Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 06:29 PM EDT

PDB ID	:	4MNE
Title	:	Crystal structure of the BRAF:MEK1 complex
Authors	:	Sudhamsu, J.; Haling, J.R.; Morales, T.; Brandhuber, B.; Hymowitz, S.G.
Deposited on	:	2013-09-10
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

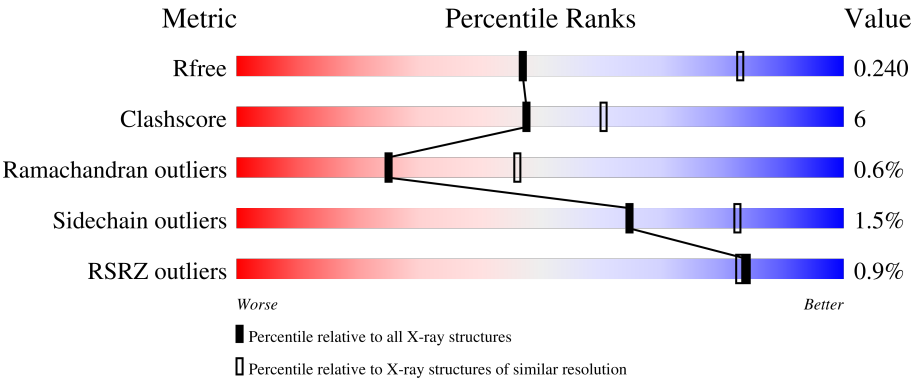
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	70% 13% 16%
1	D	341	69% 13% 16%
1	E	341	68% 15% 16%
1	H	341	65% 16% 19%
2	B	308	75% 12% 12%

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Mol	Chain	Length	Quality of chain
2	C	308	68% 16% 16%
2	F	308	73% 10% 16%
2	G	308	69% 15% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	F	801	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17682 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 Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	3	0
			2254	1442	381	414	17			
1	D	285	Total	C	N	O	S	0	0	0
			2226	1424	377	409	16			
1	E	286	Total	C	N	O	S	0	1	0
			2243	1435	378	413	17			
1	H	275	Total	C	N	O	S	0	0	0
			2146	1374	365	392	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	-	initiating methionine	UNP Q02750
A	394	LEU	-	expression tag	UNP Q02750
A	395	GLU	-	expression tag	UNP Q02750
A	396	HIS	-	expression tag	UNP Q02750
A	397	HIS	-	expression tag	UNP Q02750
A	398	HIS	-	expression tag	UNP Q02750
A	399	HIS	-	expression tag	UNP Q02750
A	400	HIS	-	expression tag	UNP Q02750
A	401	HIS	-	expression tag	UNP Q02750
D	61	MET	-	initiating methionine	UNP Q02750
D	394	LEU	-	expression tag	UNP Q02750
D	395	GLU	-	expression tag	UNP Q02750
D	396	HIS	-	expression tag	UNP Q02750
D	397	HIS	-	expression tag	UNP Q02750
D	398	HIS	-	expression tag	UNP Q02750
D	399	HIS	-	expression tag	UNP Q02750
D	400	HIS	-	expression tag	UNP Q02750
D	401	HIS	-	expression tag	UNP Q02750
E	61	MET	-	initiating methionine	UNP Q02750
E	394	LEU	-	expression tag	UNP Q02750
E	395	GLU	-	expression tag	UNP Q02750

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Chain	Residue	Modelled	Actual	Comment	Reference
E	396	HIS	-	expression tag	UNP Q02750
E	397	HIS	-	expression tag	UNP Q02750
E	398	HIS	-	expression tag	UNP Q02750
E	399	HIS	-	expression tag	UNP Q02750
E	400	HIS	-	expression tag	UNP Q02750
E	401	HIS	-	expression tag	UNP Q02750
H	61	MET	-	initiating methionine	UNP Q02750
H	394	LEU	-	expression tag	UNP Q02750
H	395	GLU	-	expression tag	UNP Q02750
H	396	HIS	-	expression tag	UNP Q02750
H	397	HIS	-	expression tag	UNP Q02750
H	398	HIS	-	expression tag	UNP Q02750
H	399	HIS	-	expression tag	UNP Q02750
H	400	HIS	-	expression tag	UNP Q02750
H	401	HIS	-	expression tag	UNP Q02750

- Molecule 2 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	1	0
			2175	1394	383	385	13			
2	C	260	Total	C	N	O	S	0	1	0
			2096	1348	363	372	13			
2	F	258	Total	C	N	O	S	0	1	0
			2075	1332	361	368	14			
2	G	259	Total	C	N	O	S	0	1	0
			2082	1334	363	372	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	420	MET	-	expression tag	UNP P15056
B	421	ASP	-	expression tag	UNP P15056
B	422	ARG	-	expression tag	UNP P15056
B	423	GLY	-	expression tag	UNP P15056
B	424	SER	-	expression tag	UNP P15056
B	425	HIS	-	expression tag	UNP P15056
B	426	HIS	-	expression tag	UNP P15056
B	427	HIS	-	expression tag	UNP P15056
B	428	HIS	-	expression tag	UNP P15056
B	429	HIS	-	expression tag	UNP P15056
B	430	HIS	-	expression tag	UNP P15056

