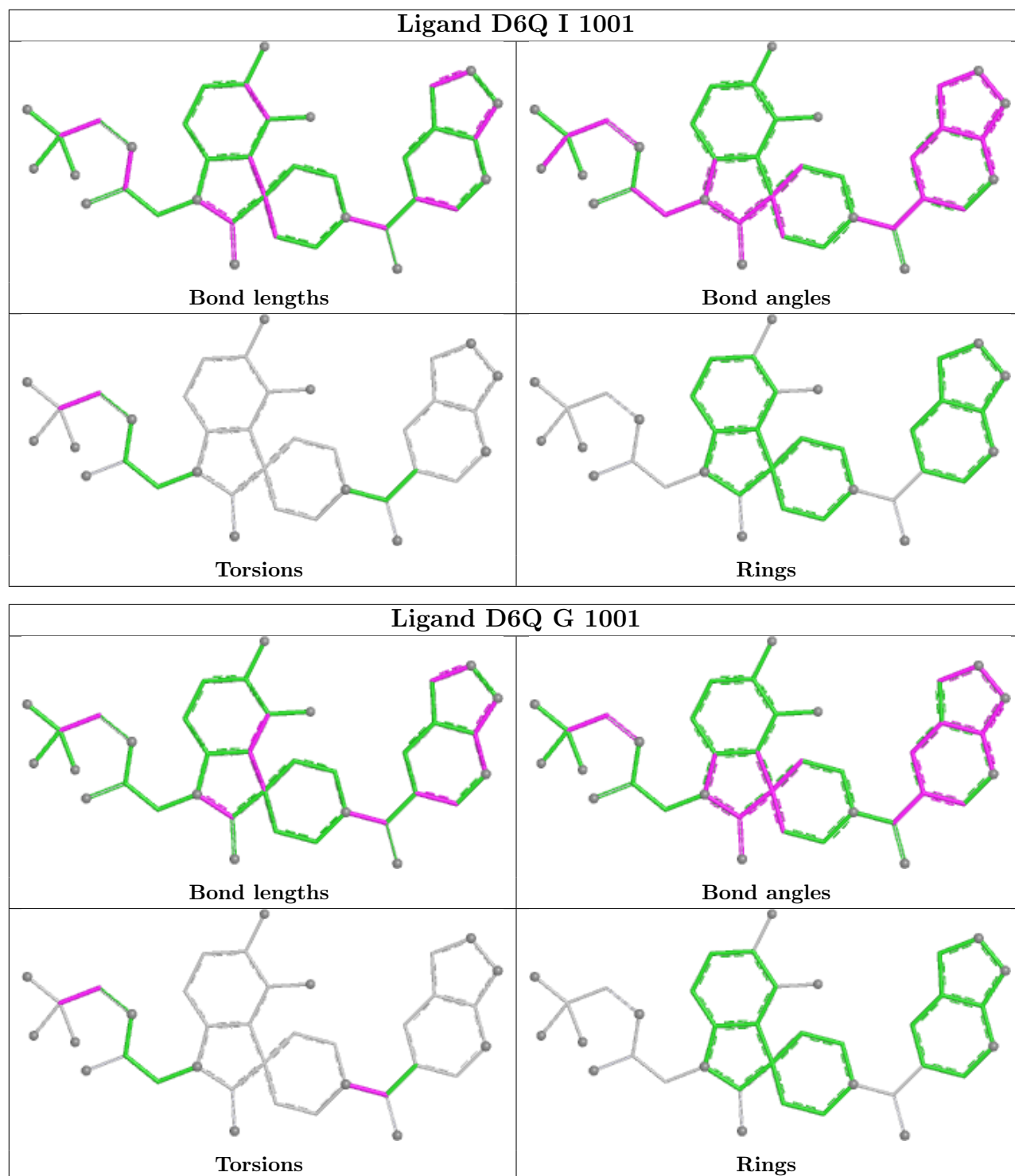
There are no ring outliers.

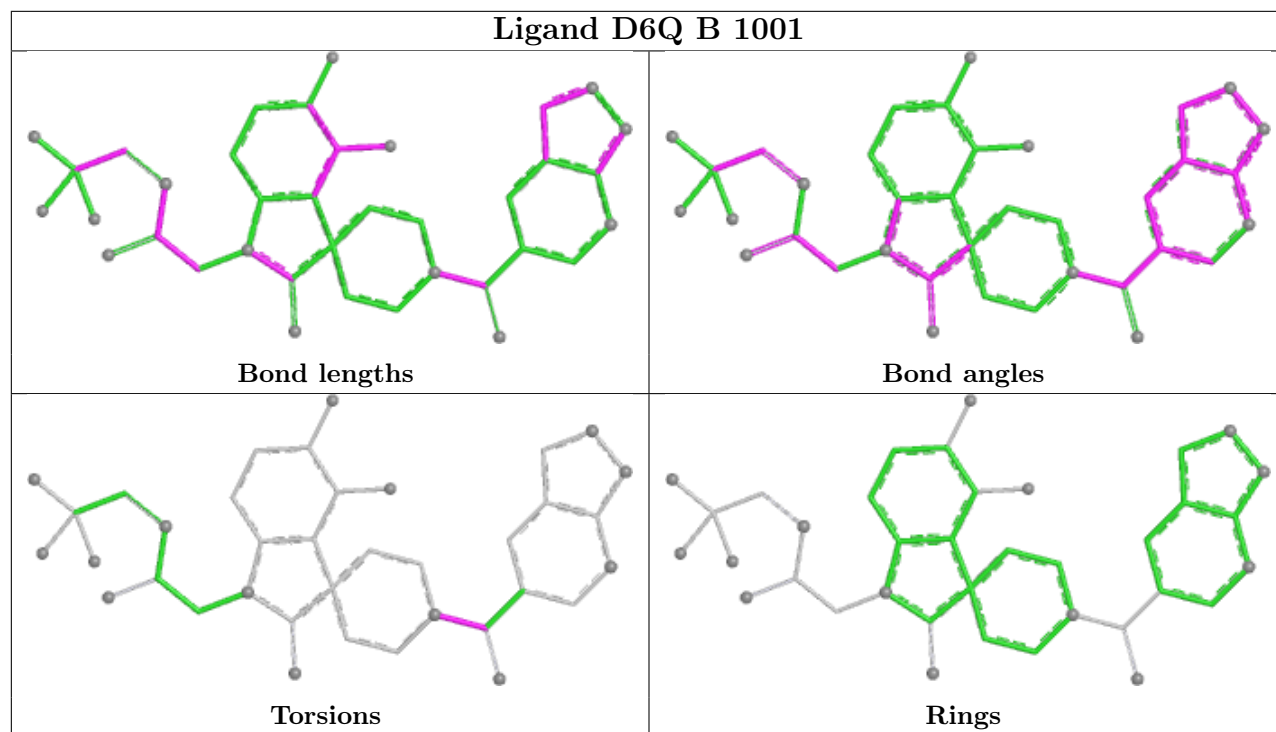
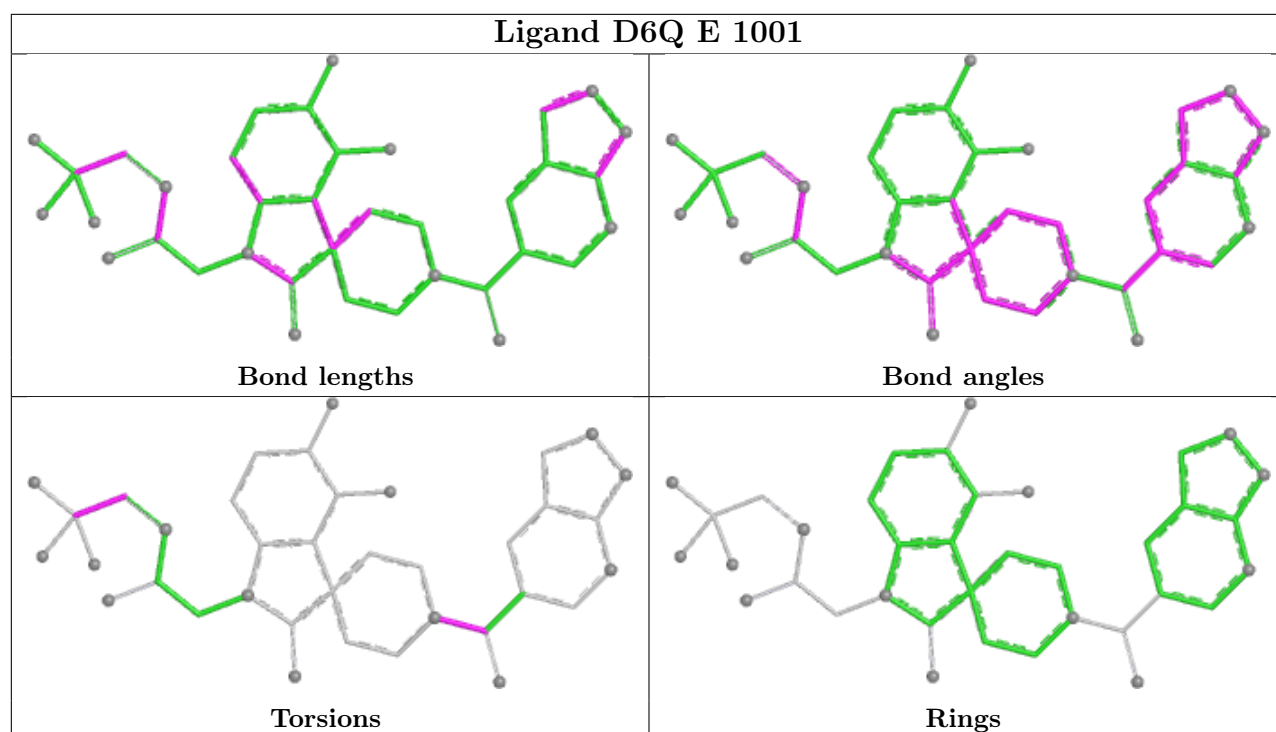
7 monomers are involved in 8 short contacts:

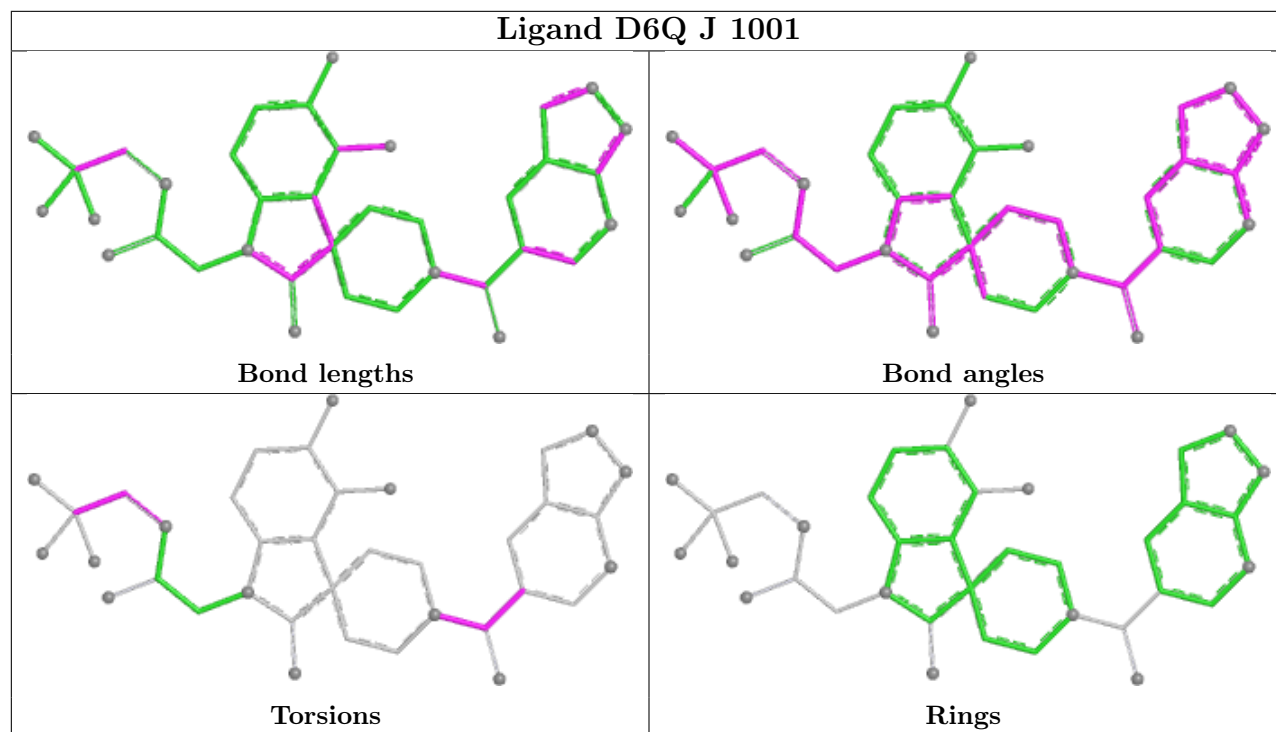
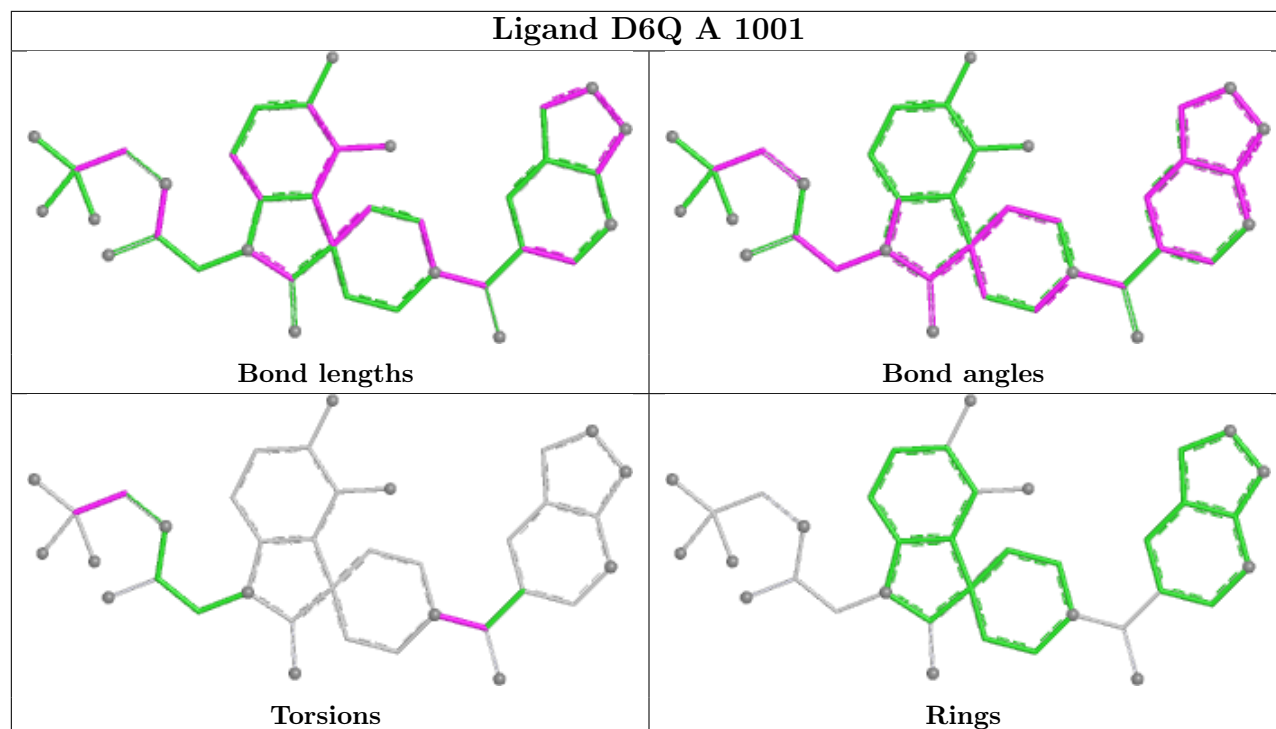
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1001	D6Q	2	0
2	E	1001	D6Q	1	0
2	A	1001	D6Q	1	0
2	J	1001	D6Q	1	0
2	F	1001	D6Q	1	0
2	K	1001	D6Q	1	0
2	D	1001	D6Q	1	0

