Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:19 am BST

PDB ID	:	6FER
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 following versions of software and data (see references ⓘ) were used in the production of this report:

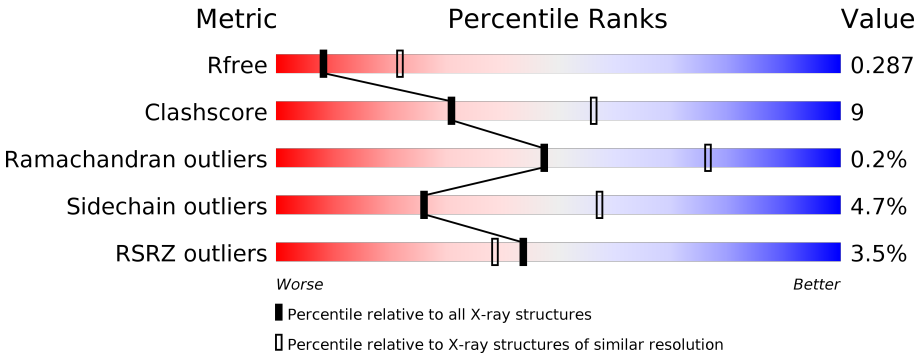
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (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 on 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	309	4% 64% 22% • 12%
1	B	309	2% 71% 19% • 10%
1	C	309	3% 66% 21% • 12%
1	D	309	% 70% 19% • 9%
1	E	309	% 64% 24% 12%
1	F	309	70% 18% • 11%

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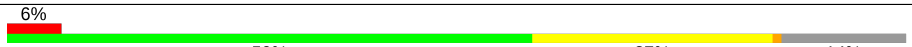
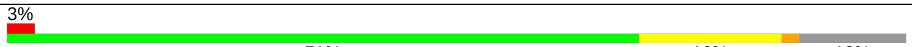
Mol	Chain	Length	Quality of chain
1	G	309	
1	H	309	
1	I	309	
1	J	309	
1	K	309	
1	L	309	

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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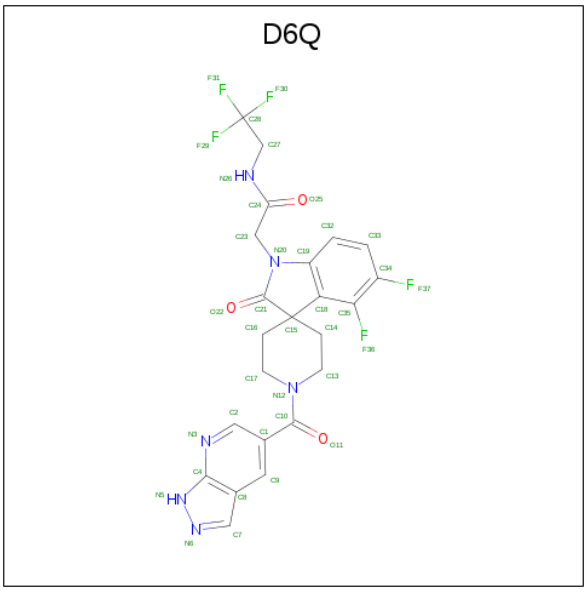
Chain	Residue	Modelled	Actual	Comment	Reference
H	908	HIS	-	expression tag	UNP Q16832
I	903	HIS	-	expression tag	UNP Q16832
I	904	HIS	-	expression tag	UNP Q16832
I	905	HIS	-	expression tag	UNP Q16832
I	906	HIS	-	expression tag	UNP Q16832
I	907	HIS	-	expression tag	UNP Q16832
I	908	HIS	-	expression tag	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-yl carbonyl)spiro[indole-3,4'-piperidine]-1-yl]- {N}-[2,2,2-tris(fluoranyl)ethyl]ethanamide (three-letter code: D6Q) (formula: $C_{23}H_{19}F_5N_6O_3$).



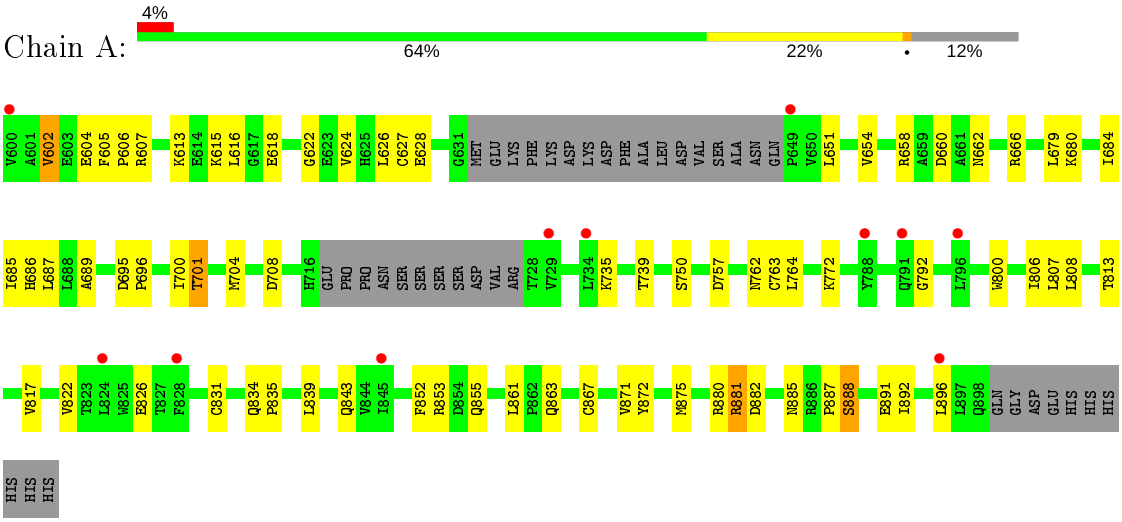
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	B	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	C	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	D	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	E	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	F	1	Total	C	F	N	O	0	0
			37	23	5	6	3		
2	G	1	Total	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 and DNA 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.

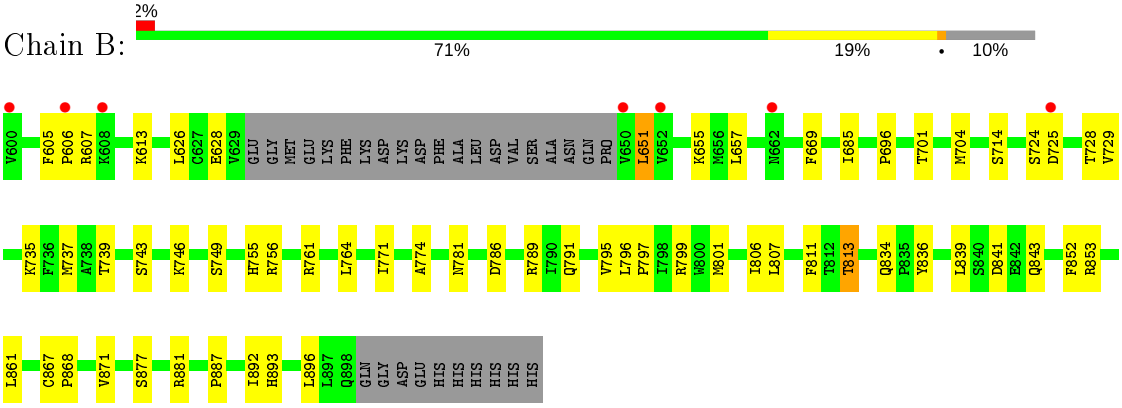
- Molecule 1: Discoidin domain-containing receptor 2

Chain A:



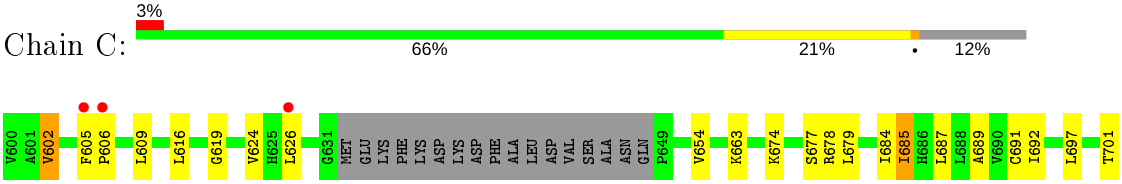
- Molecule 1: Discoidin domain-containing receptor 2

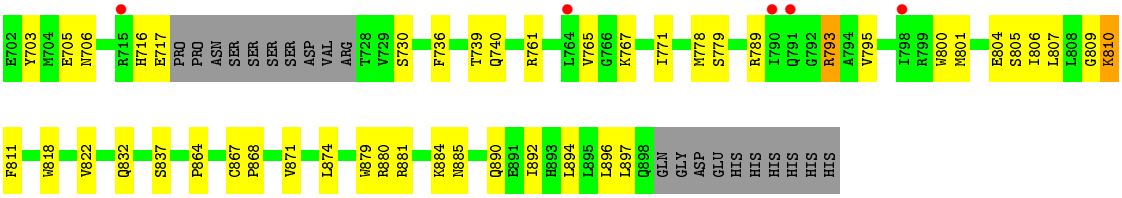
Chain B:



- Molecule 1: Discoidin domain-containing receptor 2

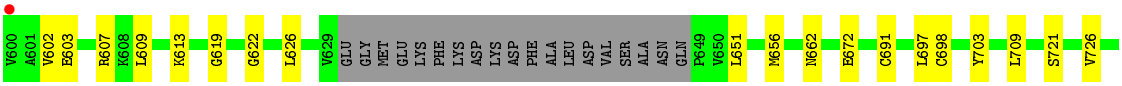
Chain C:

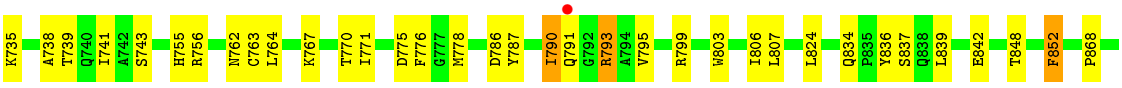


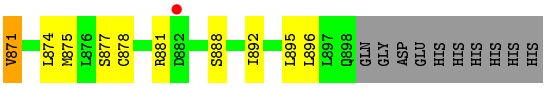


• Molecule 1: Discoidin domain-containing receptor 2

Chain D:

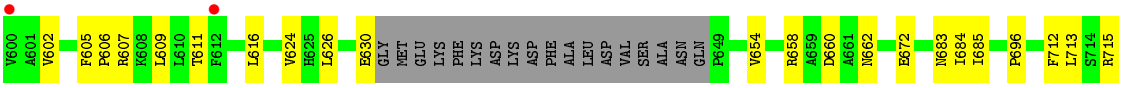


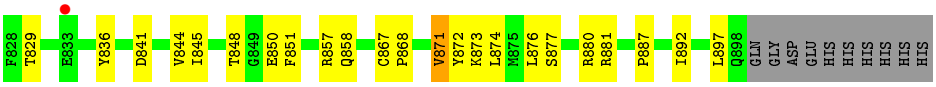




• Molecule 1: Discoidin domain-containing receptor 2

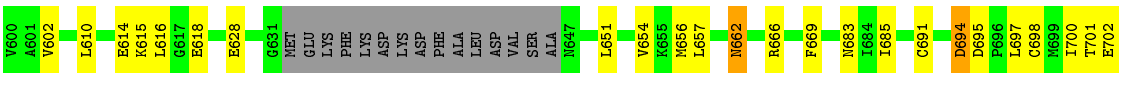
Chain E:

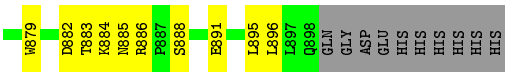




• Molecule 1: Discoidin domain-containing receptor 2

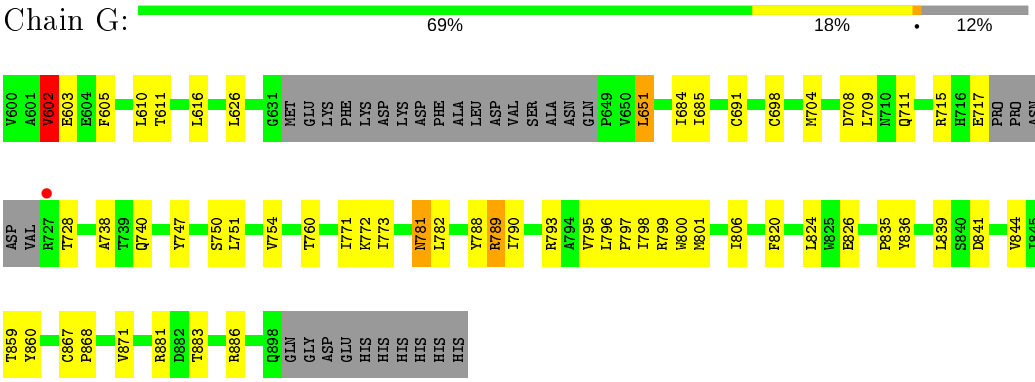
Chain F:





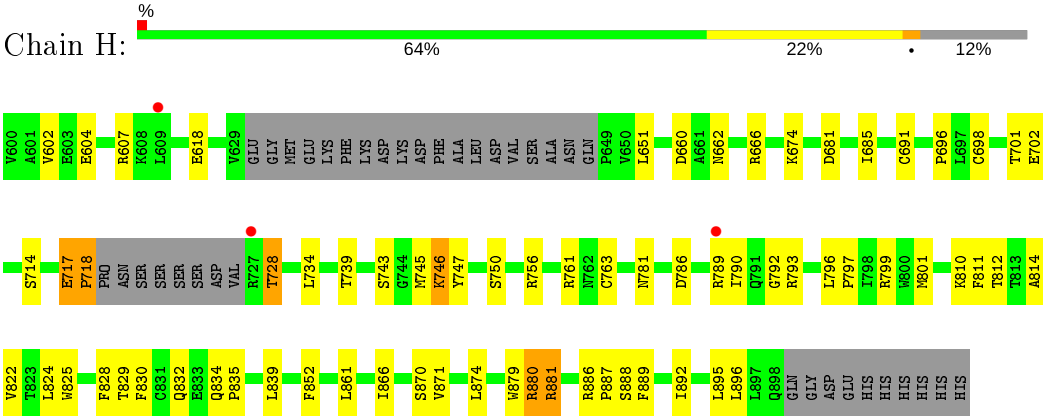
• Molecule 1: Discoidin domain-containing receptor 2

Chain G:



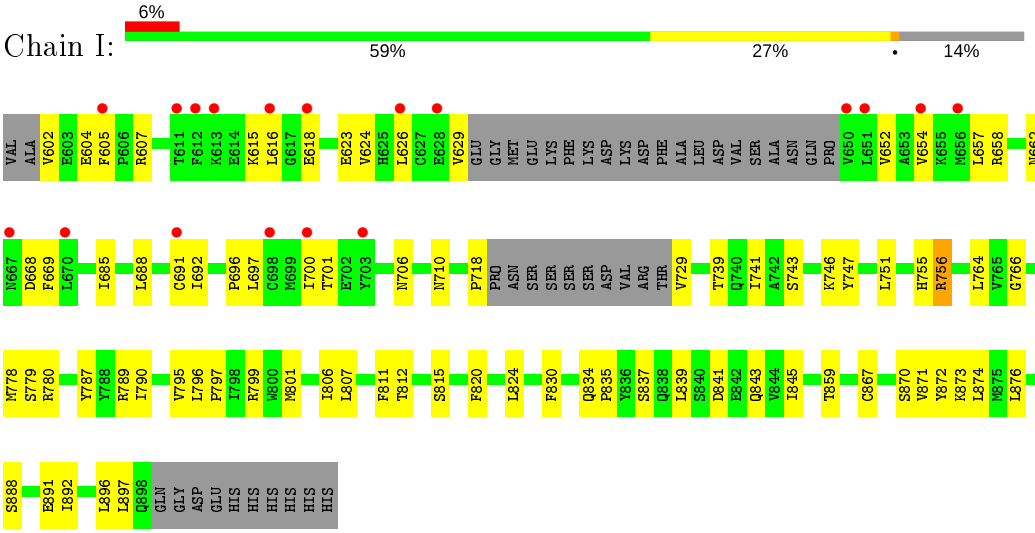
• Molecule 1: Discoidin domain-containing receptor 2

Chain H:



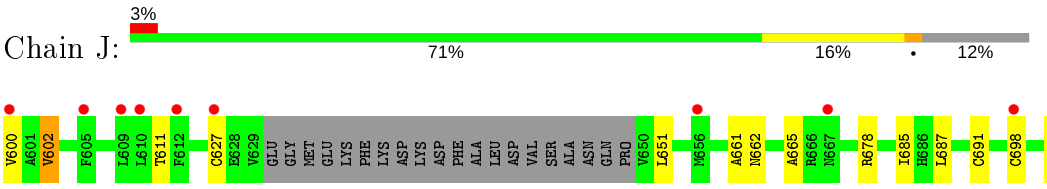
• Molecule 1: Discoidin domain-containing receptor 2

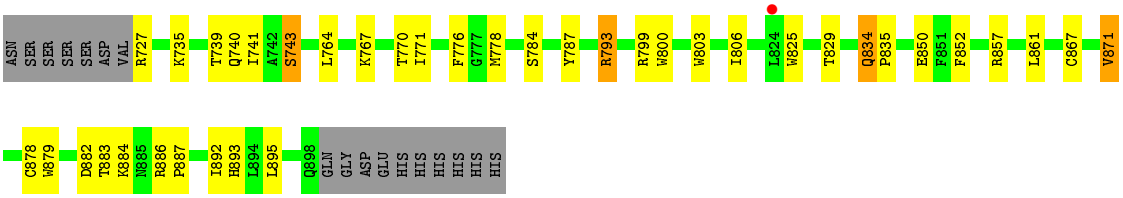
Chain I:



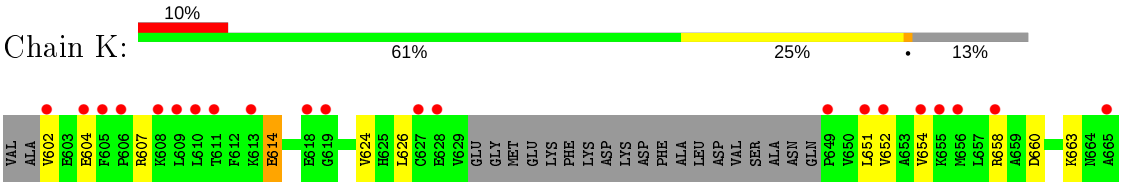
• Molecule 1: Discoidin domain-containing receptor 2

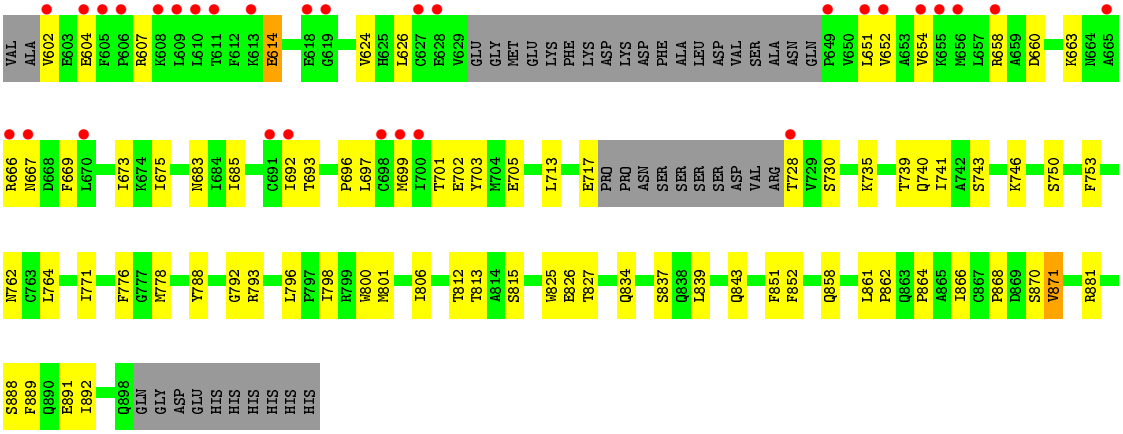
Chain J:



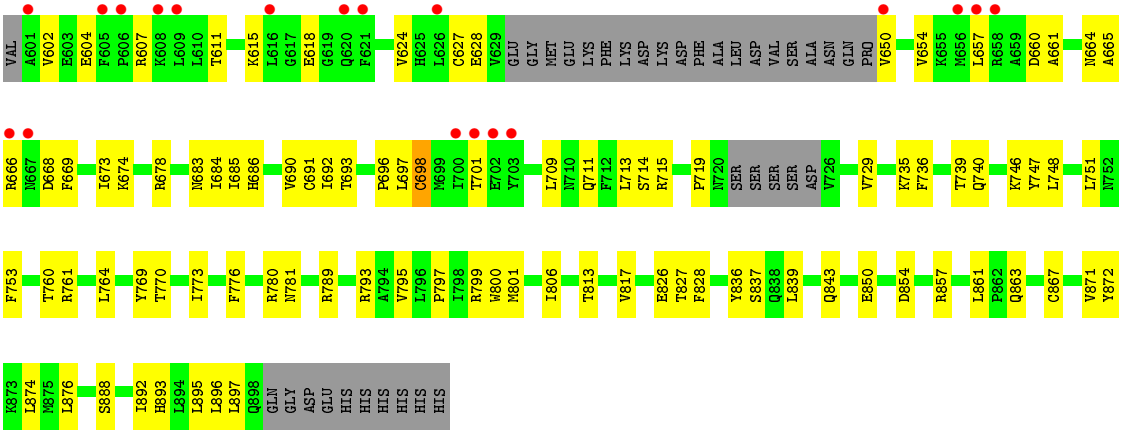


• Molecule 1: Discoidin domain-containing receptor 2





• Molecule 1: Discoidin domain-containing receptor 2



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.35 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.11_2558	Depositor
R, R_{free}	0.200 , 0.287 0.200 , 0.287	Depositor DCC
R_{free} test set	4484 reflections (4.92%)	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)	0.31 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/2247	0.58	0/3034
1	B	0.45	0/2310	0.63	0/3123
1	C	0.40	0/2256	0.58	0/3046
1	D	0.44	0/2318	0.63	0/3134
1	E	0.46	0/2271	0.65	0/3067
1	F	0.44	0/2281	0.62	0/3082
1	G	0.46	0/2267	0.65	0/3060
1	H	0.46	0/2262	0.63	0/3055
1	I	0.44	0/2224	0.60	0/3003
1	J	0.42	0/2262	0.64	0/3056
1	K	0.39	0/2231	0.57	0/3012
1	L	0.43	0/2270	0.59	0/3067
All	All	0.43	0/27199	0.62	0/36739

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

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	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2261	0	2247	35	0
1	C	2209	0	2197	40	0
1	D	2268	0	2255	37	0
1	E	2223	0	2214	42	0
1	F	2233	0	2217	33	0
1	G	2220	0	2210	35	0
1	H	2214	0	2208	49	0
1	I	2177	0	2166	53	0
1	J	2214	0	2207	34	0
1	K	2184	0	2174	45	0
1	L	2222	0	2213	59	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	0	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	486	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 9.

All (486) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:F:662:ASN:OD1	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: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:L:664:ASN:O	1:L:668:ASP:HB2	1.97	0.64
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:N	1:F:694:ASP:OD1	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
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:685:ILE:HG12	1:L:773:ILE:O	2.05	0.57
1:E:850:GLU:OE1	1:E:857:ARG:HB2	2.04	0.57
1:A:807:LEU:HD13	1:K:692:ILE:HG13	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:H:710:ASN:O	1:H:714:SER:OG	2.20	0.53
1:D:852:PHE:CE2	1:I:604:GLU:HB2	2.43	0.53
1:K:614:GLU:HG3	1:K:626:LEU:HD23	1.90	0.53
1:H:781:ASN:ND2	1:L:618:GLU:OE2	2.35	0.53
1:D:739:THR:HG22	1:D:896:LEU:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:656:MET:HG2	1:F:698:CYS:SG	2.49	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:E:734:LEU:HA	1:E:737:MET:HE2	1.92	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: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:A:604:GLU:HB2	1:H:852:PHE:CE2	2.44	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
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: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:G:781:ASN:N	1:G:781:ASN:OD1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:H:681:ASP:HB2	1:H:747:TYR:CD2	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: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:861:LEU:HD12	1:H:879:TRP:CZ2	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:850:GLU:OE1	1:L:857:ARG:HB2	2.16	0.46
1:L:895:LEU:HA	1:L:895:LEU:HD23	1.63	0.46
1:L:747:TYR:CE2	1:L:751:LEU:HD11	2.51	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:798:ILE:HD12	1:G:844:VAL:CG1	2.46	0.45
1:G:796:LEU:HB3	1:G:801:MET:SD	2.55	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:HE3	1:D:613:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:609:LEU:HD22	1:E:630:GLU:HB2	1.99	0.45
1:G:717:GLU:HG3	1:G:717:GLU:O	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: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: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:D:764:LEU:HD21	1:D:776:PHE:CZ	2.51	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:I:604:GLU:CD	1:I:692:ILE:H	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:852:PHE:CD1	1:D:852:PHE:C	2.90	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
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:HB2	1:I:615:LYS:HE3	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: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: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:HA	1:L:876:LEU:HD23	1.77	0.43
1:F:858:GLN:OE1	1:F:858:GLN:N	2.51	0.43
1:E:810:LYS:O	1:E:810:LYS:HG3	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:A:666:ARG:HH22	1:A:695:ASP:CG	2.23	0.42
1:B:655:LYS:HE2	1:B:669:PHE:CE1	2.54	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:E:760:THR:HG23	1:E:826:GLU:OE1	2.19	0.42
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:HE2	1:C:663:LYS:HB3	1.84	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: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: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:HA	1:F:616:LEU:HD23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:LEU:HD23	1:C:897:LEU:HA	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:H:618:GLU:CD	1:L:781:ASN:HD22	2.24	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:HA	1:I:897:LEU:HD23	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:HA	1:L:685:ILE:HD13	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:B:749:SER:OG	1:B:813:THR:HG21	2.20	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:L:764:LEU:HD21	1:L:776:PHE:HZ	1.86	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:C:805:SER:HB2	1:C:811:PHE:CE2	2.56	0.41
1:K:839:LEU:HB3	1:K:843:GLN:HB2	2.03	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
1:F:776:PHE:CE2	2:F:1001:D6Q:C10	3.04	0.41
1:G:685:ILE:HA	1:G:685:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:686:HIS:O	1:L:701:THR:HG23	2.20	0.40
1:L:654:VAL:HG12	1:L:698:CYS:HB3	2.03	0.40
1:D:852:PHE:O	1:D:852:PHE:HD1	2.04	0.40
1:E:713:LEU:HD11	1:E:827:THR:HG23	2.03	0.40
1:L:828:PHE:HD2	1:L:867:CYS:HG	1.66	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	64
1	G	267/309 (86%)	253 (95%)	13 (5%)	1 (0%)	34	64
1	H	266/309 (86%)	258 (97%)	8 (3%)	0	100	100
1	I	261/309 (84%)	249 (95%)	10 (4%)	2 (1%)	19	48
1	J	266/309 (86%)	254 (96%)	11 (4%)	1 (0%)	34	64
1	K	262/309 (85%)	252 (96%)	10 (4%)	0	100	100
1	L	267/309 (86%)	253 (95%)	12 (4%)	2 (1%)	22	52
All	All	3207/3708 (86%)	3081 (96%)	119 (4%)	7 (0%)	47	76

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 (i)

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%)	234 (96%)	9 (4%)	34	66
1	B	252/278 (91%)	243 (96%)	9 (4%)	35	67
1	C	244/278 (88%)	234 (96%)	10 (4%)	30	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	253/278 (91%)	235 (93%)	18 (7%)	14 38
1	E	246/278 (88%)	232 (94%)	14 (6%)	20 49
1	F	247/278 (89%)	234 (95%)	13 (5%)	22 52
1	G	245/278 (88%)	233 (95%)	12 (5%)	25 55
1	H	245/278 (88%)	224 (91%)	21 (9%)	10 29
1	I	241/278 (87%)	234 (97%)	7 (3%)	42 74
1	J	245/278 (88%)	238 (97%)	7 (3%)	42 74
1	K	242/278 (87%)	229 (95%)	13 (5%)	22 51
1	L	246/278 (88%)	239 (97%)	7 (3%)	43 75
All	All	2949/3336 (88%)	2809 (95%)	140 (5%)	26 57

All (140) 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	680	LYS
1	A	701	THR
1	A	750	SER
1	A	831	CYS
1	A	881	ARG
1	A	888	SER
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	877	SER
1	B	881	ARG
1	C	602	VAL
1	C	685	ILE
1	C	730	SER
1	C	761	ARG
1	C	778	MET
1	C	793	ARG
1	C	810	LYS

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Mol	Chain	Res	Type
1	C	832	GLN
1	C	837	SER
1	C	881	ARG
1	D	602	VAL
1	D	603	GLU
1	D	609	LEU
1	D	662	ASN
1	D	672	GLU
1	D	721	SER
1	D	726	VAL
1	D	743	SER
1	D	790	ILE
1	D	793	ARG
1	D	836	TYR
1	D	837	SER
1	D	842	GLU
1	D	852	PHE
1	D	871	VAL
1	D	877	SER
1	D	881	ARG
1	D	895	LEU
1	E	602	VAL
1	E	658	ARG
1	E	662	ASN
1	E	672	GLU
1	E	715	ARG
1	E	728	THR
1	E	778	MET
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	614	GLU
1	F	657	LEU
1	F	662	ASN
1	F	694	ASP
1	F	717	GLU
1	F	743	SER