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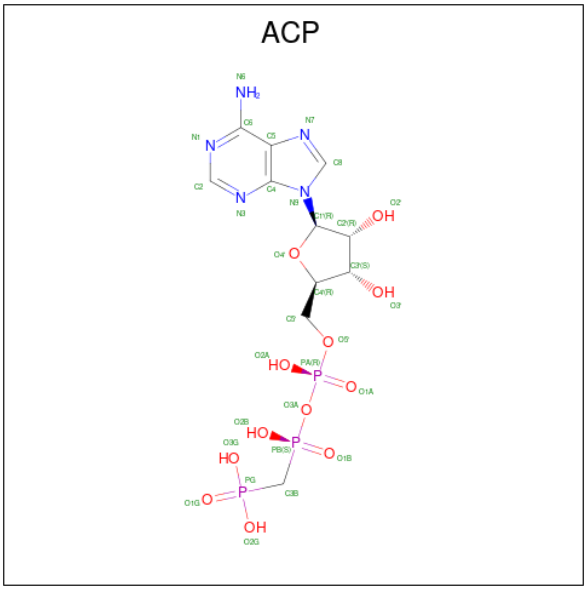
Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLY	-	expression tag	UNP P15056
B	727	LYS	-	expression tag	UNP P15056
C	420	MET	-	expression tag	UNP P15056
C	421	ASP	-	expression tag	UNP P15056
C	422	ARG	-	expression tag	UNP P15056
C	423	GLY	-	expression tag	UNP P15056
C	424	SER	-	expression tag	UNP P15056
C	425	HIS	-	expression tag	UNP P15056
C	426	HIS	-	expression tag	UNP P15056
C	427	HIS	-	expression tag	UNP P15056
C	428	HIS	-	expression tag	UNP P15056
C	429	HIS	-	expression tag	UNP P15056
C	430	HIS	-	expression tag	UNP P15056
C	431	GLY	-	expression tag	UNP P15056
C	727	LYS	-	expression tag	UNP P15056
F	420	MET	-	expression tag	UNP P15056
F	421	ASP	-	expression tag	UNP P15056
F	422	ARG	-	expression tag	UNP P15056
F	423	GLY	-	expression tag	UNP P15056
F	424	SER	-	expression tag	UNP P15056
F	425	HIS	-	expression tag	UNP P15056
F	426	HIS	-	expression tag	UNP P15056
F	427	HIS	-	expression tag	UNP P15056
F	428	HIS	-	expression tag	UNP P15056
F	429	HIS	-	expression tag	UNP P15056
F	430	HIS	-	expression tag	UNP P15056
F	431	GLY	-	expression tag	UNP P15056
F	727	LYS	-	expression tag	UNP P15056
G	420	MET	-	expression tag	UNP P15056
G	421	ASP	-	expression tag	UNP P15056
G	422	ARG	-	expression tag	UNP P15056
G	423	GLY	-	expression tag	UNP P15056
G	424	SER	-	expression tag	UNP P15056
G	425	HIS	-	expression tag	UNP P15056
G	426	HIS	-	expression tag	UNP P15056
G	427	HIS	-	expression tag	UNP P15056
G	428	HIS	-	expression tag	UNP P15056
G	429	HIS	-	expression tag	UNP P15056
G	430	HIS	-	expression tag	UNP P15056
G	431	GLY	-	expression tag	UNP P15056
G	727	LYS	-	expression tag	UNP P15056

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-

letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

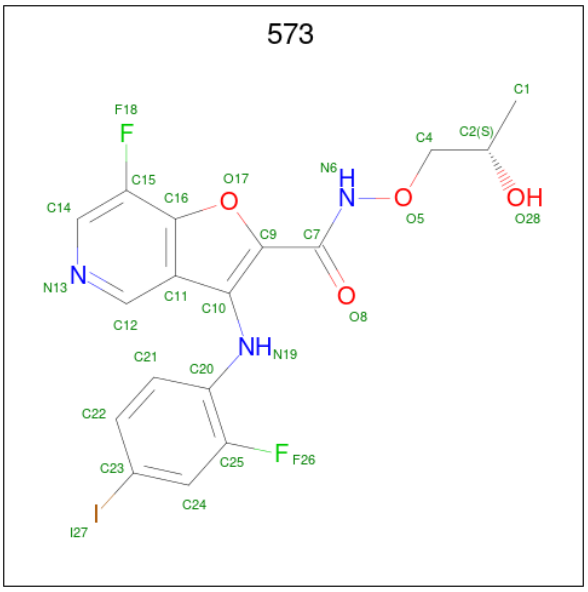


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 11 5 12 3	0	0
3	D	1	Total C N O P 31 11 5 12 3	0	0
3	E	1	Total C N O P 31 11 5 12 3	0	0
3	H	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

- Molecule 5 is 7-fluoro-3-[(2-fluoro-4-iodophenyl)amino]-N-{[(2S)-2-hydroxypropyl]oxy}furo[3,2-c]pyridine-2-carboxamide (three-letter code: 573) (formula: $C_{17}H_{14}F_2IN_3O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	I	N	O	0	0
			27	17	2	1	3	4		
5	D	1	Total	C	F	I	N	O	0	0
			27	17	2	1	3	4		
5	E	1	Total	C	F	I	N	O	0	0
			27	17	2	1	3	4		
5	H	1	Total	C	F	I	N	O	0	0
			27	17	2	1	3	4		
5	H	1	Total	C	F	I	N	O	0	0
			27	17	2	1	3	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	28	Total	O	0	0
			28	28		
7	C	17	Total	O	0	0
			17	17		