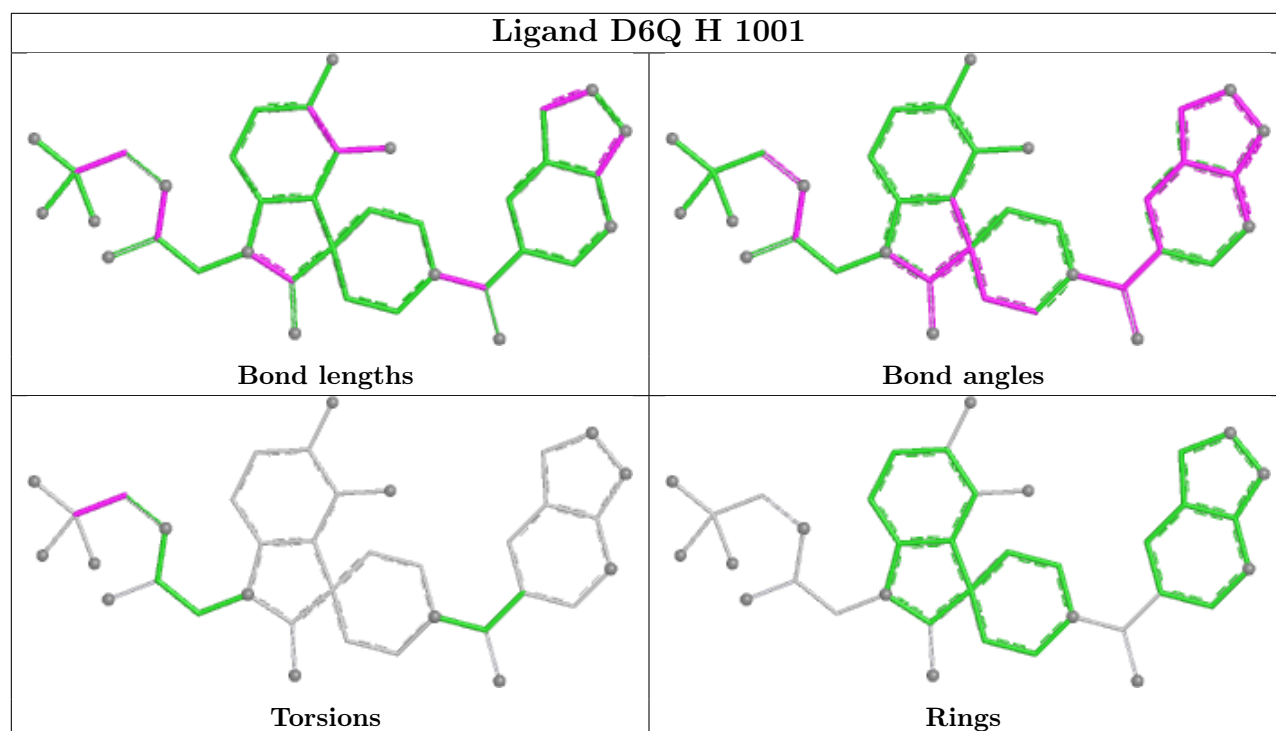
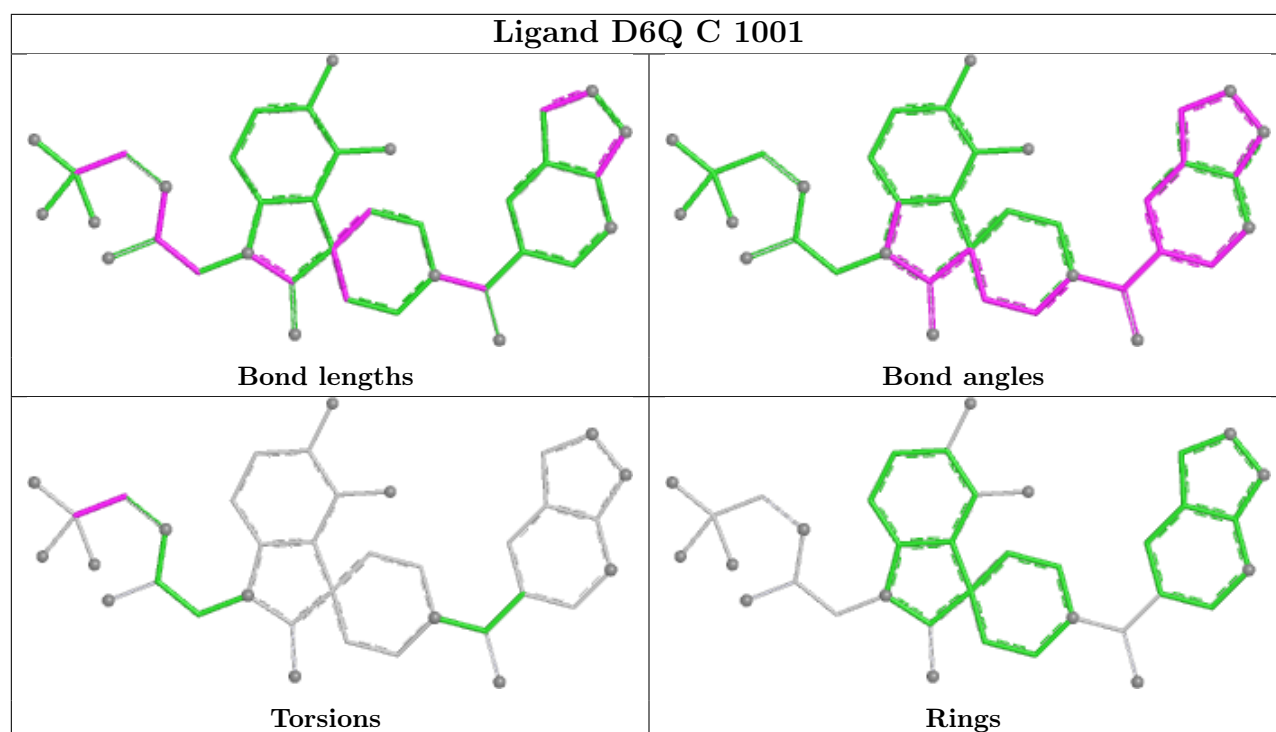
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