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Mol	Chain	Res	Type
1	F	778	MET
1	F	813	THR
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	708	ASP
1	G	728	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	G	881	ARG
1	H	602	VAL
1	H	651	LEU
1	H	662	ASN
1	H	674	LYS
1	H	698	CYS
1	H	717	GLU
1	H	718	PRO
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	870	SER
1	H	871	VAL
1	H	880	ARG
1	H	881	ARG
1	H	888	SER
1	H	895	LEU
1	I	602	VAL
1	I	710	ASN
1	I	790	ILE

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Mol	Chain	Res	Type
1	I	837	SER
1	I	859	THR
1	I	881	ARG
1	I	883	THR
1	J	602	VAL
1	J	651	LEU
1	J	743	SER
1	J	784	SER
1	J	793	ARG
1	J	834	GLN
1	J	871	VAL
1	K	602	VAL
1	K	614	GLU
1	K	705	GLU
1	K	730	SER
1	K	750	SER
1	K	778	MET
1	K	812	THR
1	K	813	THR
1	K	815	SER
1	K	866	ILE
1	K	870	SER
1	K	871	VAL
1	K	881	ARG
1	L	602	VAL
1	L	698	CYS
1	L	714	SER
1	L	746	LYS
1	L	789	ARG
1	L	837	SER
1	L	888	SER

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

Mol	Chain	Res	Type
1	A	834	GLN
1	B	710	ASN
1	B	791	GLN
1	D	706	ASN
1	D	791	GLN
1	E	716	HIS
1	E	791	GLN

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Mol	Chain	Res	Type
1	K	667	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	J	1001	-	41,41,41	1.75	6 (14%)	48,63,63	1.97	14 (29%)
2	D6Q	D	1001	-	41,41,41	1.71	5 (12%)	48,63,63	2.03	11 (22%)
2	D6Q	B	1001	-	41,41,41	2.19	9 (21%)	48,63,63	1.79	11 (22%)
2	D6Q	F	1001	-	41,41,41	1.89	10 (24%)	48,63,63	1.83	11 (22%)
2	D6Q	K	1001	-	41,41,41	1.99	8 (19%)	48,63,63	1.93	12 (25%)
2	D6Q	I	1001	-	41,41,41	1.78	9 (21%)	48,63,63	2.35	13 (27%)
2	D6Q	C	1001	-	41,41,41	1.73	7 (17%)	48,63,63	1.93	12 (25%)
2	D6Q	A	1001	-	41,41,41	1.67	14 (34%)	48,63,63	1.95	9 (18%)
2	D6Q	H	1001	-	41,41,41	1.73	7 (17%)	48,63,63	1.84	10 (20%)
2	D6Q	G	1001	-	41,41,41	1.79	7 (17%)	48,63,63	1.83	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D6Q	E	1001	-	41,41,41	1.65	7 (17%)	48,63,63	1.95	13 (27%)
2	D6Q	L	1001	-	41,41,41	1.77	10 (24%)	48,63,63	1.92	12 (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	J	1001	-	-	6/18/50/50	0/5/5/5
2	D6Q	D	1001	-	-	2/18/50/50	0/5/5/5
2	D6Q	B	1001	-	-	1/18/50/50	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	I	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	C	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	A	1001	-	-	2/18/50/50	0/5/5/5
2	D6Q	H	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	G	1001	-	-	3/18/50/50	0/5/5/5
2	D6Q	E	1001	-	-	4/18/50/50	0/5/5/5
2	D6Q	L	1001	-	-	9/18/50/50	0/5/5/5

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	D6Q	C21-N20	7.44	1.45	1.36
2	K	1001	D6Q	C21-N20	6.47	1.43	1.36
2	C	1001	D6Q	C27-C28	6.32	1.60	1.49
2	G	1001	D6Q	C21-N20	6.09	1.43	1.36
2	H	1001	D6Q	C27-C28	6.06	1.59	1.49
2	F	1001	D6Q	C21-N20	5.86	1.43	1.36
2	J	1001	D6Q	C21-N20	5.73	1.43	1.36
2	D	1001	D6Q	C21-N20	5.73	1.43	1.36
2	K	1001	D6Q	C10-N12	5.15	1.46	1.34
2	I	1001	D6Q	C27-C28	5.07	1.58	1.49
2	K	1001	D6Q	C27-C28	4.89	1.57	1.49
2	D	1001	D6Q	C27-C28	4.82	1.57	1.49
2	B	1001	D6Q	C27-C28	4.60	1.57	1.49
2	B	1001	D6Q	C10-N12	4.59	1.45	1.34
2	F	1001	D6Q	C27-C28	4.56	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1001	D6Q	C10-N12	4.52	1.44	1.34
2	L	1001	D6Q	C21-N20	4.50	1.41	1.36
2	G	1001	D6Q	C27-C28	4.48	1.57	1.49
2	H	1001	D6Q	C21-N20	4.43	1.41	1.36
2	E	1001	D6Q	C15-C18	-4.36	1.46	1.51
2	L	1001	D6Q	C10-N12	4.34	1.44	1.34
2	B	1001	D6Q	C23-C24	4.18	1.58	1.52
2	A	1001	D6Q	C21-N20	4.11	1.41	1.36
2	F	1001	D6Q	C10-N12	4.09	1.43	1.34
2	E	1001	D6Q	C27-C28	4.07	1.56	1.49
2	L	1001	D6Q	C2-C1	3.98	1.45	1.39
2	I	1001	D6Q	C24-N26	3.92	1.42	1.33
2	E	1001	D6Q	C21-N20	3.86	1.41	1.36
2	J	1001	D6Q	C10-N12	3.82	1.43	1.34
2	H	1001	D6Q	C10-N12	3.82	1.43	1.34
2	C	1001	D6Q	C21-N20	3.69	1.40	1.36
2	B	1001	D6Q	C18-C35	-3.68	1.34	1.39
2	J	1001	D6Q	C27-C28	3.59	1.55	1.49
2	D	1001	D6Q	C24-N26	3.58	1.41	1.33
2	C	1001	D6Q	C24-N26	3.51	1.41	1.33
2	I	1001	D6Q	C15-C18	-3.45	1.47	1.51
2	D	1001	D6Q	C10-N12	3.42	1.42	1.34
2	K	1001	D6Q	C24-N26	3.42	1.41	1.33
2	C	1001	D6Q	C23-C24	3.34	1.57	1.52
2	K	1001	D6Q	C2-C1	3.33	1.44	1.39
2	J	1001	D6Q	C15-C18	-3.30	1.47	1.51
2	F	1001	D6Q	C24-N26	3.29	1.40	1.33
2	B	1001	D6Q	C4-N5	3.15	1.39	1.34
2	J	1001	D6Q	C15-C21	-3.15	1.49	1.53
2	B	1001	D6Q	F36-C35	-3.14	1.30	1.35
2	G	1001	D6Q	C18-C35	-3.04	1.35	1.39
2	I	1001	D6Q	C21-N20	3.02	1.40	1.36
2	E	1001	D6Q	C4-N5	3.00	1.39	1.34
2	A	1001	D6Q	C10-N12	3.00	1.41	1.34
2	H	1001	D6Q	C4-N5	2.96	1.39	1.34
2	F	1001	D6Q	C1-C10	-2.96	1.45	1.50
2	G	1001	D6Q	C10-N12	2.95	1.41	1.34
2	F	1001	D6Q	F36-C35	-2.91	1.30	1.35
2	H	1001	D6Q	C24-N26	2.90	1.40	1.33
2	G	1001	D6Q	C2-C1	2.87	1.43	1.39
2	G	1001	D6Q	C4-N5	2.86	1.39	1.34
2	B	1001	D6Q	C24-N26	2.82	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1001	D6Q	C27-C28	2.82	1.54	1.49
2	E	1001	D6Q	C16-C15	-2.81	1.51	1.55
2	F	1001	D6Q	C23-C24	2.79	1.56	1.52
2	L	1001	D6Q	C34-C35	2.79	1.43	1.37
2	A	1001	D6Q	C16-C15	-2.78	1.51	1.55
2	A	1001	D6Q	C27-C28	2.77	1.54	1.49
2	E	1001	D6Q	C24-N26	2.73	1.39	1.33
2	L	1001	D6Q	C4-N5	2.70	1.39	1.34
2	A	1001	D6Q	C17-N12	2.68	1.51	1.47
2	K	1001	D6Q	C19-C18	2.68	1.42	1.39
2	D	1001	D6Q	C2-C1	2.66	1.43	1.39
2	G	1001	D6Q	C15-C18	-2.66	1.48	1.51
2	J	1001	D6Q	C2-C1	2.64	1.43	1.39
2	L	1001	D6Q	F36-C35	-2.62	1.30	1.35
2	I	1001	D6Q	C34-C35	2.59	1.42	1.37
2	F	1001	D6Q	C4-N5	2.57	1.38	1.34
2	A	1001	D6Q	C2-C1	2.52	1.43	1.39
2	A	1001	D6Q	C34-C35	2.51	1.42	1.37
2	A	1001	D6Q	F36-C35	-2.50	1.31	1.35
2	K	1001	D6Q	C4-N5	2.49	1.38	1.34
2	L	1001	D6Q	C24-N26	2.49	1.39	1.33
2	I	1001	D6Q	C14-C15	-2.48	1.51	1.55
2	A	1001	D6Q	C24-N26	2.45	1.39	1.33
2	K	1001	D6Q	C34-C35	2.43	1.42	1.37
2	C	1001	D6Q	C14-C15	-2.42	1.51	1.55
2	A	1001	D6Q	C4-N5	2.41	1.38	1.34
2	L	1001	D6Q	C2-N3	2.41	1.35	1.31
2	F	1001	D6Q	C16-C15	-2.30	1.51	1.55
2	I	1001	D6Q	C2-C1	2.29	1.42	1.39
2	E	1001	D6Q	C32-C19	-2.25	1.35	1.39
2	A	1001	D6Q	C18-C35	-2.20	1.36	1.39
2	A	1001	D6Q	C2-N3	2.19	1.35	1.31
2	C	1001	D6Q	C10-N12	2.17	1.39	1.34
2	A	1001	D6Q	C15-C18	-2.14	1.49	1.51
2	B	1001	D6Q	C34-C35	2.13	1.42	1.37
2	H	1001	D6Q	C34-C35	2.07	1.41	1.37
2	H	1001	D6Q	F36-C35	-2.07	1.31	1.35
2	F	1001	D6Q	C19-C18	2.07	1.42	1.39
2	L	1001	D6Q	C15-C18	-2.03	1.49	1.51
2	I	1001	D6Q	O22-C21	-2.02	1.19	1.22
2	C	1001	D6Q	C16-C15	-2.02	1.52	1.55
2	A	1001	D6Q	C32-C19	-2.00	1.36	1.39