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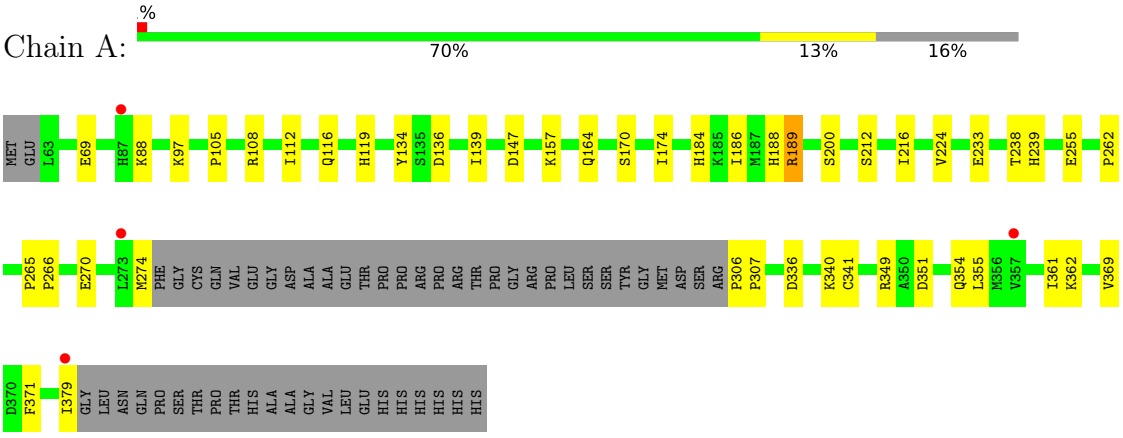
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	19	Total O 19 19	0	0
7	E	8	Total O 8 8	0	0
7	F	18	Total O 18 18	0	0
7	G	12	Total O 12 12	0	0
7	H	7	Total O 7 7	0	0

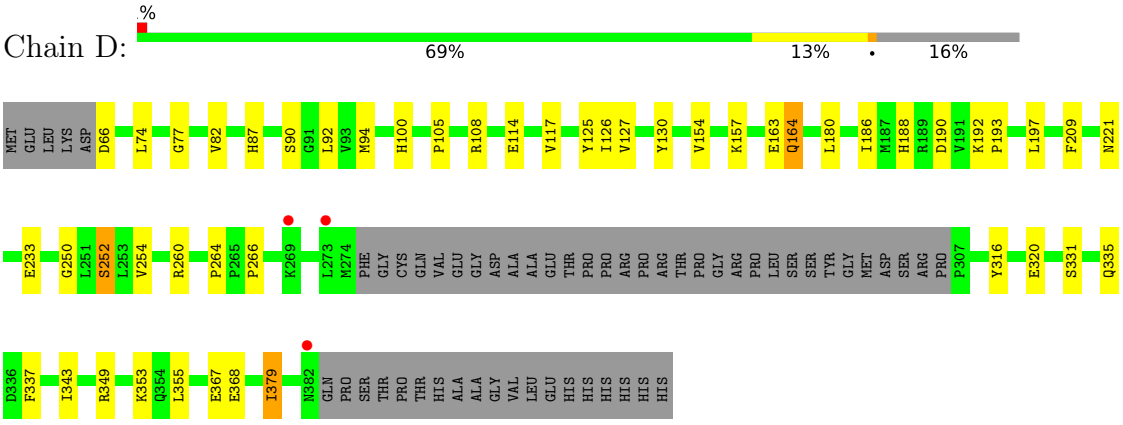
3 Residue-property plots (i)

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

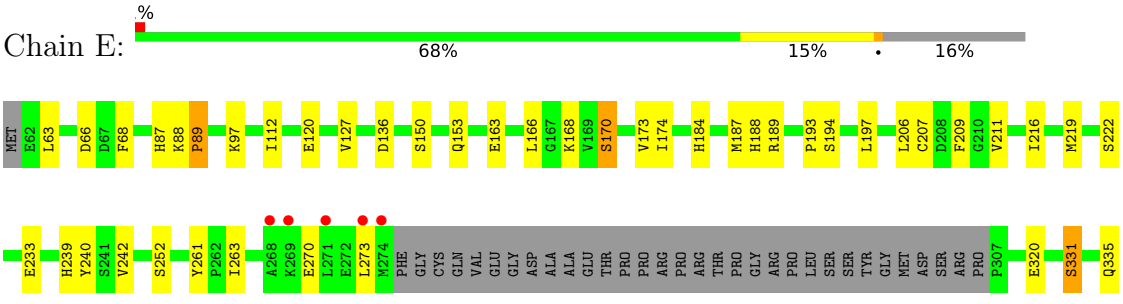
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