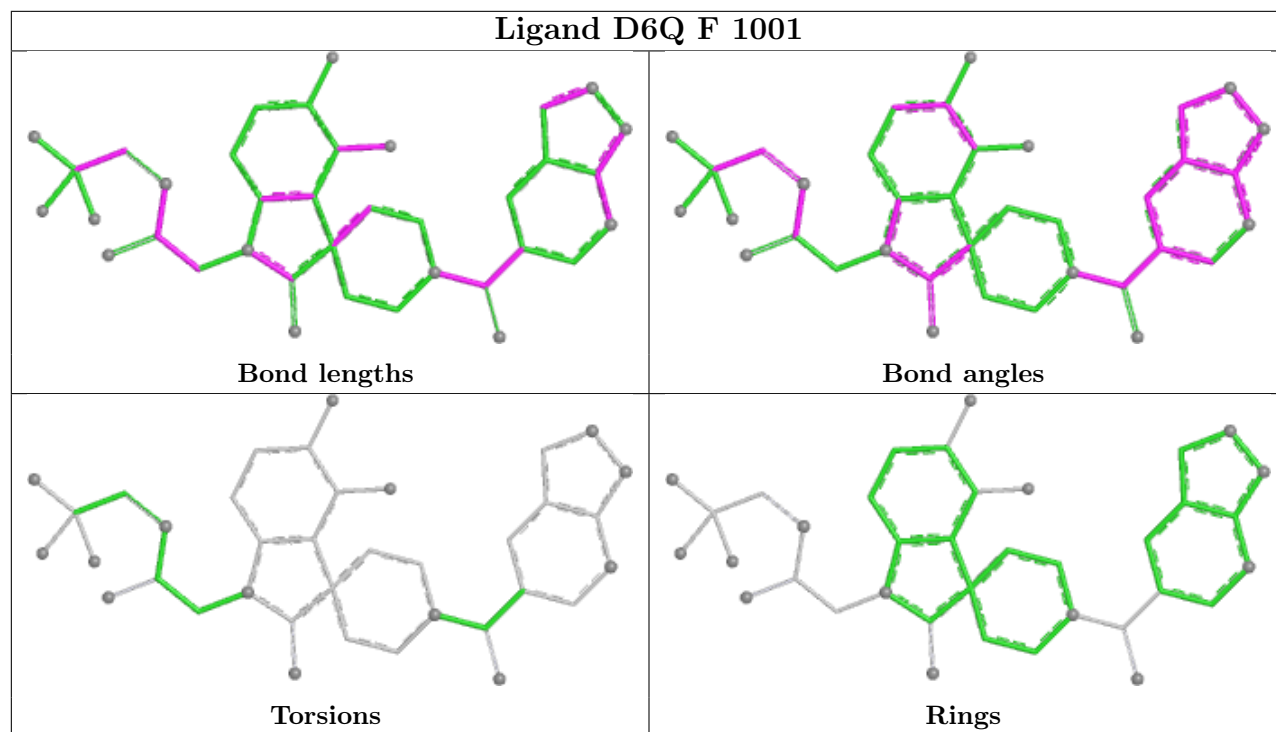
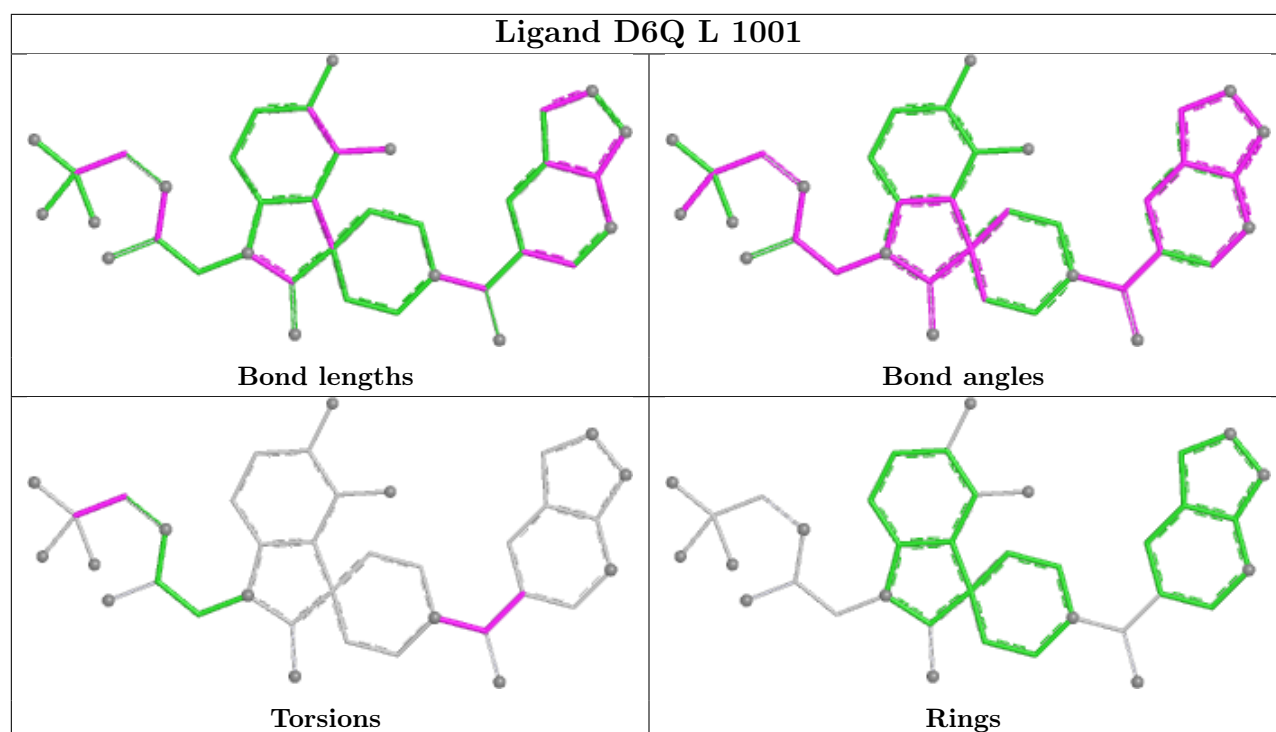
equivalents in the CSD to analyse the geometry.