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1001	D6Q	C28-C27-N26	8.58	123.29	111.79
2	J	1001	D6Q	C27-N26-C24	-7.04	113.08	123.33
2	D	1001	D6Q	C28-C27-N26	-6.76	102.74	111.79
2	E	1001	D6Q	O22-C21-C15	6.25	132.22	126.30
2	A	1001	D6Q	C28-C27-N26	-6.12	103.59	111.79
2	C	1001	D6Q	O22-C21-N20	-6.08	119.81	125.81
2	H	1001	D6Q	O22-C21-N20	-6.04	119.86	125.81
2	G	1001	D6Q	C28-C27-N26	-5.67	104.19	111.79
2	A	1001	D6Q	O22-C21-N20	-5.55	120.34	125.81
2	I	1001	D6Q	O22-C21-N20	-5.55	120.35	125.81
2	F	1001	D6Q	O22-C21-N20	-5.38	120.51	125.81
2	A	1001	D6Q	O22-C21-C15	5.32	131.34	126.30
2	H	1001	D6Q	O22-C21-C15	5.27	131.29	126.30
2	K	1001	D6Q	C28-C27-N26	5.26	118.84	111.79
2	D	1001	D6Q	O22-C21-N20	-5.11	120.77	125.81
2	C	1001	D6Q	O22-C21-C15	4.93	130.97	126.30
2	F	1001	D6Q	C9-C1-C2	4.91	121.76	116.87
2	G	1001	D6Q	C9-C1-C2	4.82	121.66	116.87
2	D	1001	D6Q	C2-N3-C4	-4.79	111.89	116.69
2	L	1001	D6Q	O22-C21-N20	-4.77	121.11	125.81
2	D	1001	D6Q	C9-C1-C2	4.63	121.47	116.87
2	B	1001	D6Q	C19-N20-C21	-4.59	108.54	111.16
2	L	1001	D6Q	C2-N3-C4	-4.51	112.17	116.69
2	I	1001	D6Q	C9-C1-C2	4.49	121.34	116.87
2	K	1001	D6Q	O22-C21-N20	-4.42	121.46	125.81
2	D	1001	D6Q	O22-C21-C15	4.41	130.48	126.30
2	I	1001	D6Q	C19-N20-C21	-4.21	108.76	111.16
2	F	1001	D6Q	O22-C21-C15	4.19	130.27	126.30
2	E	1001	D6Q	C9-C1-C2	4.18	121.03	116.87
2	L	1001	D6Q	C1-C10-N12	4.18	124.03	118.72
2	L	1001	D6Q	C18-C15-C21	-4.12	99.50	101.95
2	K	1001	D6Q	C2-N3-C4	-4.10	112.58	116.69
2	B	1001	D6Q	O22-C21-N20	-4.04	121.83	125.81
2	B	1001	D6Q	C9-C1-C2	4.03	120.88	116.87
2	C	1001	D6Q	C2-N3-C4	-4.02	112.66	116.69
2	I	1001	D6Q	O22-C21-C15	3.94	130.03	126.30
2	G	1001	D6Q	C1-C9-C8	-3.92	115.18	121.24
2	G	1001	D6Q	C2-N3-C4	-3.90	112.78	116.69
2	E	1001	D6Q	O22-C21-N20	-3.87	122.00	125.81
2	F	1001	D6Q	C19-N20-C21	-3.86	108.96	111.16
2	I	1001	D6Q	C2-N3-C4	-3.83	112.85	116.69
2	D	1001	D6Q	C1-C9-C8	-3.81	115.36	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1001	D6Q	C19-N20-C21	-3.79	109.00	111.16
2	C	1001	D6Q	C1-C9-C8	-3.73	115.48	121.24
2	C	1001	D6Q	C9-C1-C2	3.67	120.53	116.87
2	B	1001	D6Q	C1-C9-C8	-3.64	115.62	121.24
2	H	1001	D6Q	C18-C15-C21	-3.62	99.79	101.95
2	E	1001	D6Q	C1-C9-C8	-3.53	115.79	121.24
2	A	1001	D6Q	C9-C1-C2	3.53	120.38	116.87
2	J	1001	D6Q	C2-N3-C4	-3.51	113.17	116.69
2	E	1001	D6Q	C18-C15-C21	3.43	103.99	101.95
2	K	1001	D6Q	C9-C1-C2	3.41	120.26	116.87
2	K	1001	D6Q	O22-C21-C15	3.41	129.53	126.30
2	B	1001	D6Q	C1-C10-N12	3.38	123.01	118.72
2	C	1001	D6Q	C18-C35-C34	-3.35	117.83	122.22
2	C	1001	D6Q	C19-N20-C21	-3.34	109.25	111.16
2	H	1001	D6Q	C2-N3-C4	-3.33	113.35	116.69
2	I	1001	D6Q	C1-C10-N12	3.28	122.88	118.72
2	L	1001	D6Q	O22-C21-C15	3.24	129.37	126.30
2	B	1001	D6Q	O22-C21-C15	3.22	129.34	126.30
2	G	1001	D6Q	O22-C21-C15	3.21	129.34	126.30
2	L	1001	D6Q	C24-C23-N20	-3.16	102.97	112.41
2	A	1001	D6Q	C1-C9-C8	-3.10	116.45	121.24
2	L	1001	D6Q	C19-N20-C21	-3.07	109.41	111.16
2	H	1001	D6Q	C9-C1-C2	3.05	119.91	116.87
2	B	1001	D6Q	C2-N3-C4	-3.04	113.64	116.69
2	H	1001	D6Q	C1-C10-N12	3.00	122.52	118.72
2	E	1001	D6Q	C14-C15-C18	-2.98	101.10	111.07
2	I	1001	D6Q	C1-C9-C8	-2.98	116.64	121.24
2	J	1001	D6Q	F31-C28-F30	-2.97	95.51	106.43
2	J	1001	D6Q	C9-C1-C2	2.97	119.83	116.87
2	A	1001	D6Q	C2-N3-C4	-2.95	113.73	116.69
2	J	1001	D6Q	C1-C10-N12	2.95	122.46	118.72
2	D	1001	D6Q	C18-C15-C21	-2.95	100.19	101.95
2	E	1001	D6Q	C2-N3-C4	-2.94	113.74	116.69
2	F	1001	D6Q	C27-N26-C24	-2.92	119.07	123.33
2	I	1001	D6Q	F29-C28-C27	2.92	119.86	111.85
2	I	1001	D6Q	C18-C35-C34	-2.91	118.41	122.22
2	J	1001	D6Q	C24-C23-N20	-2.90	103.75	112.41
2	G	1001	D6Q	O22-C21-N20	-2.87	122.98	125.81
2	K	1001	D6Q	C24-C23-N20	-2.86	103.85	112.41
2	G	1001	D6Q	C18-C35-C34	-2.85	118.48	122.22
2	I	1001	D6Q	C24-C23-N20	-2.84	103.92	112.41
2	L	1001	D6Q	O11-C10-N12	-2.81	117.69	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1001	D6Q	C18-C35-C34	-2.79	118.56	122.22
2	J	1001	D6Q	C1-C9-C8	-2.79	116.93	121.24
2	H	1001	D6Q	C27-N26-C24	-2.78	119.28	123.33
2	K	1001	D6Q	C1-C10-N12	2.78	122.24	118.72
2	F	1001	D6Q	C2-N3-C4	-2.74	113.95	116.69
2	L	1001	D6Q	F29-C28-C27	2.72	119.31	111.85
2	F	1001	D6Q	C1-C9-C8	-2.72	117.05	121.24
2	E	1001	D6Q	C18-C35-C34	-2.72	118.66	122.22
2	H	1001	D6Q	C1-C9-C8	-2.71	117.06	121.24
2	J	1001	D6Q	C18-C19-N20	-2.68	107.63	109.62
2	L	1001	D6Q	C9-C1-C2	2.67	119.53	116.87
2	C	1001	D6Q	O11-C10-N12	-2.62	118.01	122.34
2	B	1001	D6Q	C28-C27-N26	-2.60	108.30	111.79
2	H	1001	D6Q	C18-C35-C34	-2.59	118.83	122.22
2	I	1001	D6Q	C19-C18-C35	2.59	120.58	118.01
2	K	1001	D6Q	C1-C9-C8	-2.58	117.25	121.24
2	L	1001	D6Q	C1-C9-C8	-2.57	117.28	121.24
2	F	1001	D6Q	C1-C10-N12	2.56	121.97	118.72
2	J	1001	D6Q	O22-C21-C15	2.51	128.68	126.30
2	E	1001	D6Q	C16-C17-N12	-2.45	106.09	110.92
2	C	1001	D6Q	C9-C1-C10	2.44	125.30	120.52
2	J	1001	D6Q	C18-C35-C34	-2.43	119.04	122.22
2	B	1001	D6Q	O25-C24-C23	2.43	125.33	121.08
2	C	1001	D6Q	C1-C10-N12	2.43	121.80	118.72
2	E	1001	D6Q	C27-N26-C24	-2.41	119.82	123.33
2	G	1001	D6Q	C2-C1-C10	-2.40	113.95	121.01
2	L	1001	D6Q	C27-N26-C24	-2.37	119.88	123.33
2	C	1001	D6Q	C2-C1-C10	-2.35	114.09	121.01
2	J	1001	D6Q	C19-C18-C35	2.34	120.34	118.01
2	K	1001	D6Q	F29-C28-C27	2.31	118.18	111.85
2	E	1001	D6Q	C2-C1-C10	-2.31	114.22	121.01
2	A	1001	D6Q	C19-N20-C21	-2.29	109.85	111.16
2	J	1001	D6Q	C16-C17-N12	-2.29	106.41	110.92
2	E	1001	D6Q	C19-C18-C35	2.28	120.28	118.01
2	A	1001	D6Q	C13-N12-C10	-2.28	115.56	122.78
2	D	1001	D6Q	C1-C10-N12	2.27	121.60	118.72
2	K	1001	D6Q	F31-C28-F30	-2.25	98.16	106.43
2	C	1001	D6Q	C13-N12-C10	-2.22	115.76	122.78
2	D	1001	D6Q	C2-C1-C10	-2.19	114.58	121.01
2	B	1001	D6Q	C2-C1-C10	-2.16	114.64	121.01
2	A	1001	D6Q	C18-C35-C34	-2.16	119.39	122.22
2	F	1001	D6Q	C2-C1-C10	-2.12	114.77	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1001	D6Q	C33-C34-C35	-2.11	119.26	121.18
2	I	1001	D6Q	C23-N20-C19	2.11	128.42	125.18
2	G	1001	D6Q	C19-N20-C21	-2.10	109.96	111.16
2	E	1001	D6Q	C9-C1-C10	2.07	124.58	120.52
2	J	1001	D6Q	O11-C10-N12	-2.06	118.93	122.34
2	J	1001	D6Q	F31-C28-C27	-2.04	106.25	111.85
2	D	1001	D6Q	C19-N20-C21	-2.04	110.00	111.16
2	F	1001	D6Q	C28-C27-N26	-2.04	109.06	111.79
2	H	1001	D6Q	O11-C10-N12	-2.03	118.98	122.34
2	B	1001	D6Q	C9-C1-C10	2.02	124.49	120.52
2	D	1001	D6Q	C18-C35-C34	-2.00	119.60	122.22

There are no chirality outliers.

All (37) torsion outliers are listed below:

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

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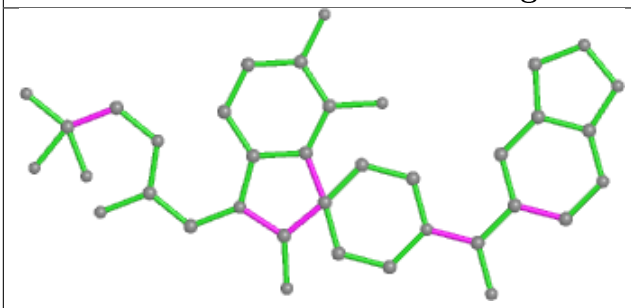
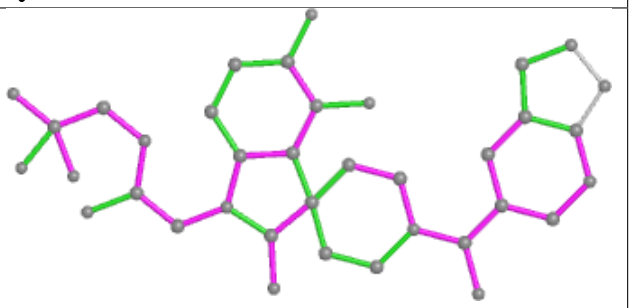
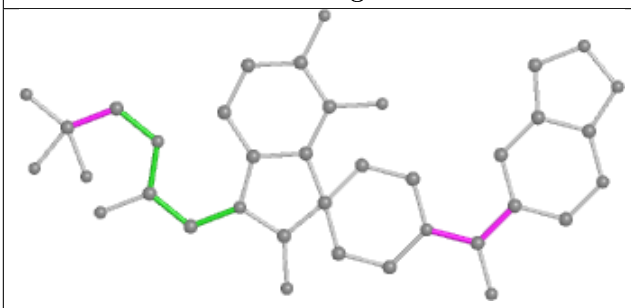
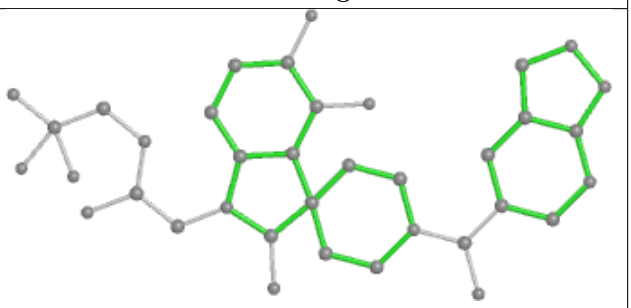
Mol	Chain	Res	Type	Atoms
2	E	1001	D6Q	N26-C27-C28-F29
2	A	1001	D6Q	O11-C10-N12-C17
2	D	1001	D6Q	C28-C27-N26-C24
2	D	1001	D6Q	O11-C10-N12-C13
2	J	1001	D6Q	N26-C27-C28-F30
2	L	1001	D6Q	C1-C10-N12-C17
2	B	1001	D6Q	O11-C10-N12-C13
2	K	1001	D6Q	N26-C27-C28-F30
2	G	1001	D6Q	N26-C27-C28-F30
2	L	1001	D6Q	C9-C1-C10-N12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

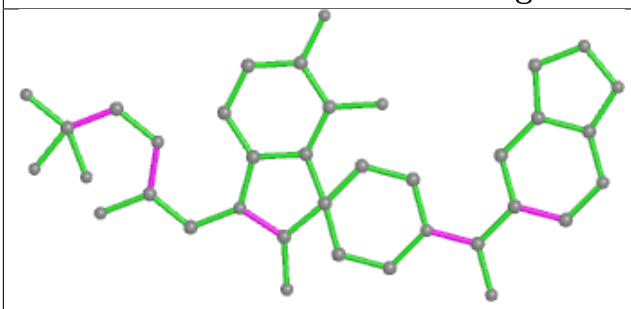
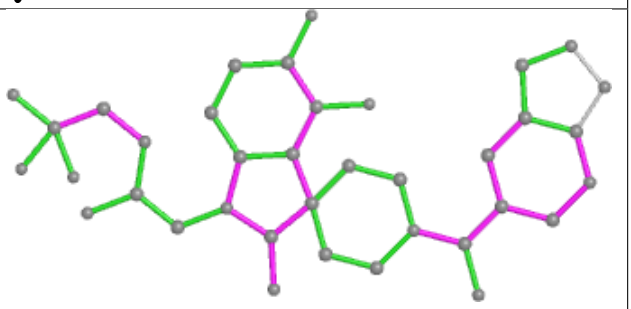
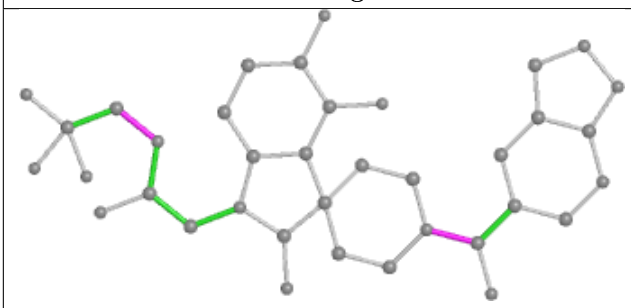
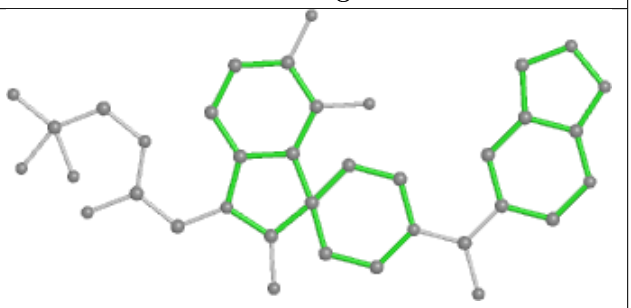
There are no ring outliers.