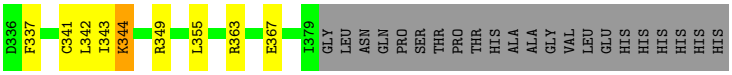


• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1



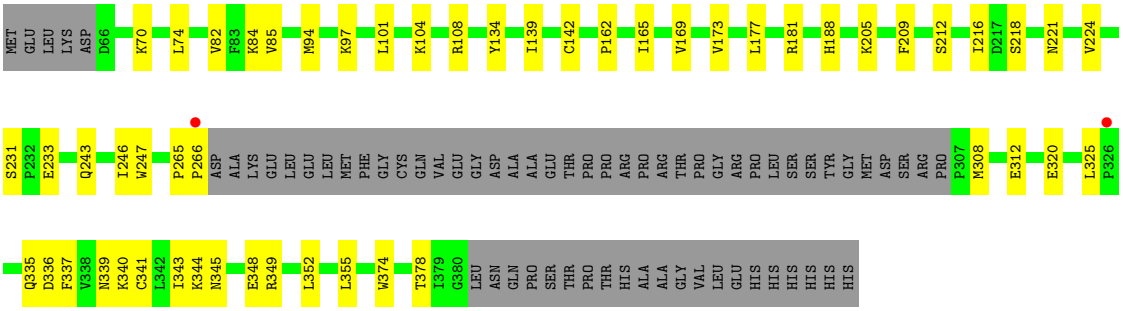
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1





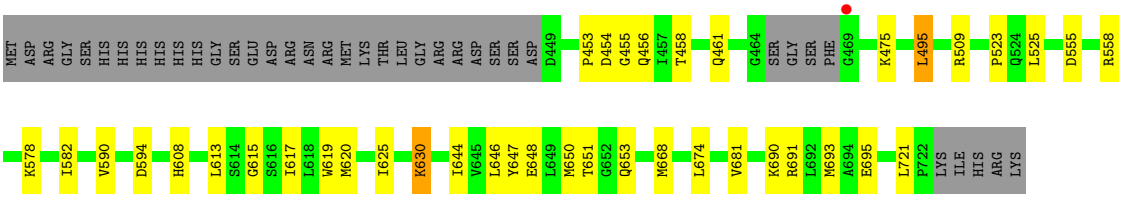
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

Chain H:



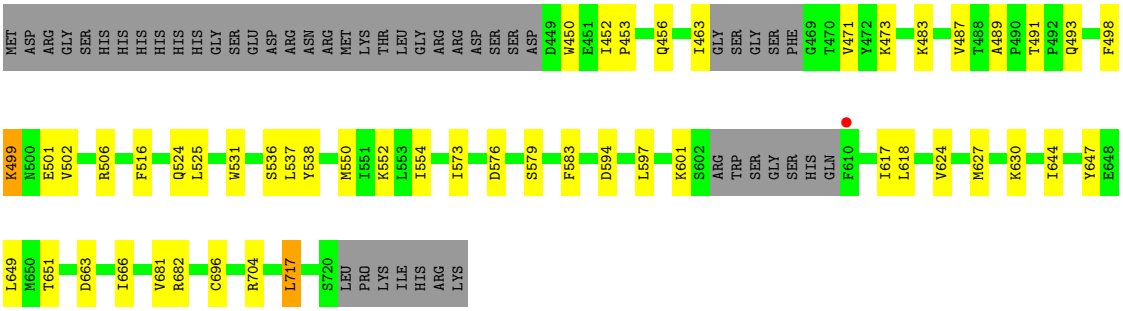
• Molecule 2: Serine/threonine-protein kinase B-raf

Chain B:



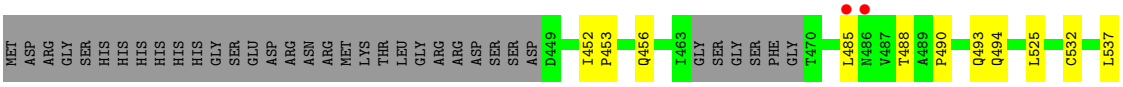
• Molecule 2: Serine/threonine-protein kinase B-raf

Chain C:

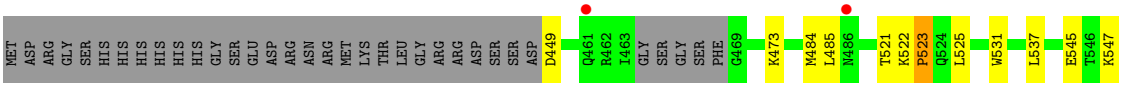


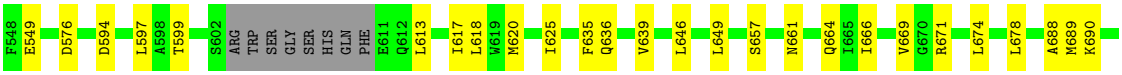
• Molecule 2: Serine/threonine-protein kinase B-raf

Chain F:



• Molecule 2: Serine/threonine-protein kinase B-raf





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.50Å 135.66Å 256.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.85 39.59 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.59-2.85) 94.5 (39.59-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.185 , 0.240 0.185 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17682	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: CL, ACP, 573, MG

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	0.42	0/2308	0.58	0/3112
1	D	0.44	0/2272	0.59	0/3063
1	E	0.42	0/2292	0.56	0/3089
1	H	0.38	0/2192	0.57	0/2956
2	B	0.46	0/2226	0.62	0/3004
2	C	0.45	0/2143	0.62	0/2890
2	F	0.45	0/2120	0.61	0/2860
2	G	0.45	0/2127	0.62	0/2869
All	All	0.43	0/17680	0.60	0/23843

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	2254	0	2277	29	0
1	D	2226	0	2254	28	0
1	E	2243	0	2273	32	0
1	H	2146	0	2172	33	0
2	B	2175	0	2217	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2096	0	2140	29	0
2	F	2075	0	2129	17	0
2	G	2082	0	2128	26	0
3	A	31	0	14	0	0
3	D	31	0	14	1	0
3	E	31	0	14	1	0
3	H	31	0	14	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
5	A	27	0	14	2	0
5	D	27	0	14	0	0
5	E	27	0	14	1	0
5	H	54	0	28	6	0
6	F	1	0	0	0	0
7	A	12	0	0	0	0
7	B	28	0	0	0	0
7	C	17	0	0	0	0
7	D	19	0	0	0	0
7	E	8	0	0	0	0
7	F	18	0	0	1	0
7	G	12	0	0	0	0
7	H	7	0	0	0	0
All	All	17682	0	17716	216	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 6.