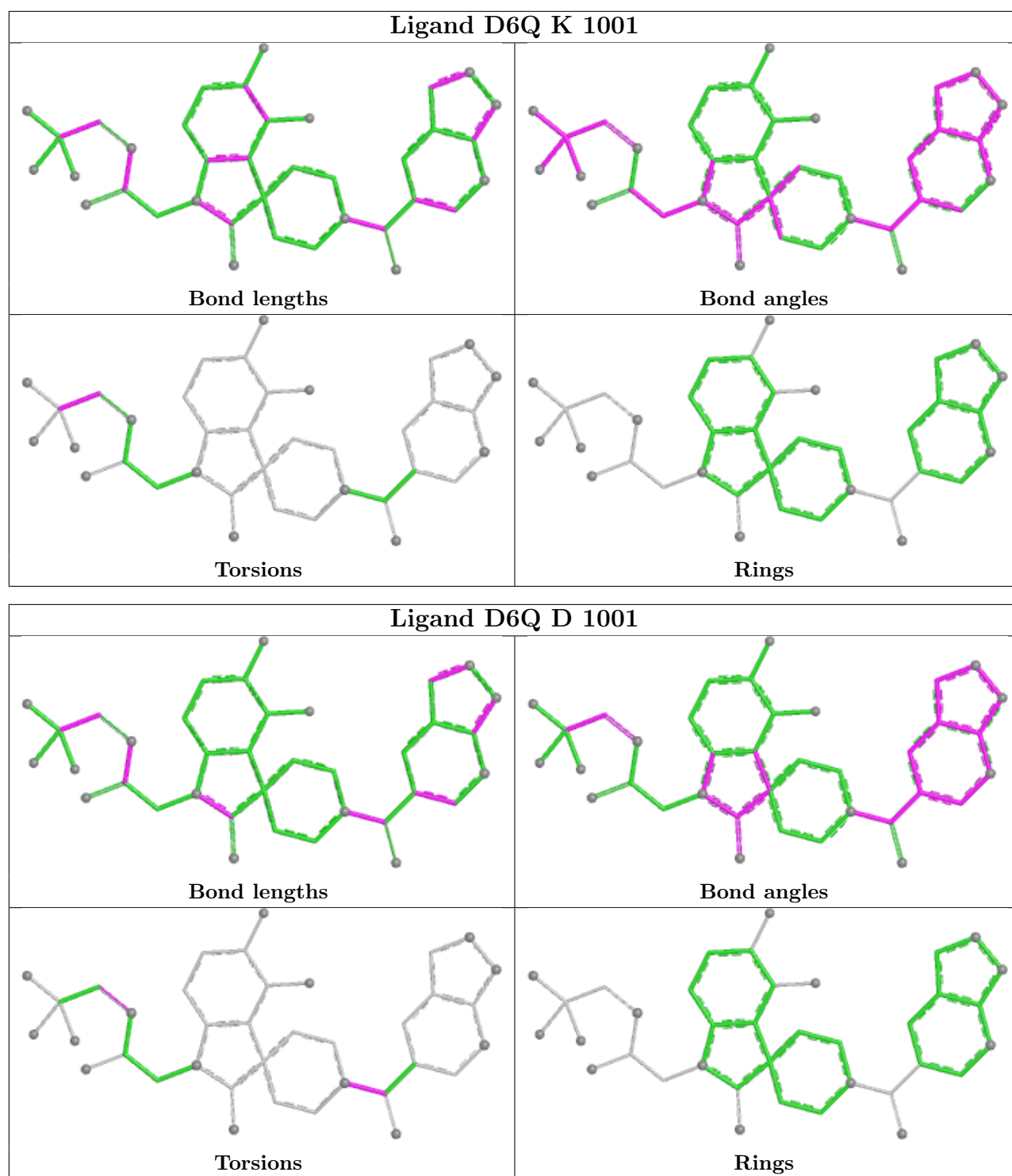












5.7 Other polymers [i](#)

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	271/309 (87%)	-0.21	0 100 100	39, 69, 109, 145	0
1	B	279/309 (90%)	-0.23	4 (1%) 73 66	32, 57, 113, 165	0
1	C	272/309 (88%)	-0.23	2 (0%) 84 80	40, 63, 103, 170	0
1	D	280/309 (90%)	-0.39	1 (0%) 88 86	32, 53, 92, 173	0
1	E	273/309 (88%)	-0.41	2 (0%) 84 80	29, 48, 100, 168	0
1	F	275/309 (88%)	-0.46	0 100 100	32, 53, 93, 127	0
1	G	273/309 (88%)	-0.42	2 (0%) 84 80	30, 49, 91, 150	0
1	H	272/309 (88%)	-0.44	1 (0%) 88 86	27, 49, 90, 164	0
1	I	267/309 (86%)	0.02	22 (8%) 17 14	29, 58, 146, 186	0
1	J	272/309 (88%)	-0.29	3 (1%) 78 72	31, 55, 107, 164	0
1	K	268/309 (86%)	0.09	17 (6%) 26 20	39, 65, 163, 212	0
1	L	273/309 (88%)	-0.16	4 (1%) 72 64	33, 63, 119, 225	0
All	All	3275/3708 (88%)	-0.26	58 (1%) 67 60	27, 57, 119, 225	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	691	CYS	4.8
1	K	654	VAL	4.1
1	I	656	MET	4.1
1	J	600	VAL	4.0
1	K	652	VAL	3.8
1	G	600	VAL	3.8
1	K	605	PHE	3.7
1	K	656	MET	3.6
1	K	698	CYS	3.6
1	K	659	ALA	3.5
1	E	600	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	602	VAL	3.2
1	C	631	GLY	3.1
1	I	621	PHE	3.1
1	I	657	LEU	3.1
1	I	667	ASN	2.9
1	K	665	ALA	2.9
1	I	670	LEU	2.9
1	I	698	CYS	2.8
1	L	621	PHE	2.7
1	I	701	THR	2.7
1	K	610	LEU	2.7
1	K	649	PRO	2.7
1	D	649	PRO	2.6
1	I	690	VAL	2.6
1	I	610	LEU	2.5
1	J	602	VAL	2.5
1	K	691	CYS	2.5
1	B	725	ASP	2.5
1	H	602	VAL	2.4
1	B	652	VAL	2.4
1	I	666	ARG	2.4
1	L	702	GLU	2.4
1	B	619	GLY	2.3
1	K	621	PHE	2.3
1	K	728	THR	2.3
1	L	650	VAL	2.3
1	C	621	PHE	2.3
1	B	601	ALA	2.3
1	K	702	GLU	2.3
1	I	697	LEU	2.2
1	I	616	LEU	2.2
1	K	650	VAL	2.2
1	K	655	LYS	2.2
1	E	621	PHE	2.2
1	I	626	LEU	2.2
1	I	617	GLY	2.1
1	I	665	ALA	2.1
1	I	700	ILE	2.1
1	J	656	MET	2.1
1	L	703	TYR	2.1
1	K	670	LEU	2.1
1	I	605	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	790	ILE	2.1
1	I	651	LEU	2.0
1	I	702	GLU	2.0
1	I	664	ASN	2.0
1	I	612	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](#)

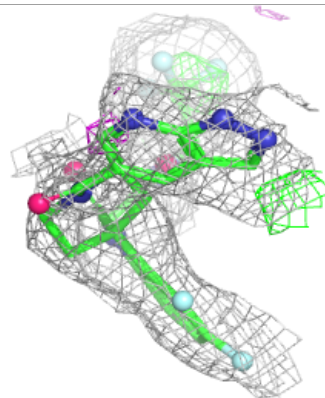
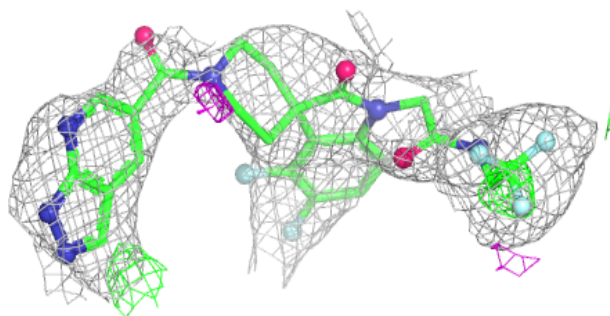
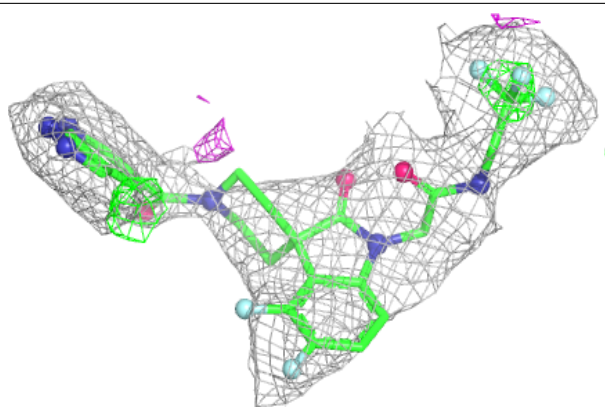
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	D6Q	K	1001	37/37	0.92	0.12	31,81,95,104	0
2	D6Q	I	1001	37/37	0.93	0.13	13,68,92,101	0
2	D6Q	A	1001	37/37	0.94	0.07	26,45,63,64	0
2	D6Q	C	1001	37/37	0.94	0.08	40,60,78,81	0
2	D6Q	J	1001	37/37	0.95	0.07	22,48,63,70	0
2	D6Q	L	1001	37/37	0.95	0.09	25,62,79,87	0
2	D6Q	B	1001	37/37	0.96	0.06	26,43,57,60	0
2	D6Q	E	1001	37/37	0.96	0.06	17,42,61,74	0
2	D6Q	F	1001	37/37	0.96	0.07	17,37,47,54	0
2	D6Q	G	1001	37/37	0.96	0.06	19,43,56,59	0
2	D6Q	D	1001	37/37	0.97	0.05	27,39,55,61	0
2	D6Q	H	1001	37/37	0.97	0.05	9,38,51,57	0