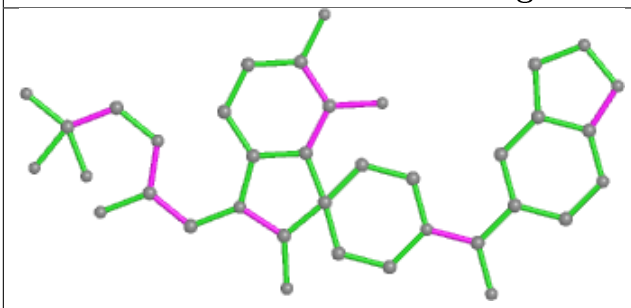
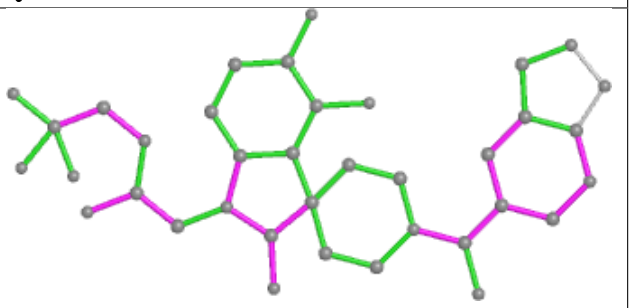
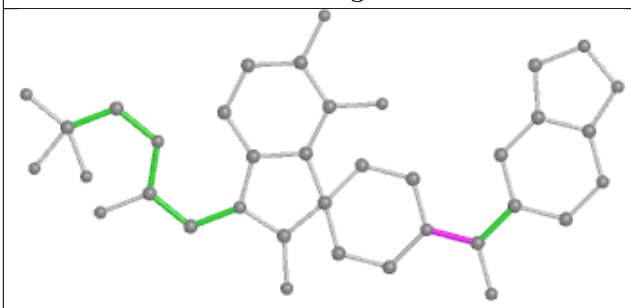
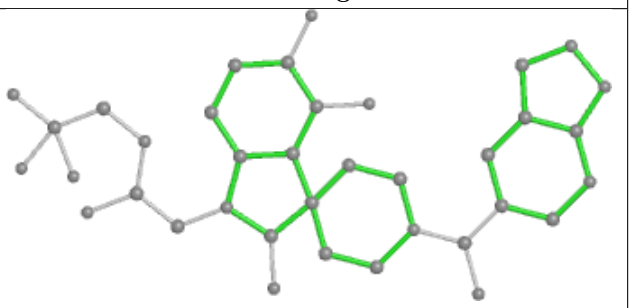
6 monomers are involved in 7 short contacts:

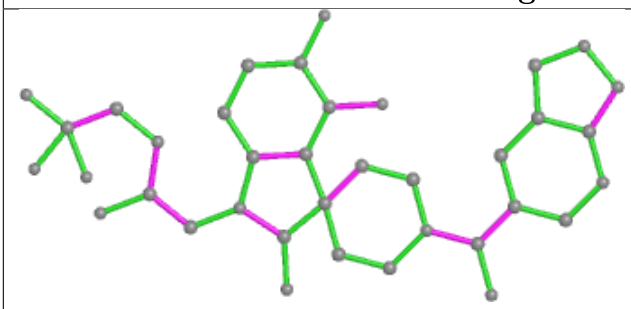
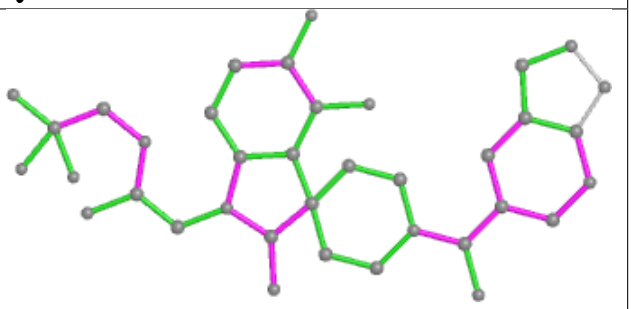
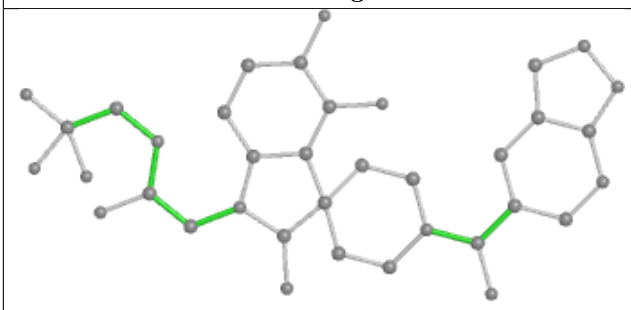
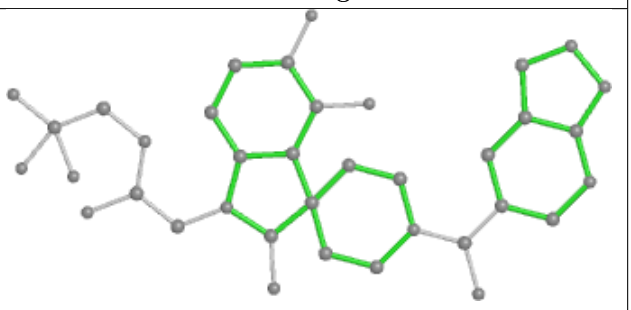
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1001	D6Q	1	0
2	F	1001	D6Q	1	0
2	K	1001	D6Q	1	0
2	I	1001	D6Q	2	0
2	A	1001	D6Q	1	0
2	E	1001	D6Q	1	0

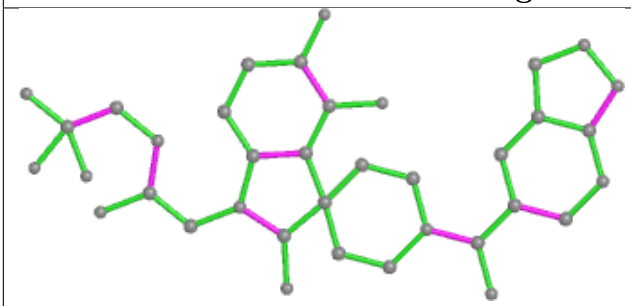
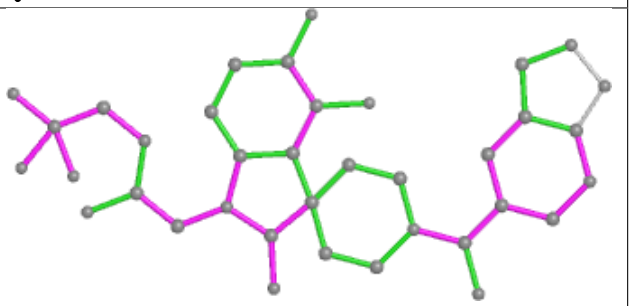
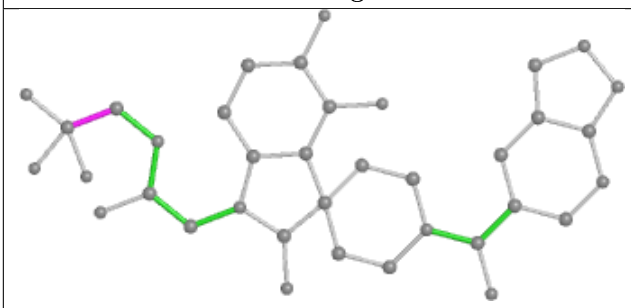
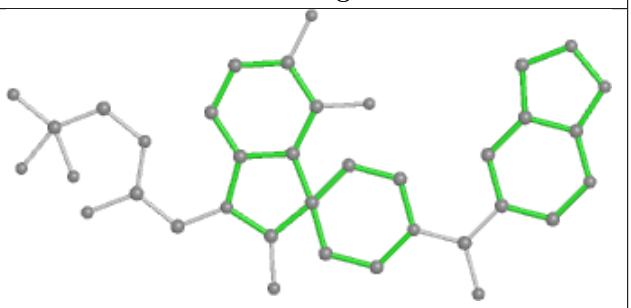
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

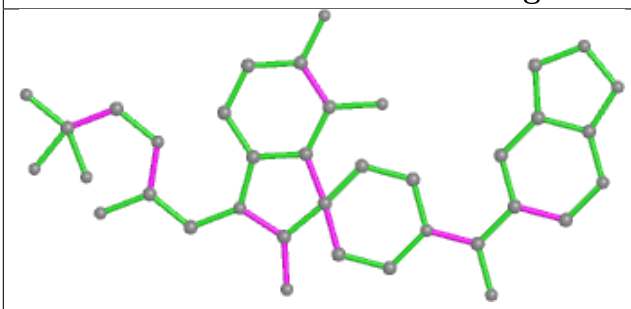
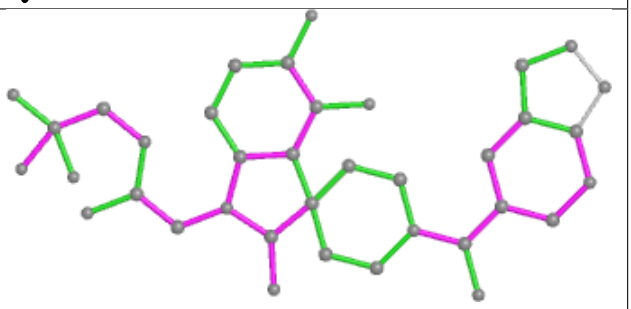
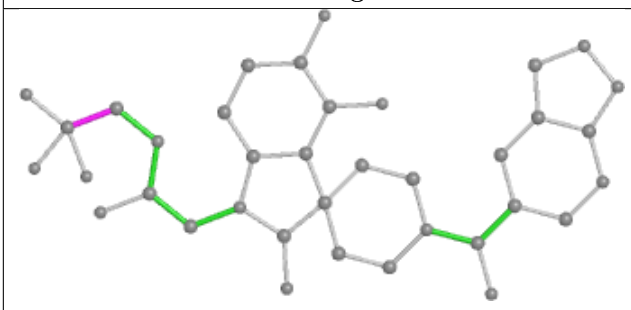
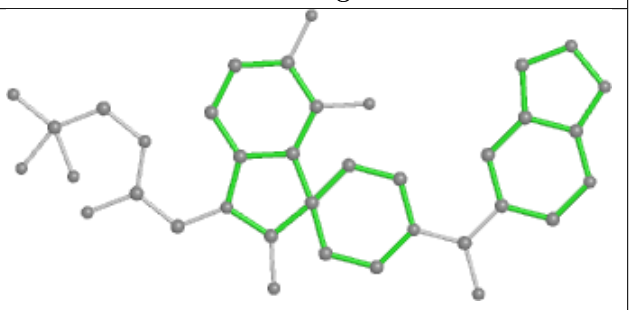
Ligand D6Q J 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

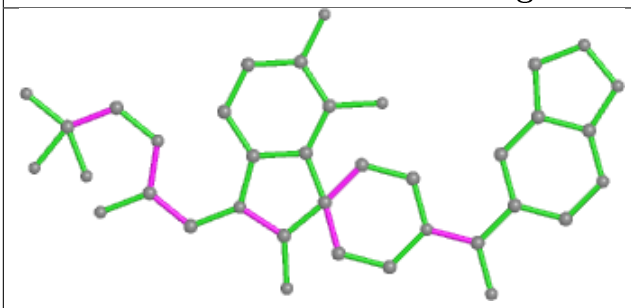
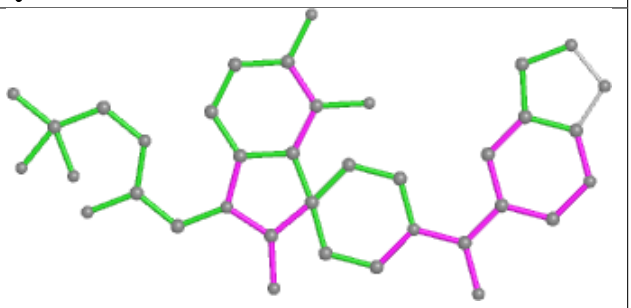
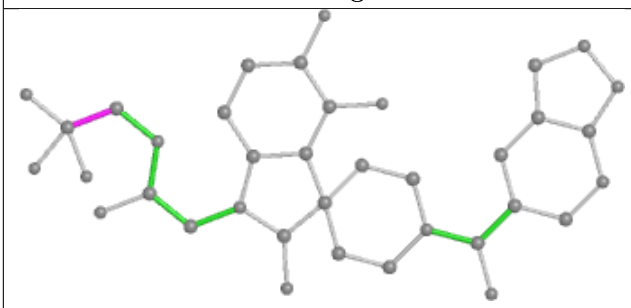
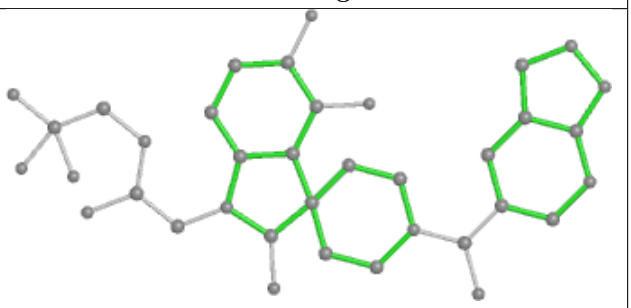
Ligand D6Q D 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

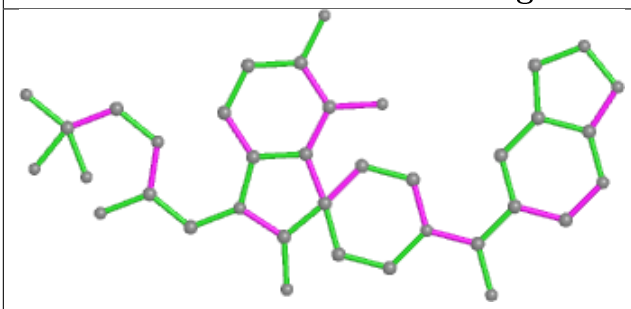
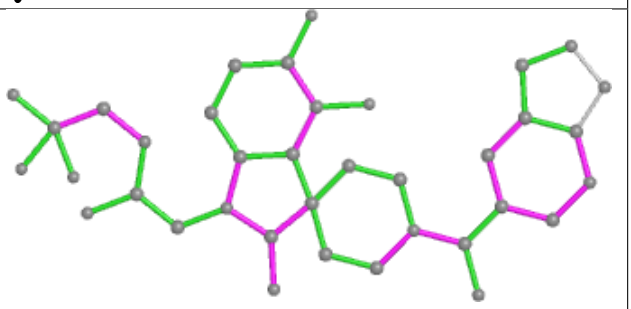
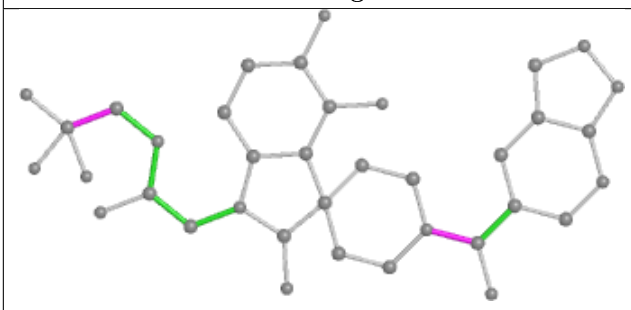
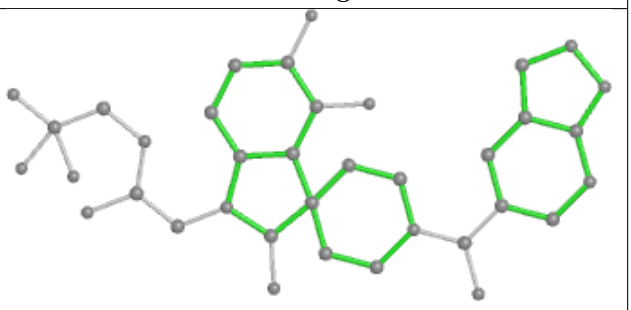
Ligand D6Q B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