All (216) 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:H:320:GLU:O	1:H:344:LYS:NZ	1.91	1.04
1:E:66:ASP:O	1:E:88:LYS:NZ	1.94	0.99
2:B:555:ASP:OD1	2:B:558[A]:ARG:NH1	2.00	0.93
1:D:157:LYS:HE3	1:D:379:ILE:HG23	1.53	0.91
1:E:163:GLU:OE2	1:E:331:SER:HB3	1.76	0.86
1:A:336:ASP:OD2	1:A:340:LYS:NZ	2.09	0.84
1:D:87:HIS:ND1	1:D:90:SER:OG	2.12	0.83
2:C:487:VAL:HG12	2:C:489:ALA:H	1.50	0.77
2:C:491:THR:HG22	2:C:493:GLN:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:HG3	1:A:88:LYS:HD2	1.69	0.75
1:D:77:GLY:HA3	3:D:901:ACP:H3B1	1.72	0.71
1:D:163:GLU:OE2	1:D:331:SER:HB3	1.93	0.69
1:E:189:ARG:NE	1:E:240:TYR:OH	2.26	0.69
1:D:193:PRO:HD3	1:D:252:SER:HB3	1.75	0.68
1:H:337:PHE:CE1	1:H:355:LEU:HD22	2.30	0.66
1:D:233:GLU:OE2	1:D:349:ARG:NH2	2.29	0.66
1:H:108:ARG:HD2	1:H:134:TYR:CG	2.32	0.65
1:H:341:CYS:O	1:H:349:ARG:HD2	1.96	0.65
1:A:164:GLN:HG2	1:A:369:VAL:HG11	1.78	0.65
2:F:555:ASP:OD1	2:F:558:ARG:NH1	2.29	0.64
1:E:188:HIS:CD2	1:E:209:PHE:HB3	2.32	0.63
2:F:576:ASP:HB2	2:F:597:LEU:HD12	1.81	0.61
2:C:576:ASP:HB2	2:C:597:LEU:HD12	1.83	0.61
2:F:709:GLN:OE1	7:F:916:HOH:O	2.16	0.61
1:H:82:VAL:HG22	1:H:97:LYS:HB2	1.83	0.60
1:D:105:PRO:HA	1:D:108:ARG:HG2	1.83	0.60
2:B:458:THR:HB	2:B:475:LYS:HB2	1.82	0.59
2:G:646:LEU:HD22	2:G:689:MET:HE1	1.83	0.59
1:E:63:LEU:HD13	1:E:68:PHE:HZ	1.67	0.59
2:C:663:ASP:HA	2:C:666:ILE:HD12	1.85	0.59
1:H:325:LEU:HD12	1:H:335:GLN:HA	1.83	0.59
1:D:316:TYR:CD1	1:D:320:GLU:HG3	2.38	0.59
1:A:341:CYS:O	1:A:349:ARG:HD2	2.03	0.58
2:C:717:LEU:O	2:C:717:LEU:HD22	2.02	0.58
2:C:502:VAL:O	2:C:506:ARG:HG3	2.04	0.57
5:H:904:573:H11	5:H:904:573:C12	2.35	0.57
1:E:233:GLU:HG3	1:E:239:HIS:HB2	1.85	0.57
1:E:320:GLU:O	1:E:344:LYS:NZ	2.38	0.57
1:A:97:LYS:NZ	5:A:903:573:H5	2.20	0.57
2:G:688:ALA:HB3	2:G:717:LEU:HG	1.87	0.56
2:B:681:VAL:HG21	2:B:690:LYS:HD2	1.88	0.56
2:G:636:GLN:NE2	2:G:706:LEU:HD21	2.21	0.56
1:D:180:LEU:HD22	1:D:186:ILE:HD11	1.88	0.56
1:H:336:ASP:O	1:H:340:LYS:HG2	2.06	0.55
2:F:649:LEU:O	2:F:682:ARG:NH1	2.39	0.55
1:E:341:CYS:O	1:E:349:ARG:HD2	2.06	0.55
1:E:153:GLN:NE2	3:E:901:ACP:O2'	2.40	0.54
1:H:101:LEU:HD12	1:H:139:ILE:HG12	1.89	0.54
1:H:97:LYS:HZ2	5:H:903:573:H5	1.72	0.54
2:G:617:ILE:HG22	1:H:224:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:MET:CE	1:H:312:GLU:HB3	2.38	0.54
1:H:212:SER:O	5:H:903:573:H9	2.08	0.53
2:B:582:ILE:HG23	2:B:590:VAL:HG13	1.90	0.53
2:F:613:LEU:HD11	2:F:620:MET:HE3	1.91	0.53
1:H:74:LEU:HD21	1:H:84:LYS:HB2	1.91	0.53
2:B:650:MET:HB2	2:B:693:MET:HE1	1.92	0.52
2:B:454:ASP:OD1	2:B:455:GLY:N	2.43	0.52
2:B:461:GLN:OE1	2:B:461:GLN:N	2.37	0.52
2:C:453:PRO:HG2	2:C:456:GLN:NE2	2.24	0.52
1:A:224:VAL:HG22	2:B:617:ILE:HG22	1.91	0.52
2:C:498:PHE:CG	2:C:525:LEU:HD13	2.46	0.51
1:D:260:ARG:NH1	1:D:266:PRO:HG3	2.25	0.51
1:D:188:HIS:CD2	1:D:209:PHE:HB3	2.45	0.51
2:B:620:MET:HE1	2:B:625:ILE:HG12	1.93	0.51
1:A:105:PRO:HA	1:A:108:ARG:HG2	1.92	0.50
2:B:613:LEU:HD21	2:B:620:MET:HE3	1.92	0.50
2:G:473:LYS:HD2	2:G:531:TRP:CZ2	2.45	0.50
5:H:904:573:H11	5:H:904:573:H8	1.93	0.50
2:G:617:ILE:HG13	2:G:618:LEU:HD23	1.94	0.50
1:H:97:LYS:NZ	5:H:903:573:H5	2.27	0.50
1:E:363:ARG:O	1:E:367:GLU:HG3	2.12	0.49
1:H:308:MET:HE3	1:H:312:GLU:HB3	1.93	0.49
2:G:669:VAL:HG23	2:G:674:LEU:HD23	1.94	0.49
2:G:545:GLU:OE2	1:H:104:LYS:HD3	2.13	0.49
1:D:337:PHE:CE1	1:D:355:LEU:HD22	2.47	0.49
2:B:608:HIS:HB2	2:B:630:LYS:HE2	1.93	0.49