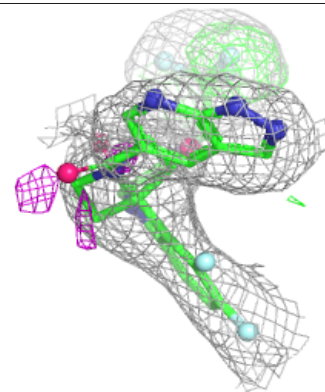
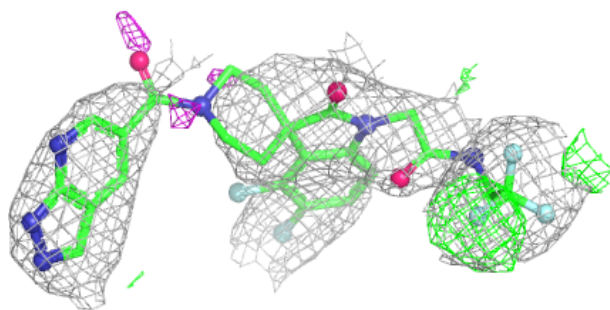
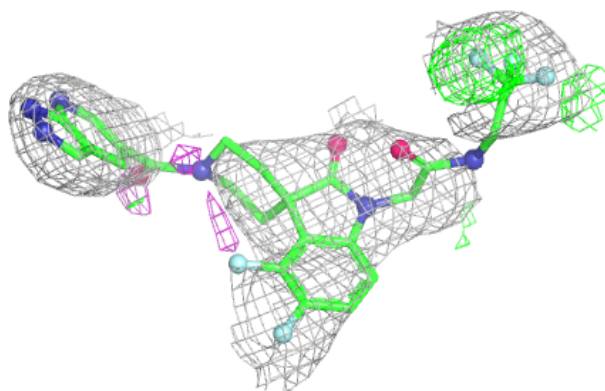
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D6Q K 1001:

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

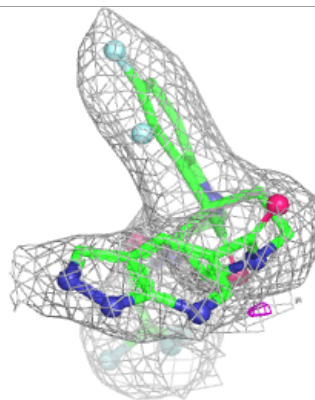
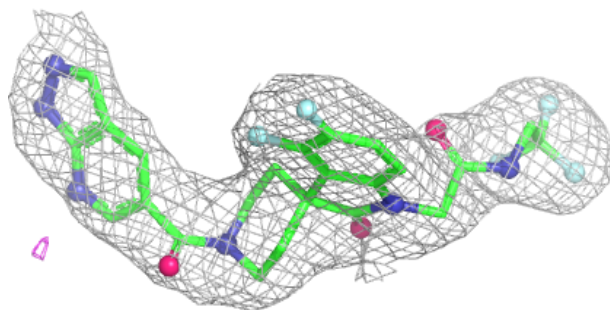
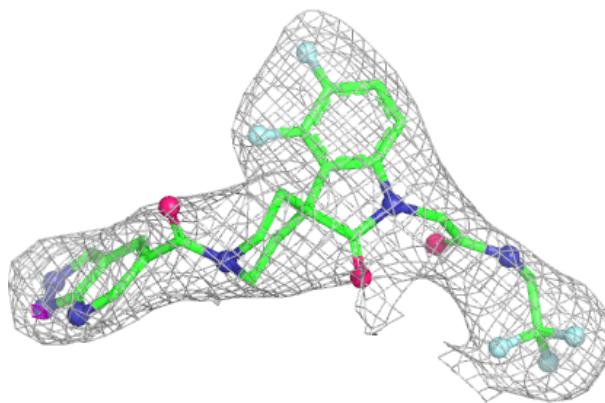
**Electron density around D6Q I 1001:**

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

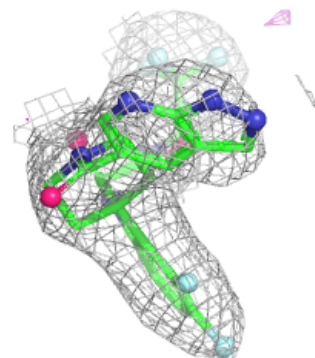
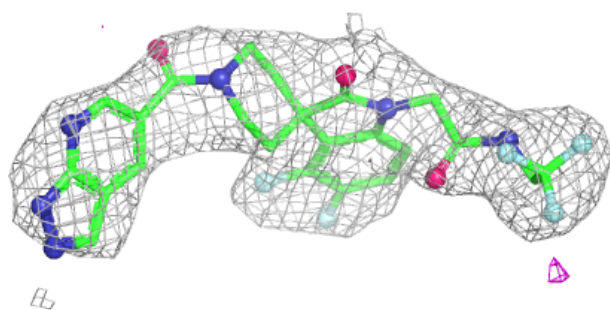
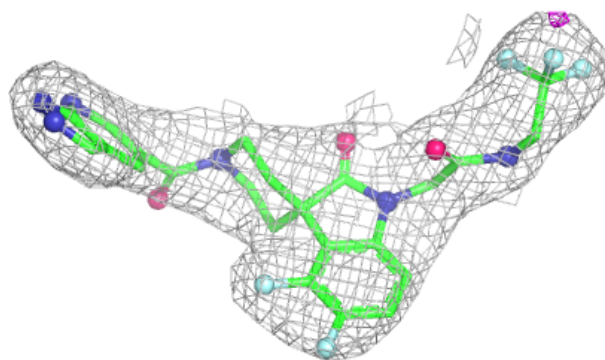


Electron density around D6Q A 1001:

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

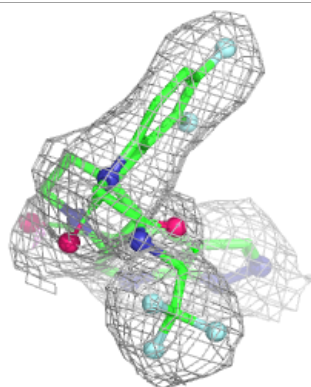
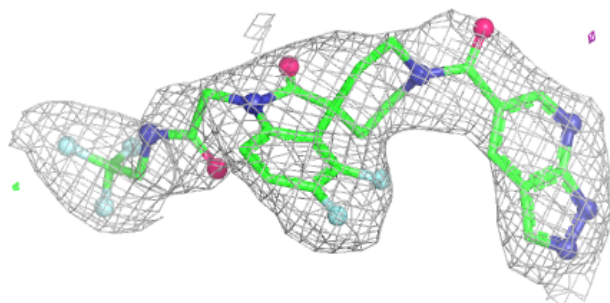
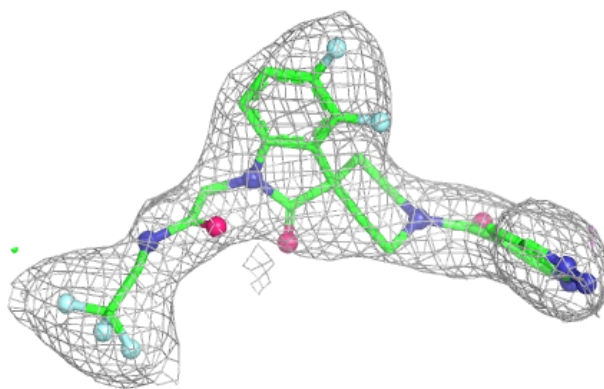
**Electron density around D6Q C 1001:**