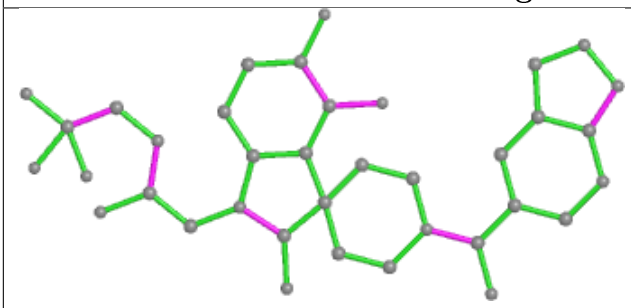
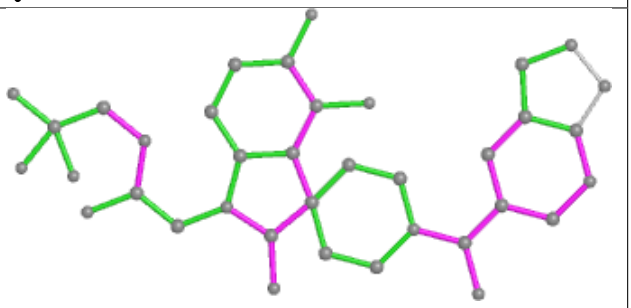
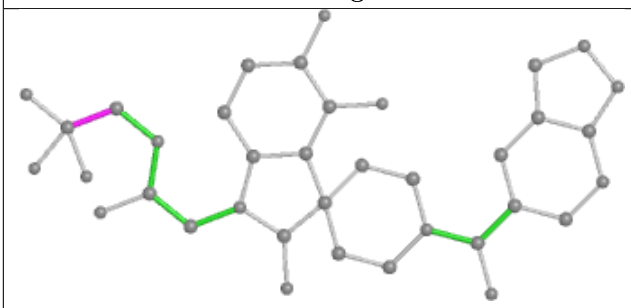
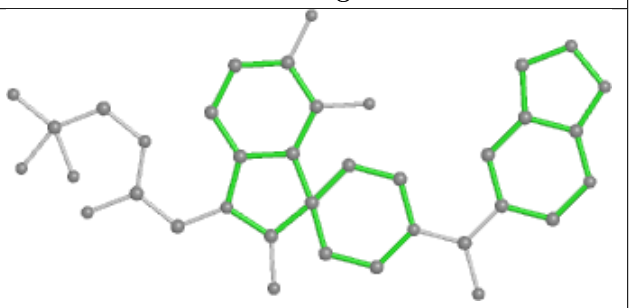
Ligand D6Q F 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

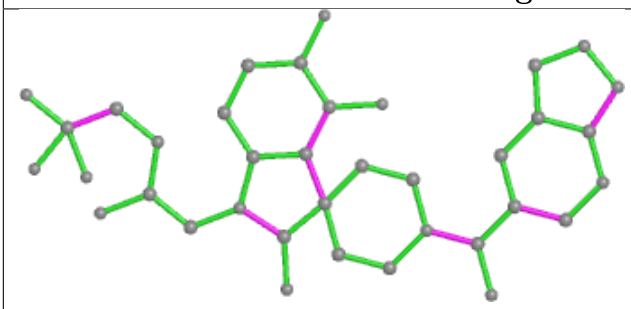
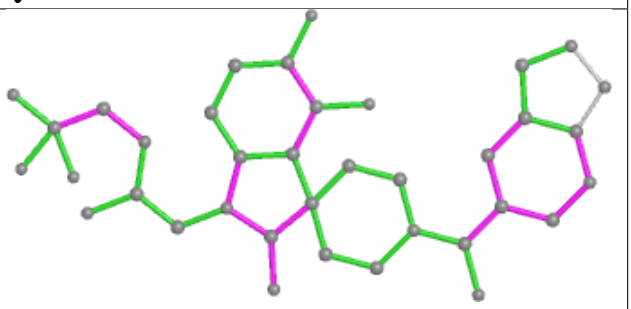
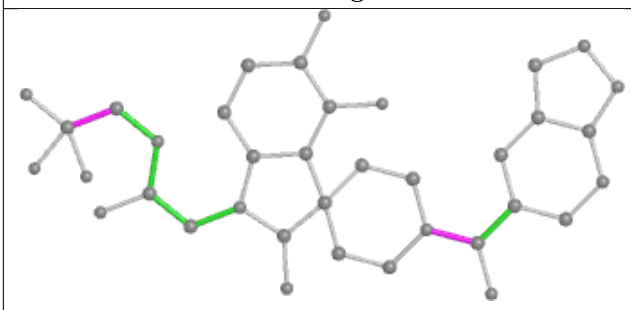
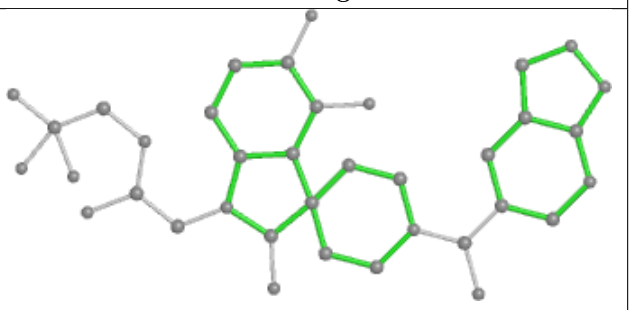
Ligand D6Q K 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D6Q I 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

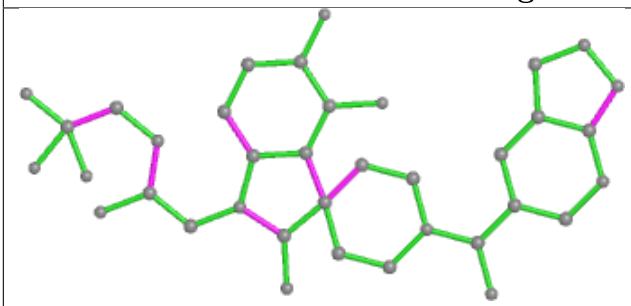
Ligand D6Q C 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D6Q A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

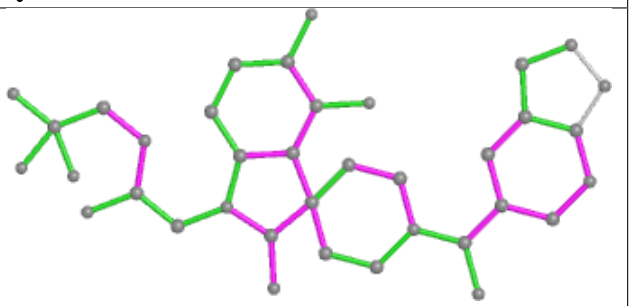
Ligand D6Q H 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D6Q G 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

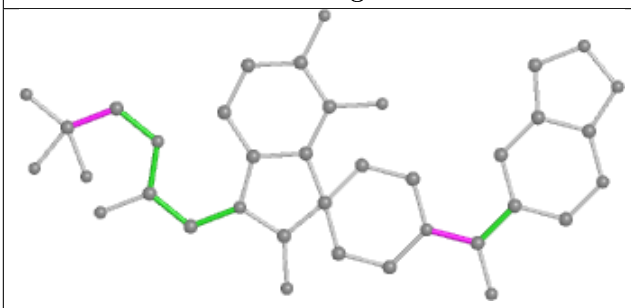
Ligand D6Q E 1001



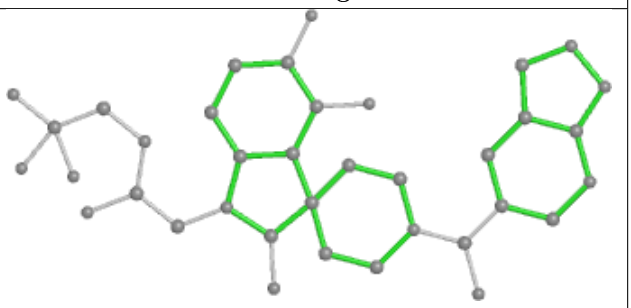
Bond lengths



Bond angles

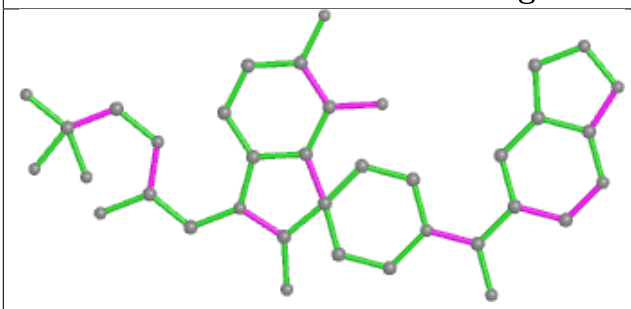


Torsions

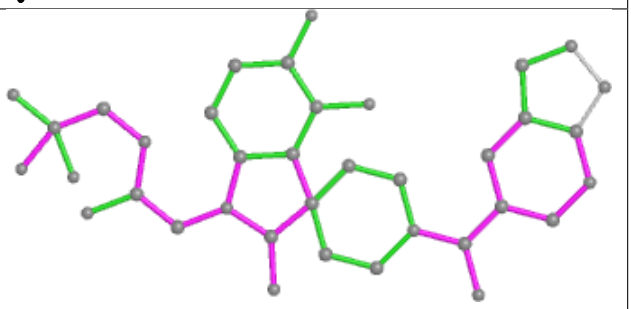


Rings

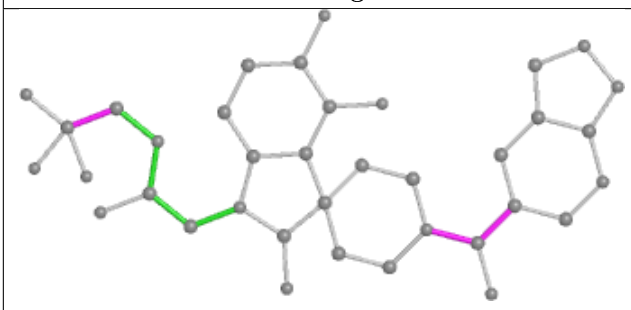
Ligand D6Q L 1001



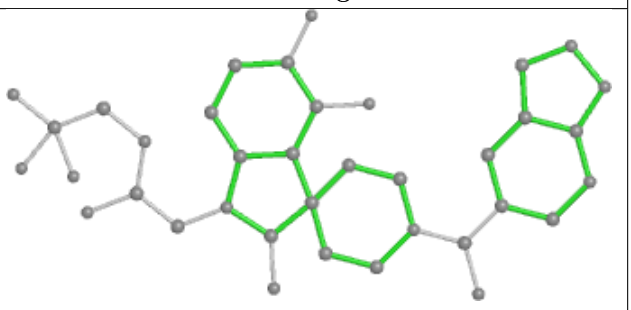
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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%)	0.12	11 (4%) 37 32	39, 69, 109, 145	0
1	B	279/309 (90%)	0.01	7 (2%) 57 55	32, 57, 113, 165	0
1	C	272/309 (88%)	0.13	8 (2%) 51 48	40, 63, 103, 170	0
1	D	280/309 (90%)	-0.06	3 (1%) 80 80	32, 53, 92, 173	0
1	E	273/309 (88%)	-0.12	4 (1%) 73 73	29, 48, 100, 168	0
1	F	275/309 (88%)	-0.12	0 100 100	32, 53, 93, 127	0
1	G	273/309 (88%)	-0.10	1 (0%) 92 92	30, 49, 91, 150	0
1	H	272/309 (88%)	-0.10	3 (1%) 80 80	27, 49, 91, 164	0
1	I	267/309 (86%)	0.34	20 (7%) 14 10	29, 58, 146, 186	0
1	J	272/309 (88%)	0.09	10 (3%) 41 37	31, 55, 107, 164	0
1	K	268/309 (86%)	0.56	30 (11%) 5 3	39, 65, 163, 212	0
1	L	273/309 (88%)	0.20	19 (6%) 16 12	33, 63, 119, 225	0
All	All	3275/3708 (88%)	0.08	116 (3%) 44 39	27, 57, 119, 225	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	691	CYS	10.5
1	K	698	CYS	9.7
1	K	654	VAL	8.2
1	K	609	LEU	6.7
1	K	652	VAL	6.3
1	K	656	MET	6.3
1	I	656	MET	6.1
1	L	608	LYS	6.0
1	K	619	GLY	5.9
1	B	600	VAL	5.9
1	K	610	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	I	698	CYS	5.5
1	K	606	PRO	5.5
1	J	600	VAL	5.2
1	A	791	GLN	5.1
1	K	611	THR	4.8
1	K	605	PHE	4.7
1	I	667	ASN	4.7
1	K	613	LYS	4.7
1	I	651	LEU	4.6
1	K	666	ARG	4.6
1	I	703	TYR	4.5
1	K	651	LEU	4.5
1	K	691	CYS	4.4
1	I	666	ARG	4.4
1	K	670	LEU	4.2
1	H	727	ARG	4.1
1	J	610	LEU	3.9
1	I	670	LEU	3.9
1	L	656	MET	3.8
1	B	652	VAL	3.8
1	I	611	THR	3.7
1	K	604	GLU	3.7
1	E	727	ARG	3.6
1	K	692	ILE	3.6
1	L	658	ARG	3.6
1	L	601	ALA	3.5
1	I	700	ILE	3.4
1	I	665	ALA	3.4
1	K	700	ILE	3.4
1	J	609	LEU	3.3
1	K	602	VAL	3.2
1	B	725	ASP	3.2
1	L	703	TYR	3.2
1	I	626	LEU	3.2
1	L	702	GLU	3.2
1	J	698	CYS	3.1
1	L	616	LEU	3.1
1	J	627	CYS	3.1
1	L	605	PHE	3.1
1	I	628	GLU	3.1
1	C	791	GLN	3.0
1	J	656	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	665	ALA	3.0
1	K	655	LYS	3.0
1	K	627	CYS	2.8
1	A	600	VAL	2.7
1	E	600	VAL	2.7
1	I	650	VAL	2.7
1	L	606	PRO	2.7
1	K	618	GLU	2.7
1	I	605	PHE	2.6
1	K	658	ARG	2.6
1	J	667	ASN	2.6
1	I	616	LEU	2.5
1	K	608	LYS	2.5
1	L	700	ILE	2.5
1	A	649	PRO	2.5
1	C	764	LEU	2.5
1	I	654	VAL	2.5
1	K	628	GLU	2.5
1	A	729	VAL	2.5
1	G	727	ARG	2.5
1	K	728	THR	2.5
1	L	666	ARG	2.4
1	B	650	VAL	2.4
1	L	667	ASN	2.4
1	C	605	PHE	2.4
1	K	649	PRO	2.4
1	B	662	ASN	2.4
1	D	882	ASP	2.4
1	A	845	ILE	2.4
1	L	657	LEU	2.3
1	L	621	PHE	2.3
1	E	833	GLU	2.3
1	H	609	LEU	2.3
1	A	734	LEU	2.3
1	L	609	LEU	2.3
1	A	828	PHE	2.3
1	A	824	LEU	2.2
1	C	798	ILE	2.2
1	L	701	THR	2.2
1	D	600	VAL	2.2
1	I	618	GLU	2.2
1	A	896	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	791	GLN	2.1
1	L	620	GLN	2.1
1	B	606	PRO	2.1
1	C	606	PRO	2.1
1	K	667	ASN	2.1
1	A	796	LEU	2.1
1	E	612	PHE	2.1
1	J	612	PHE	2.1
1	A	788	TYR	2.1
1	C	626	LEU	2.1
1	C	715	ARG	2.1
1	L	650	VAL	2.1
1	H	789	ARG	2.1
1	C	790	ILE	2.0
1	K	699	MET	2.0
1	I	612	PHE	2.0
1	J	605	PHE	2.0
1	I	613	LYS	2.0
1	L	626	LEU	2.0
1	B	608	LYS	2.0
1	J	824	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	D6Q	K	1001	37/37	0.92	0.29	31,81,95,104	0
2	D6Q	I	1001	37/37	0.92	0.30	13,68,92,101	0