1:D:250:GLY:O	1:D:254:VAL:HG23	2.13	0.49
2:F:493:GLN:HG2	2:F:494:GLN:N	2.28	0.49
1:H:108:ARG:HD2	1:H:134:TYR:CD2	2.48	0.49
1:D:74:LEU:HD12	1:D:82:VAL:HG12	1.94	0.49
2:C:550:MET:O	2:C:554:ILE:HG13	2.13	0.48
2:G:449:ASP:N	2:G:449:ASP:OD1	2.46	0.48
1:A:233:GLU:HG3	1:A:239:HIS:HB3	1.95	0.48
2:C:538:TYR:HB2	2:C:579:SER:HB3	1.95	0.48
1:A:188:HIS:O	1:A:189:ARG:HB2	2.13	0.48
2:B:613:LEU:HD11	2:B:620:MET:HE3	1.94	0.48
2:G:521:THR:HA	2:G:525:LEU:HD23	1.95	0.48
2:B:509:ARG:HD3	2:C:516:PHE:O	2.14	0.48
2:B:620:MET:HB3	2:B:620:MET:HE2	1.65	0.47
2:G:537:LEU:HD21	2:G:649:LEU:HD21	1.96	0.47
2:B:691:ARG:O	2:B:695:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:PRO:HB2	1:H:165:ILE:HG12	1.96	0.47
1:H:345:ASN:HB3	1:H:348:GLU:HB3	1.97	0.47
1:A:212:SER:O	1:A:216:ILE:HG13	2.14	0.47
2:F:575:ARG:HD2	2:F:633:TYR:CG	2.49	0.47
1:E:219:MET:O	1:E:222:SER:OG	2.32	0.47
1:A:255:GLU:HB2	1:A:262:PRO:HD3	1.97	0.47
2:B:651:THR:HG22	2:B:681:VAL:HA	1.97	0.47
1:H:169:VAL:O	1:H:173:VAL:HG23	2.15	0.46
1:A:184:HIS:O	1:A:186:ILE:HG23	2.14	0.46
2:F:453:PRO:HG2	2:F:456:GLN:NE2	2.31	0.46
1:A:157:LYS:NZ	1:A:379:ILE:HA	2.30	0.46
1:E:170:SER:O	1:E:174:ILE:HG13	2.15	0.46
1:E:337:PHE:CE1	1:E:355:LEU:HD22	2.50	0.46
1:A:170:SER:O	1:A:174:ILE:HG13	2.15	0.46
2:G:522:LYS:HA	2:G:523:PRO:C	2.36	0.46
2:G:613:LEU:HD21	2:G:620:MET:HE3	1.97	0.46
2:C:573:ILE:HD11	2:C:601:LYS:HD3	1.96	0.46
1:E:343:ILE:O	1:E:349:ARG:HD3	2.16	0.46
2:B:495:LEU:HD23	2:B:525:LEU:HD11	1.98	0.46
1:D:105:PRO:HG3	1:D:108:ARG:NH1	2.31	0.46
1:H:94:MET:CE	1:H:142:CYS:HB3	2.46	0.46
2:C:483:LYS:NZ	2:C:501:GLU:OE2	2.44	0.46
2:C:624:VAL:O	2:C:627:MET:HG2	2.16	0.45
1:A:97:LYS:HZ3	5:A:903:573:H5	1.79	0.45
1:D:343:ILE:O	1:D:349:ARG:NH1	2.49	0.45
1:D:331:SER:O	1:D:335:GLN:HG3	2.15	0.45
1:E:127:VAL:HG21	1:E:207[A]:CYS:HB3	1.99	0.45
1:A:224:VAL:HG22	2:B:617:ILE:CG2	2.47	0.45
1:E:270:GLU:HA	1:E:273:LEU:HD12	1.98	0.45
2:B:644:ILE:O	2:B:648:GLU:HG3	2.17	0.45
1:D:90:SER:HB2	1:D:92:LEU:H	1.82	0.45
1:A:134:TYR:HB2	1:A:139:ILE:HD13	1.98	0.45
1:H:173:VAL:O	1:H:177:LEU:HG	2.17	0.45
1:H:231:SER:HA	1:H:247:TRP:CD1	2.52	0.45
1:H:374:TRP:O	1:H:378:THR:HG23	2.17	0.45
2:C:649:LEU:O	2:C:682:ARG:NH1	2.50	0.45
2:C:463:ILE:HG12	2:C:471:VAL:O	2.17	0.45
2:G:635:PHE:O	2:G:639:VAL:HG23	2.16	0.44
1:E:120:GLU:O	1:E:184:HIS:HE1	2.00	0.44
5:H:904:573:H8	5:H:904:573:C21	2.48	0.44
1:A:108:ARG:O	1:A:112:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LYS:HE2	5:E:903:573:H5	1.99	0.44
1:H:181:ARG:HE	1:H:352:LEU:CD1	2.29	0.44
2:C:651:THR:HG22	2:C:681:VAL:HA	1.99	0.44
1:H:233:GLU:OE2	1:H:349:ARG:NH2	2.51	0.44
2:B:646:LEU:HD23	2:B:646:LEU:HA	1.80	0.44
1:E:261:TYR:CE2	1:E:263:ILE:HB	2.53	0.44
2:C:630:LYS:HE2	2:F:627:MET:O	2.18	0.44
2:B:668:MET:HB3	2:B:674:LEU:HB2	1.99	0.44
2:C:696:CYS:O	2:C:704:ARG:HD3	2.18	0.44
1:A:224:VAL:HG23	2:B:615:GLY:O	2.18	0.43
2:C:536:SER:HA	2:C:583[A]:PHE:HA	1.99	0.43
2:B:453:PRO:HG2	2:B:456:GLN:NE2	2.33	0.43
1:D:188:HIS:HA	1:D:209:PHE:HB2	2.00	0.43
2:G:678:LEU:O	2:G:690:LYS:NZ	2.52	0.43
1:A:369:VAL:O	1:A:371:PHE:N	2.51	0.43
1:E:187:MET:HB3	1:E:242:VAL:HG22	2.00	0.43
2:G:613:LEU:HD11	2:G:620:MET:HE3	2.00	0.43
2:C:552:LYS:HD2	2:C:552:LYS:HA	1.69	0.43
1:D:190:ASP:OD2	1:D:192:LYS:HE2	2.17	0.43
1:E:173:VAL:HG22	1:E:206:LEU:HD21	2.00	0.43
2:G:547:LYS:HA	2:G:547:LYS:HD3	1.59	0.43
1:A:265:PRO:HA	1:A:266:PRO:HD3	1.90	0.43