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

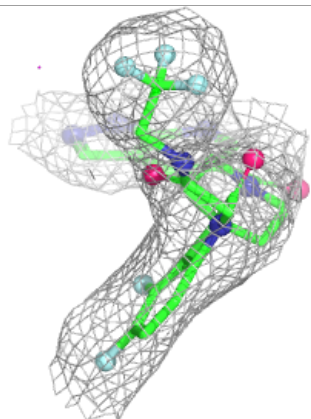
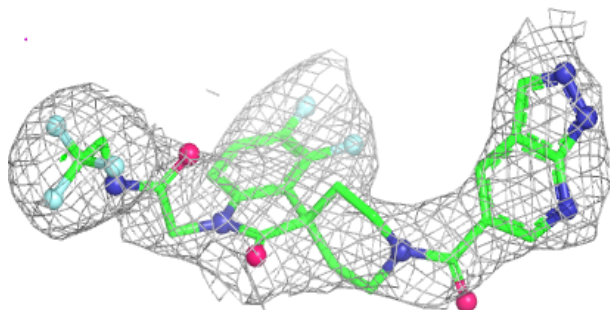
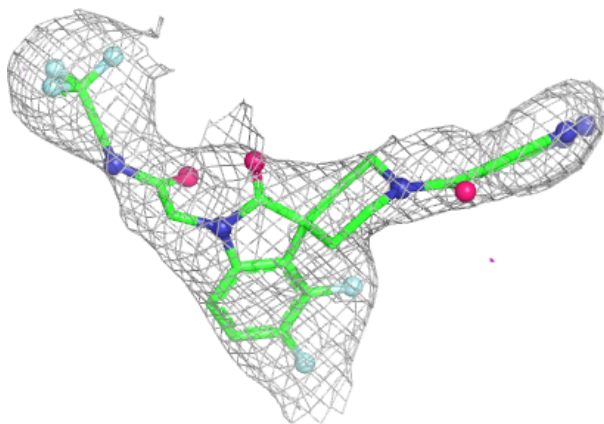


Electron density around D6Q J 1001:

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

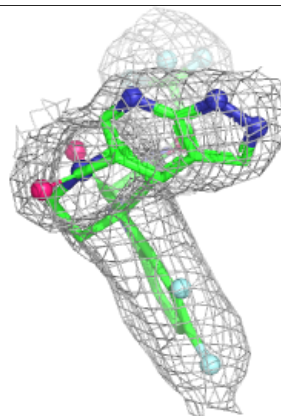
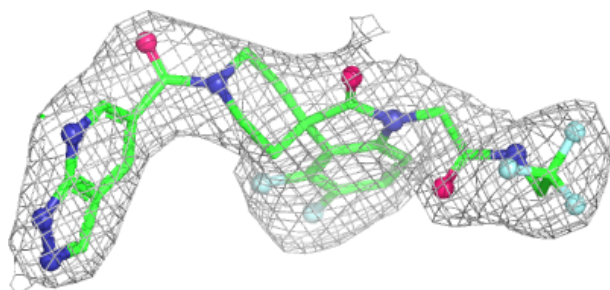
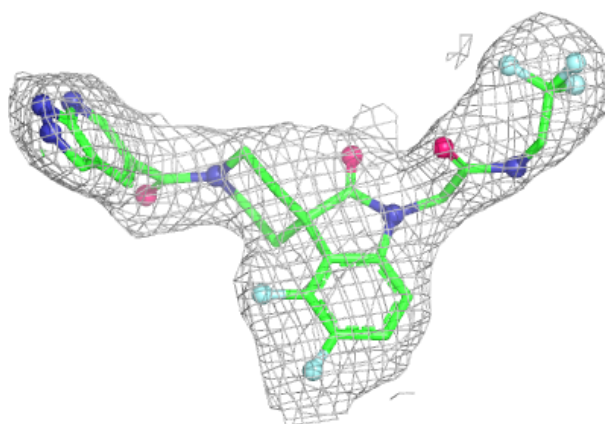
**Electron density around D6Q L 1001:**

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

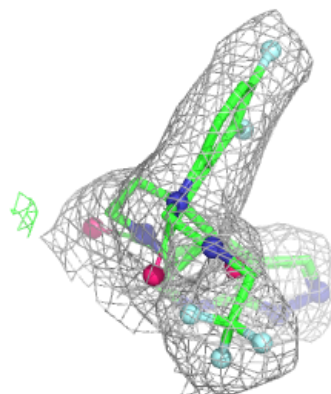
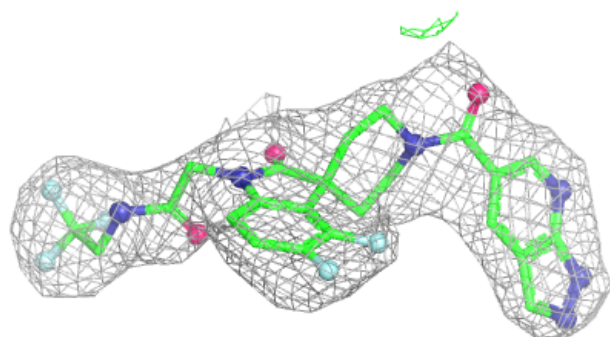
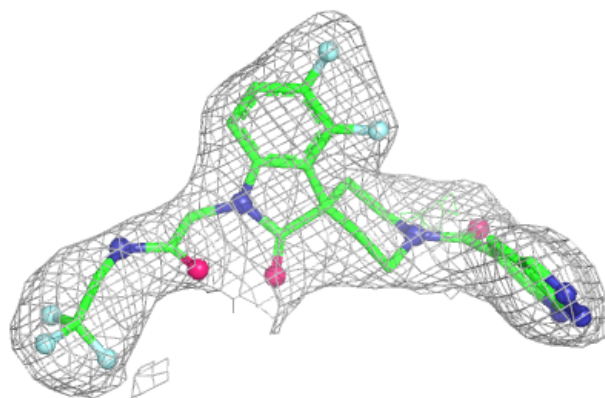


Electron density around D6Q B 1001:

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

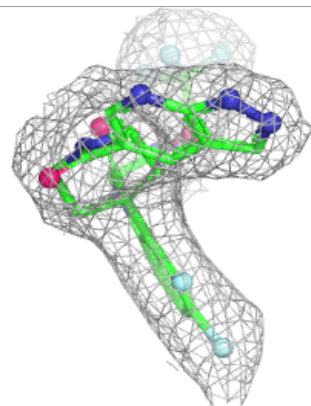
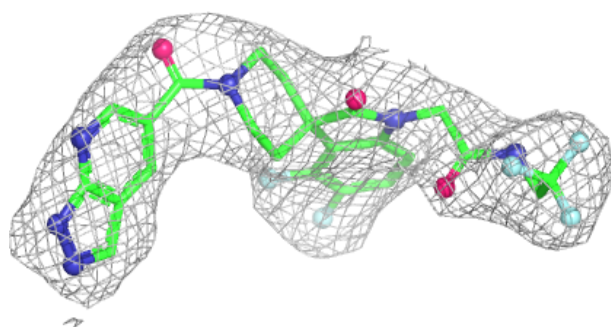
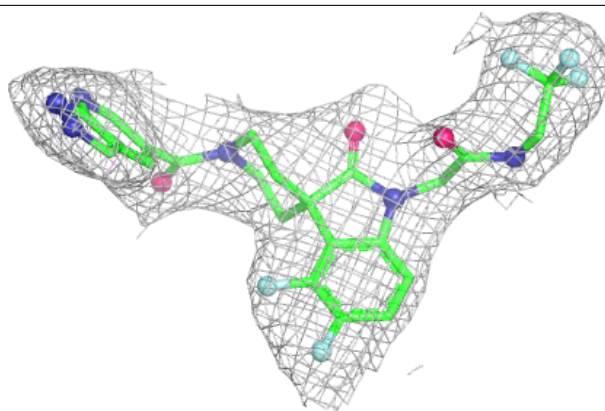
**Electron density around D6Q E 1001:**