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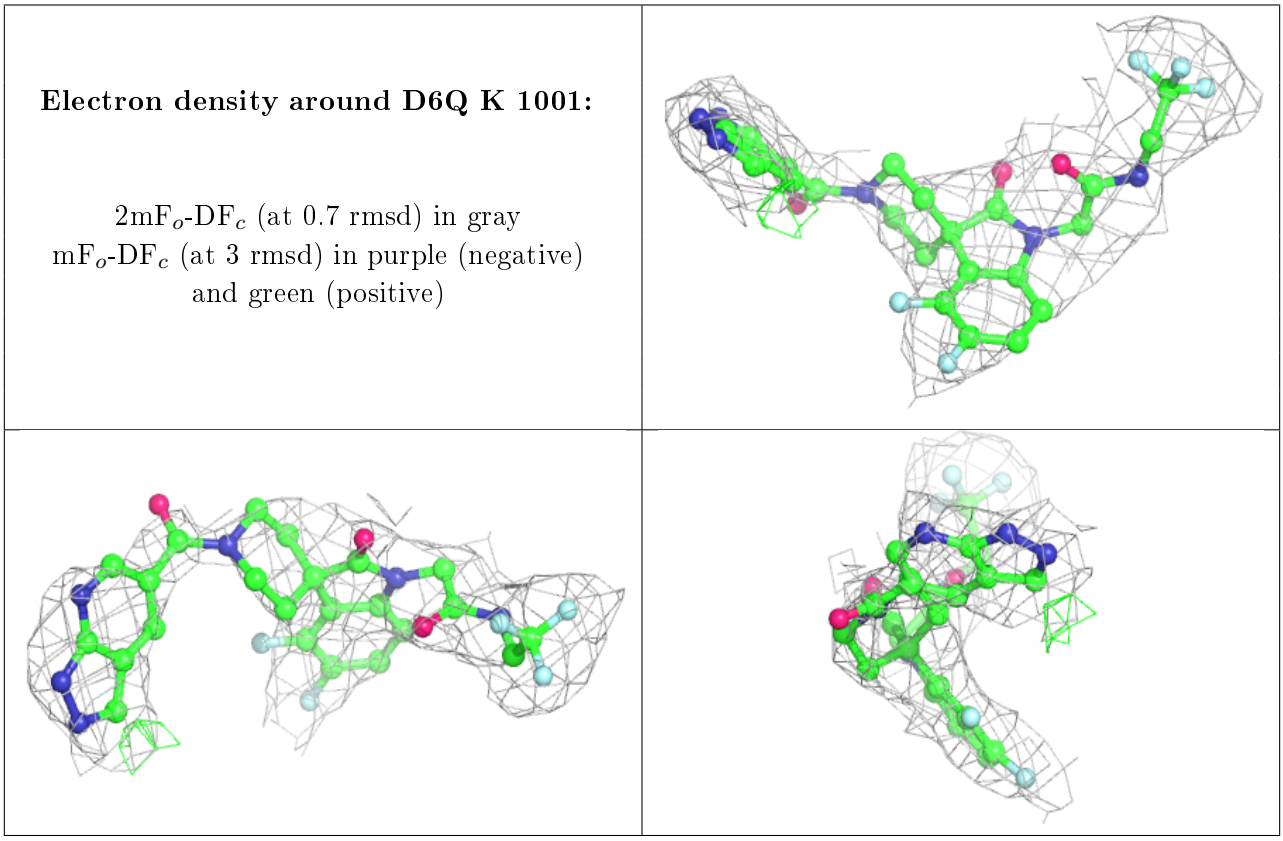
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	D6Q	C	1001	37/37	0.95	0.22	40,60,78,81	0
2	D6Q	L	1001	37/37	0.95	0.24	25,62,79,87	0
2	D6Q	A	1001	37/37	0.96	0.19	26,45,63,64	0
2	D6Q	G	1001	37/37	0.96	0.19	19,43,56,59	0
2	D6Q	J	1001	37/37	0.96	0.21	22,48,63,70	0
2	D6Q	H	1001	37/37	0.97	0.18	9,38,51,57	0
2	D6Q	B	1001	37/37	0.97	0.17	26,43,57,60	0
2	D6Q	E	1001	37/37	0.97	0.17	17,42,61,74	0
2	D6Q	F	1001	37/37	0.97	0.17	17,37,47,54	0
2	D6Q	D	1001	37/37	0.98	0.16	27,39,55,61	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.

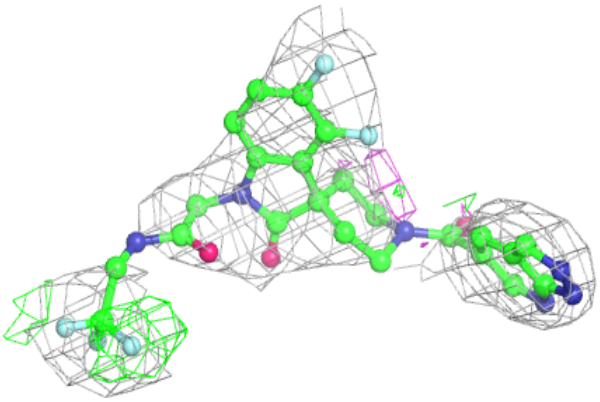
Electron density around D6Q K 1001:

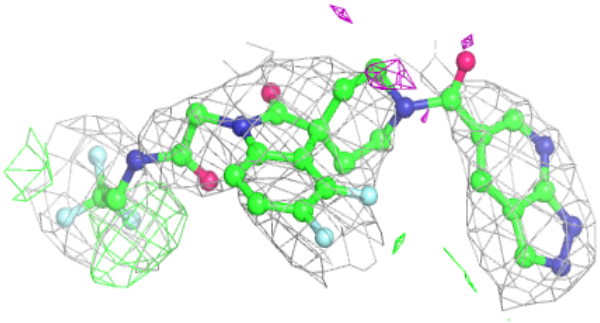
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

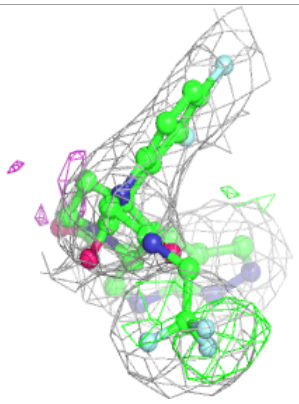


Electron density around D6Q I 1001:

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

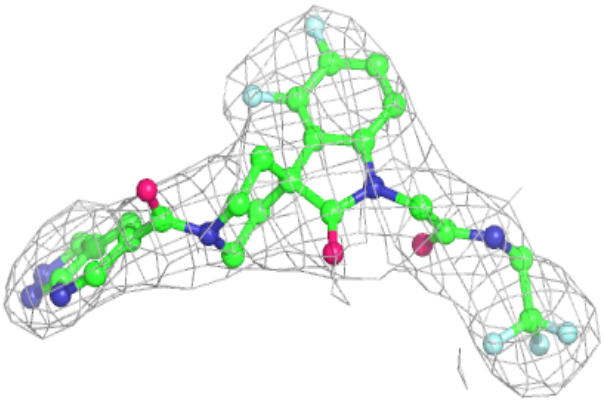


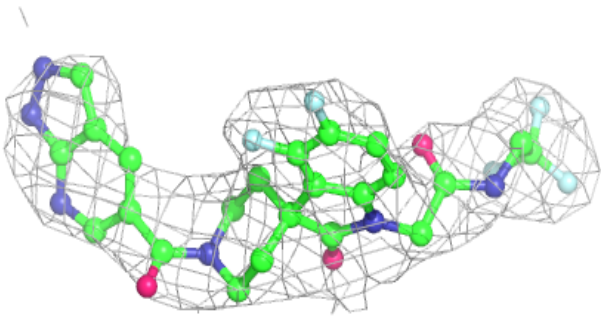


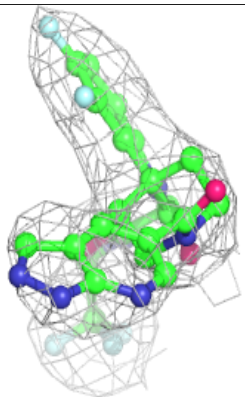


Electron density around D6Q C 1001:

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

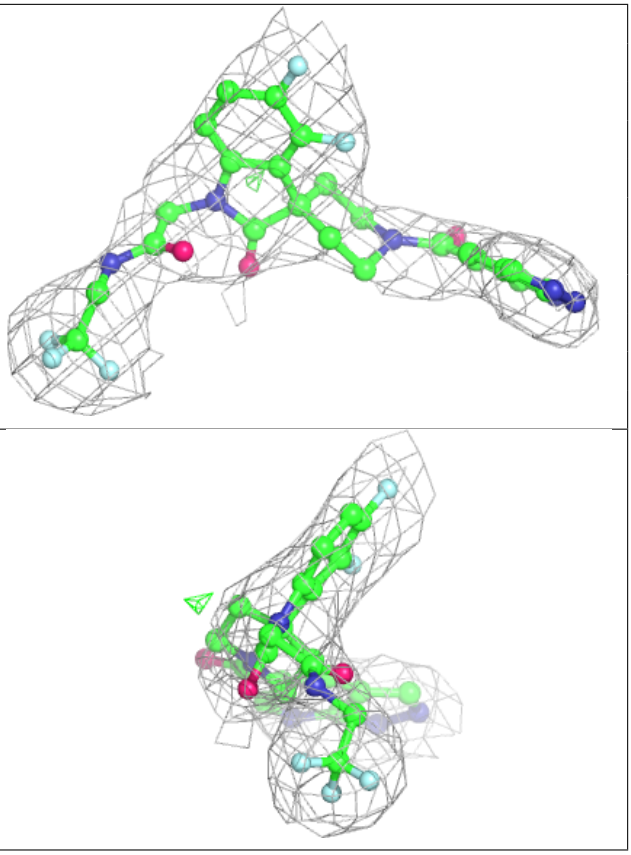






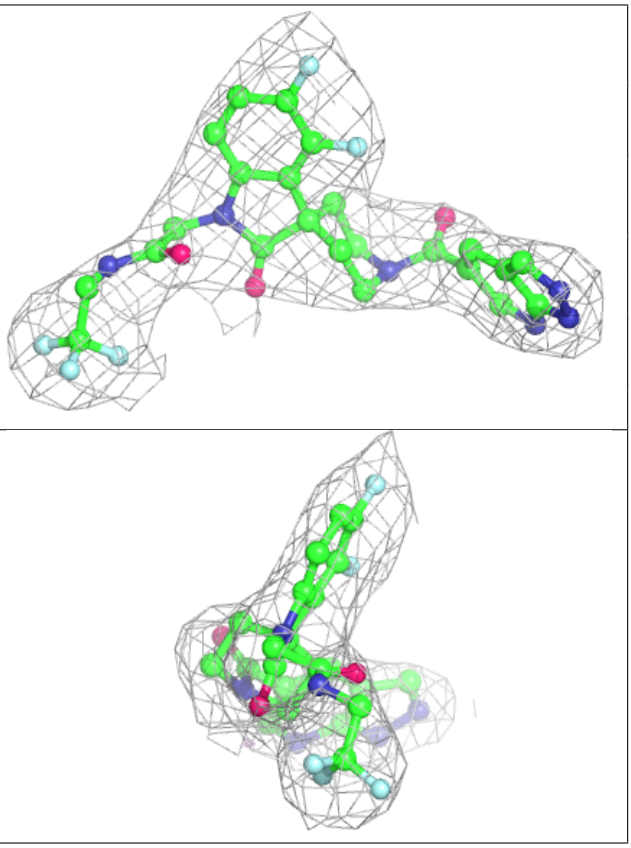
Electron density around D6Q L 1001:

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



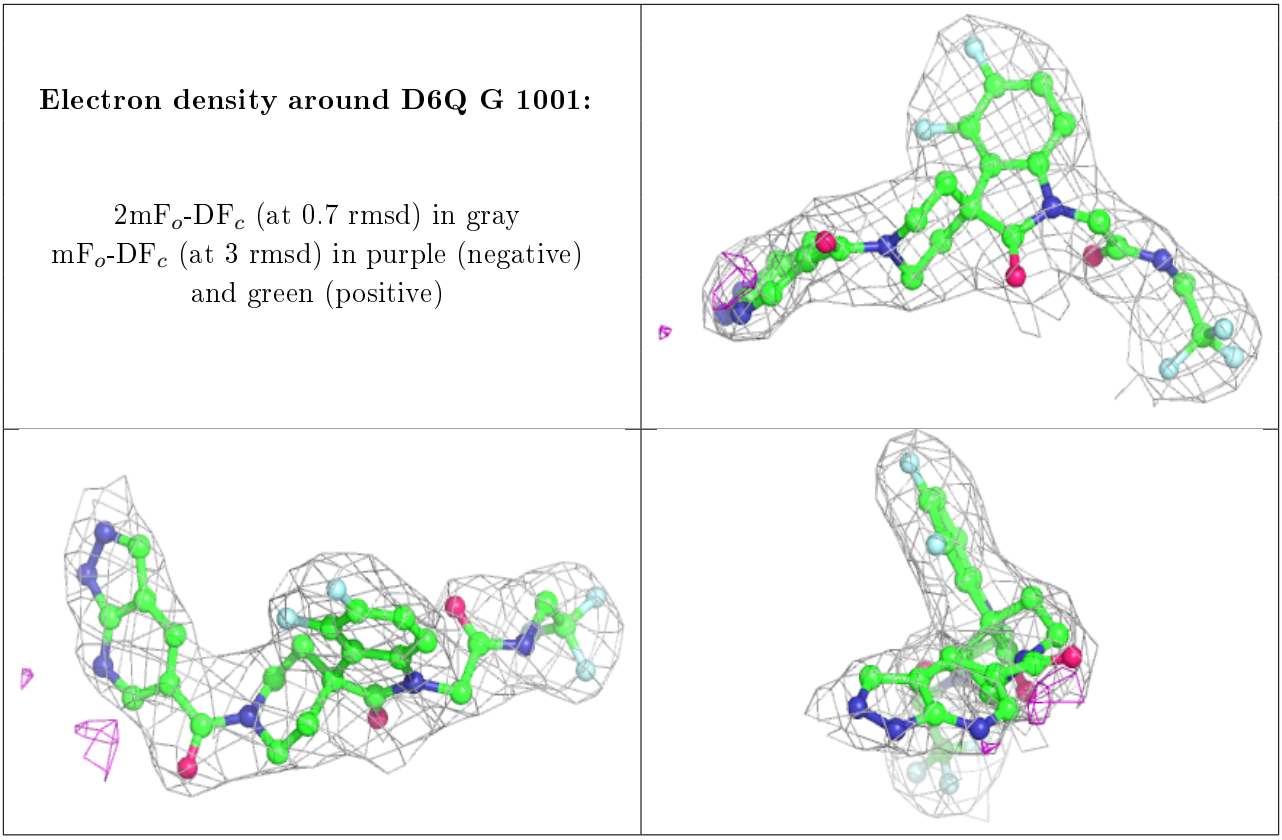
Electron density around D6Q A 1001:

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



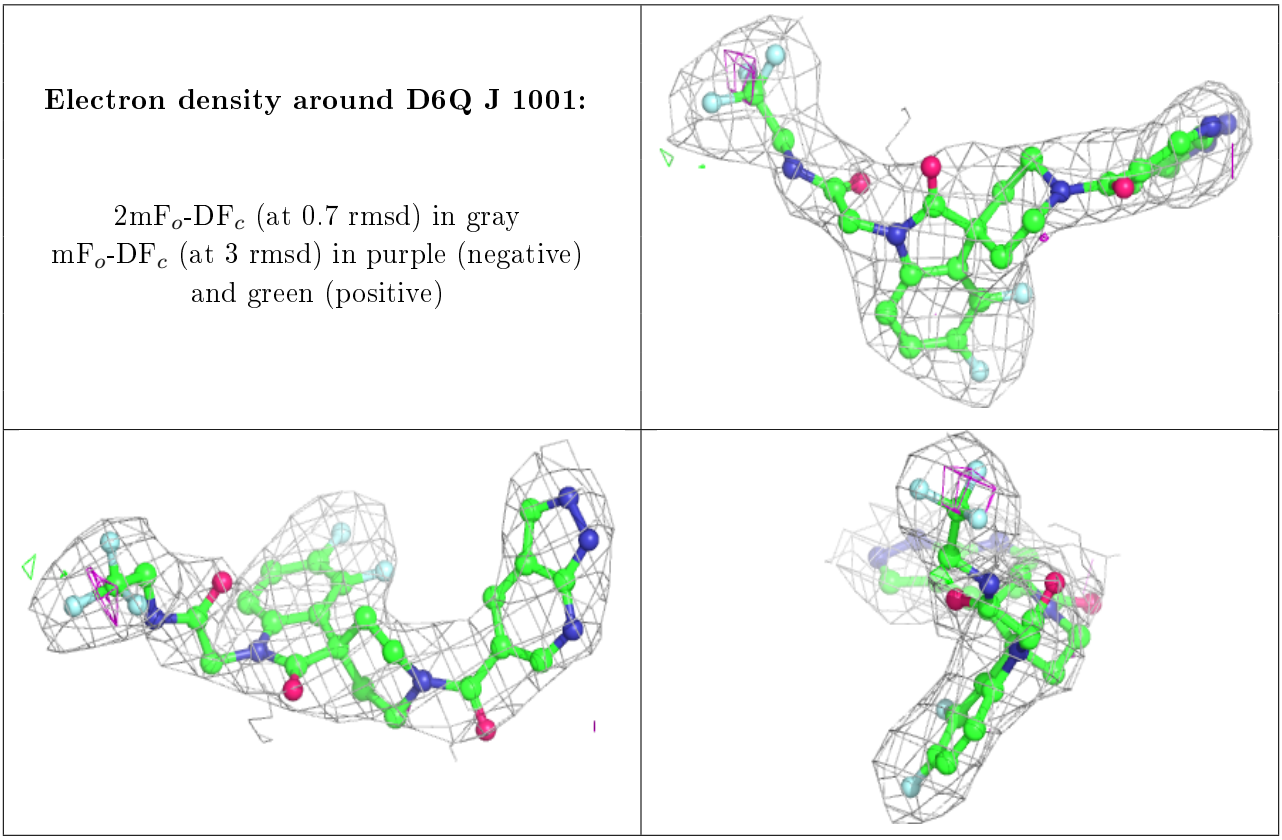
Electron density around D6Q G 1001:

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



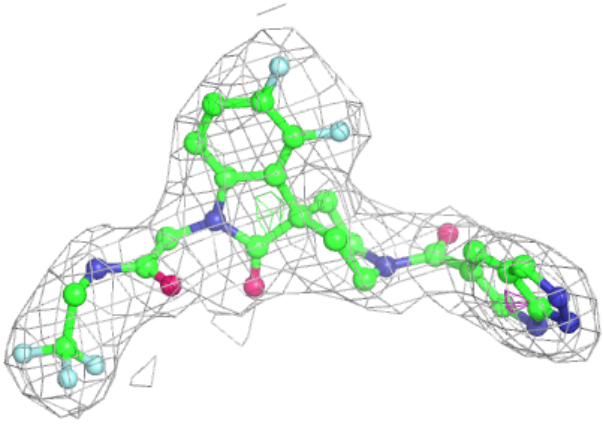
Electron density around D6Q J 1001:

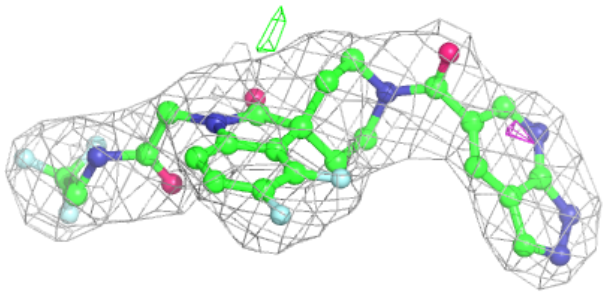
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

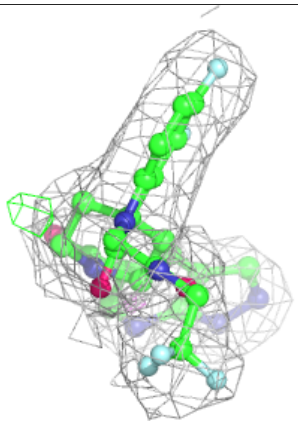


Electron density around D6Q H 1001:

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

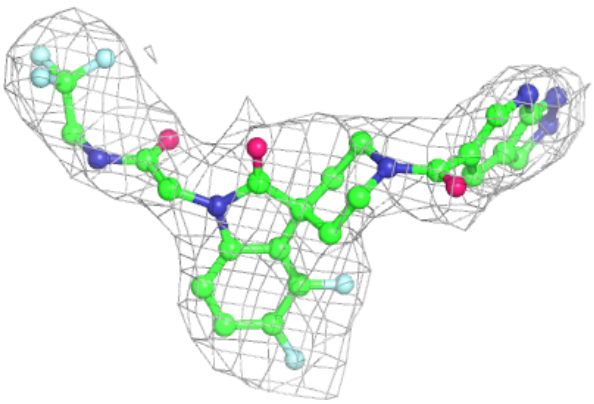


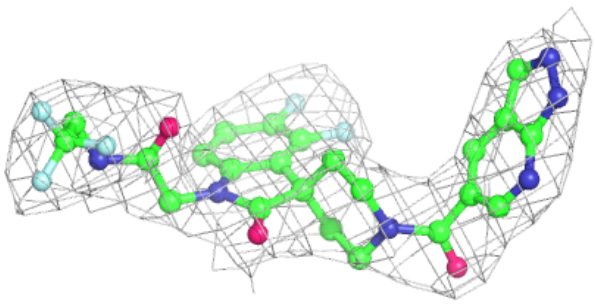


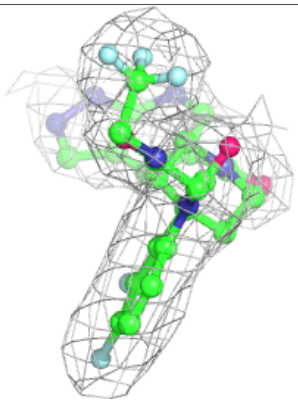


Electron density around D6Q B 1001:

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

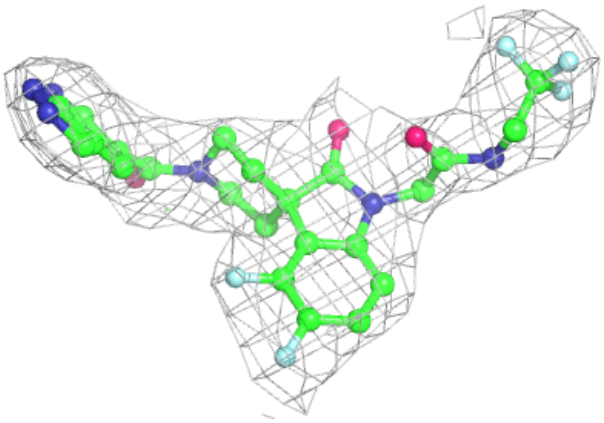


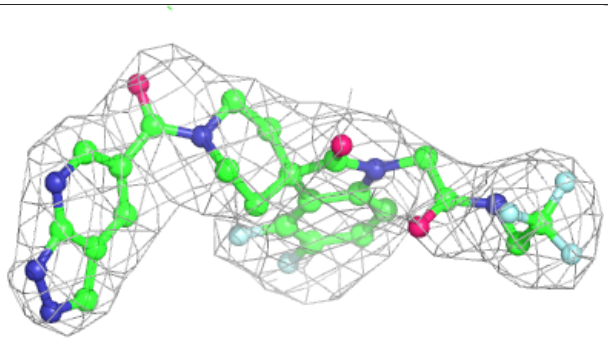


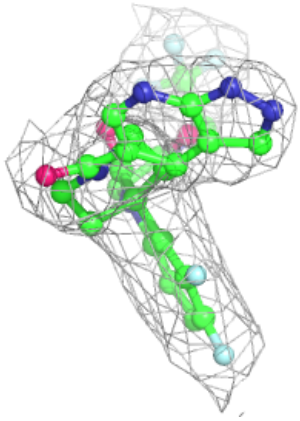


Electron density around D6Q E 1001:

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

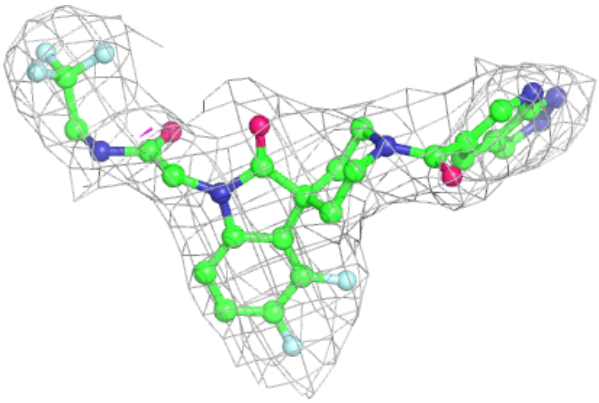


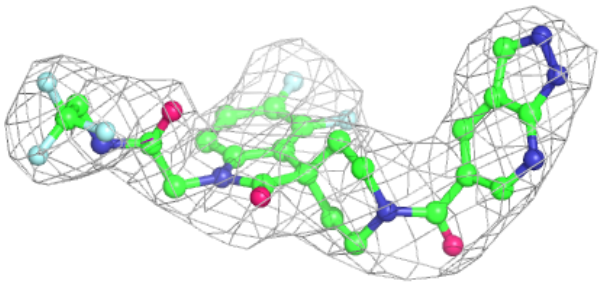


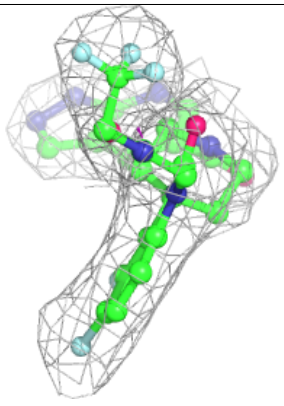


Electron density around D6Q F 1001:

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

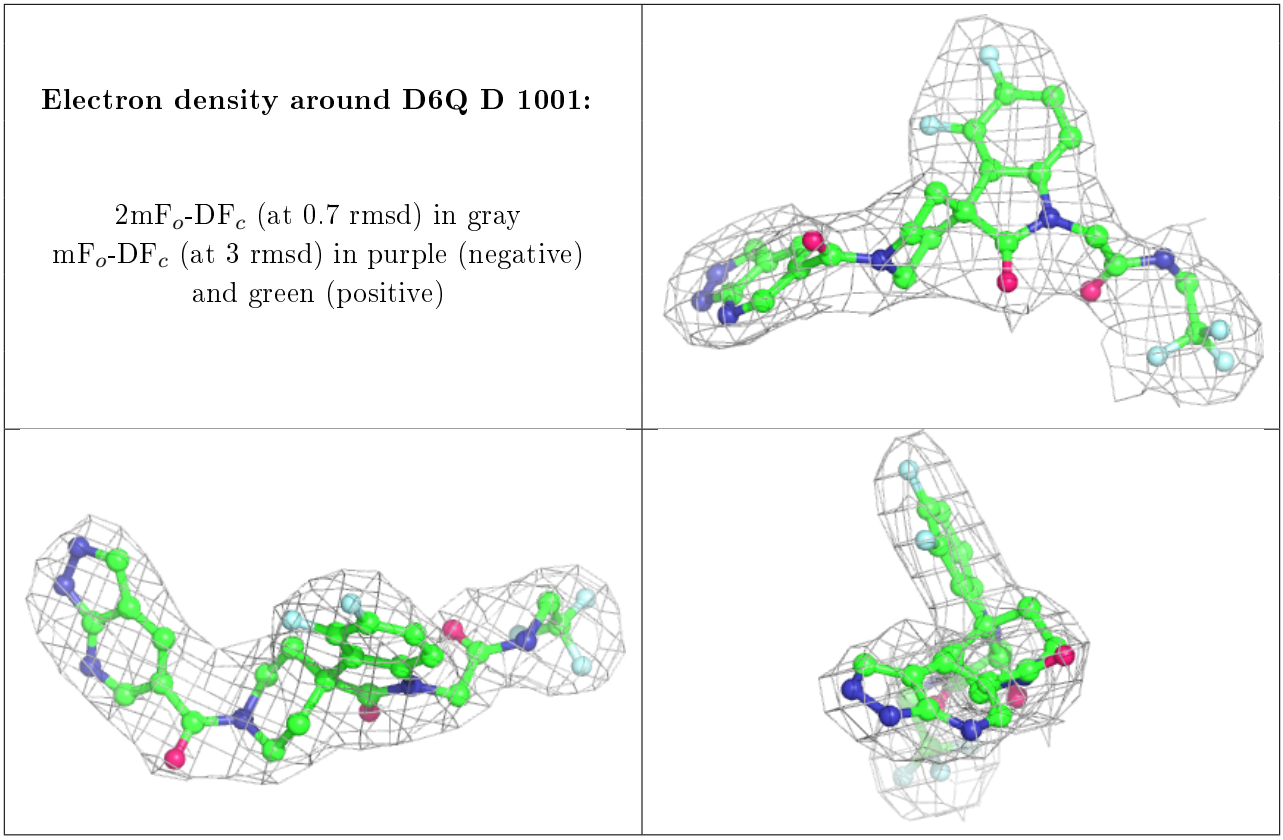






Electron density around D6Q D 1001:

$2mF_o$-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.