1:E:127:VAL:HG21	1:E:197:LEU:HD12	2.00	0.43
1:E:166:LEU:HD23	1:E:166:LEU:HA	1.80	0.43
2:F:620:MET:HE2	2:F:620:MET:HB3	1.69	0.43
2:F:646:LEU:HD23	2:F:646:LEU:HA	1.84	0.43
1:A:270:GLU:O	1:A:274:MET:HG3	2.19	0.43
2:F:539:HIS:HA	2:F:543:ILE:HG12	2.01	0.43
2:G:701:ARG:O	2:G:704:ARG:HB2	2.18	0.43
1:E:233:GLU:OE2	1:E:349:ARG:NH2	2.52	0.43
2:F:661:ASN:HB3	2:F:664:GLN:HB3	2.00	0.43
1:D:114:GLU:O	1:D:117:VAL:HG13	2.19	0.43
1:H:339:ASN:O	1:H:343:ILE:HG13	2.19	0.43
2:B:578:LYS:HB2	2:B:619:TRP:CE2	2.54	0.42
1:D:260:ARG:NH2	1:D:264:PRO:O	2.34	0.42
1:H:188:HIS:CD2	1:H:209:PHE:HB3	2.54	0.42
1:A:105:PRO:O	1:A:108:ARG:HG2	2.18	0.42
2:C:499:LYS:HE3	2:C:499:LYS:HB2	1.78	0.42
2:G:695:GLU:O	2:G:698:LYS:HG2	2.18	0.42
1:H:212:SER:O	1:H:216:ILE:HG13	2.19	0.42
2:B:647:TYR:O	2:B:651:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:VAL:HG21	1:D:197:LEU:HD12	2.00	0.42
1:A:362:LYS:HB3	1:A:362:LYS:HE2	1.83	0.42
1:D:125:TYR:O	1:D:126:ILE:HD13	2.20	0.42
1:E:150:SER:HB2	1:E:194:SER:HA	2.01	0.42
1:E:193:PRO:HD3	1:E:252:SER:HB3	2.02	0.42
2:F:488:THR:O	2:F:490:PRO:HD3	2.18	0.42
2:G:576:ASP:HB2	2:G:597:LEU:HD12	2.02	0.42
1:E:87:HIS:CD2	1:E:89:PRO:HD2	2.54	0.42
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.86	0.42
2:F:485:LEU:HD22	2:F:525:LEU:HD12	2.01	0.42
2:G:485:LEU:HD12	2:G:485:LEU:O	2.20	0.42
2:G:716:LEU:O	2:G:719:ARG:HG2	2.20	0.42
2:G:693:MET:HG2	2:G:697:LEU:HD12	2.02	0.42
1:A:147:ASP:OD1	1:A:200:SER:OG	2.36	0.41
2:C:536:SER:HA	2:C:583[B]:PHE:HA	2.01	0.41
1:A:116:GLN:HG3	1:A:119:HIS:HD2	1.85	0.41
1:D:66:ASP:N	1:D:66:ASP:OD1	2.53	0.41
1:D:154:VAL:HG22	1:D:379:ILE:HD11	2.02	0.41
1:H:181:ARG:HE	1:H:352:LEU:HD12	1.85	0.41
2:C:473:LYS:HD2	2:C:531:TRP:CZ2	2.55	0.41
2:C:644:ILE:O	2:C:647:TYR:HB3	2.21	0.41
1:E:168:LYS:HA	1:E:168:LYS:HD3	1.88	0.41
1:A:355:LEU:O	1:A:361:ILE:HG13	2.21	0.41
1:H:265:PRO:HA	1:H:266:PRO:HD3	1.79	0.41
1:A:351:ASP:OD1	1:A:354:GLN:HG3	2.21	0.41
2:C:617:ILE:HG13	2:C:618:LEU:N	2.36	0.41
1:E:331:SER:O	1:E:335:GLN:HG3	2.21	0.41
1:H:243:GLN:HA	1:H:246:ILE:HD12	2.03	0.41
2:C:452:ILE:HA	2:C:453:PRO:HD2	1.96	0.41
1:D:94:MET:HE2	1:D:130:TYR:CD2	2.56	0.41
1:E:189:ARG:HD2	1:E:216:ILE:HD13	2.03	0.41
2:G:484:MET:HB3	2:G:484:MET:HE2	2.00	0.41
1:E:342:LEU:HD23	1:E:342:LEU:HA	1.94	0.41
2:G:625:ILE:HG23	2:G:666:ILE:HG23	2.03	0.41
1:E:112:ILE:HD13	1:E:112:ILE:HA	1.82	0.40
2:G:661:ASN:HB3	2:G:664:GLN:HB3	2.02	0.40
2:C:537:LEU:HD12	2:C:537:LEU:HA	1.85	0.40
2:F:452:ILE:HA	2:F:453:PRO:HD2	1.83	0.40
2:F:537:LEU:HD21	2:F:649:LEU:HD21	2.03	0.40
1:D:164:GLN:HG3	1:D:367:GLU:OE1	2.21	0.40
2:B:495:LEU:HD23	2:B:495:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:ARG:HD2	2:C:450:TRP:CZ3	2.56	0.40
1:H:70:LYS:HA	1:H:85:VAL:HG12	2.04	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	285/341 (84%)	269 (94%)	14 (5%)	2 (1%)	22	42
1	D	281/341 (82%)	266 (95%)	13 (5%)	2 (1%)	22	42
1	E	283/341 (83%)	262 (93%)	20 (7%)	1 (0%)	34	56
1	H	271/341 (80%)	262 (97%)	8 (3%)	1 (0%)	34	56
2	B	267/308 (87%)	254 (95%)	11 (4%)	2 (1%)	22	42
2	C	255/308 (83%)	242 (95%)	12 (5%)	1 (0%)	34	56
2	F	253/308 (82%)	243 (96%)	9 (4%)	1 (0%)	34	56
2	G	254/308 (82%)	236 (93%)	15 (6%)	3 (1%)	13	28
All	All	2149/2596 (83%)	2034 (95%)	102 (5%)	13 (1%)	25	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
2	C	594	ASP
1	D	221	ASN
1	A	189	ARG
2	B	594	ASP
1	D	379	ILE
1	H	221	ASN
2	F	594	ASP