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

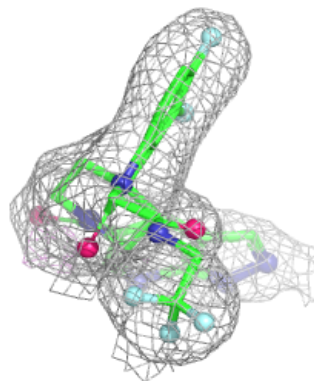
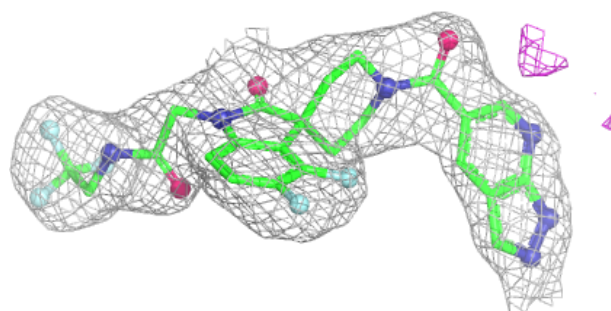
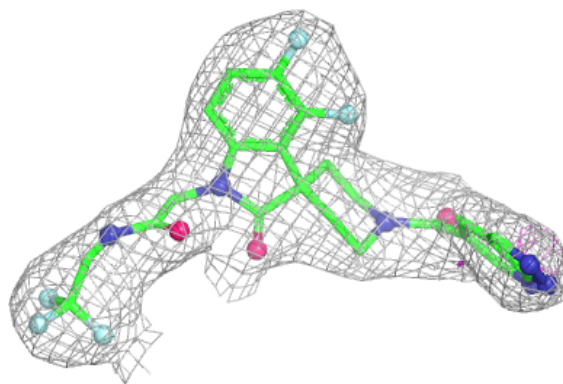


Electron density around D6Q F 1001:

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

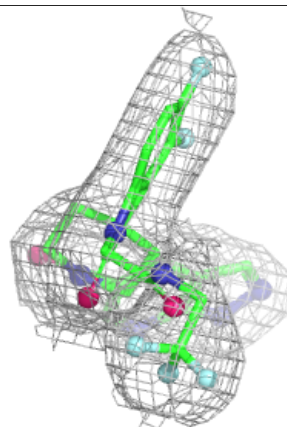
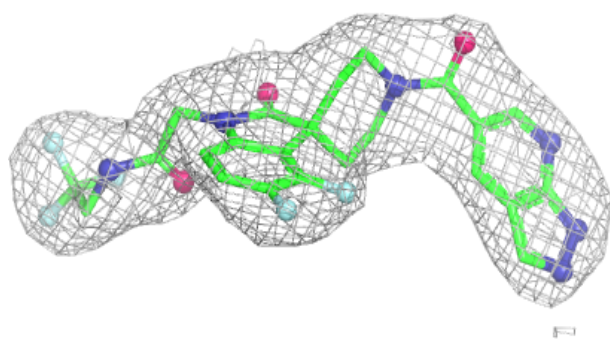
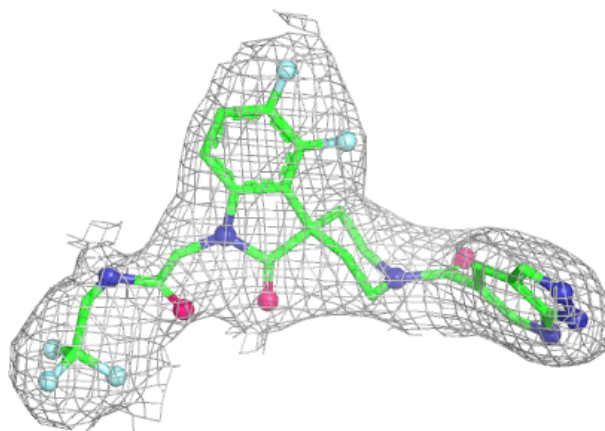
**Electron density around D6Q G 1001:**

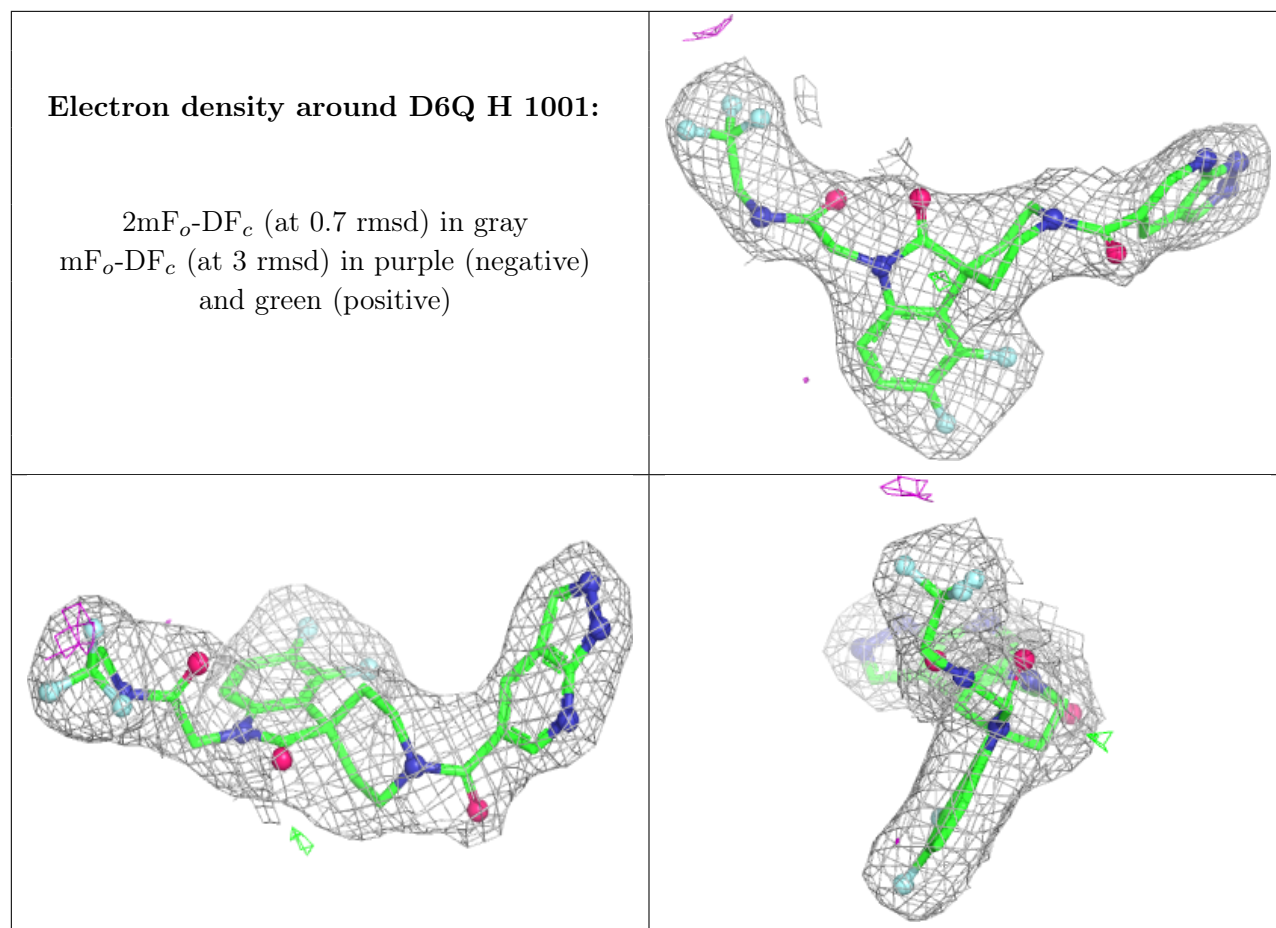
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around D6Q D 1001:

$2mF_o - DF_c$ (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.