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Mol	Chain	Res	Type
2	G	594	ASP
2	G	657	SER
2	B	523	PRO
1	E	89	PRO
2	G	523	PRO

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	251/294 (85%)	250 (100%)	1 (0%)	91 95
1	D	247/294 (84%)	242 (98%)	5 (2%)	55 76
1	E	250/294 (85%)	245 (98%)	5 (2%)	55 76
1	H	238/294 (81%)	236 (99%)	2 (1%)	81 90
2	B	239/272 (88%)	235 (98%)	4 (2%)	60 80
2	C	231/272 (85%)	228 (99%)	3 (1%)	69 84
2	F	230/272 (85%)	225 (98%)	5 (2%)	52 75
2	G	230/272 (85%)	225 (98%)	5 (2%)	52 75
All	All	1916/2264 (85%)	1886 (98%)	30 (2%)	65 81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	THR
2	B	495	LEU
2	B	630	LYS
2	B	653	GLN
2	B	721	LEU
2	C	499	LYS
2	C	524	GLN
2	C	717	LEU
1	D	100	HIS
1	D	164	GLN

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Mol	Chain	Res	Type
1	D	252	SER
1	D	353	LYS
1	D	368	GLU
1	E	136	ASP
1	E	170	SER
1	E	211	VAL
1	E	331	SER
1	E	344	LYS
2	F	532[A]	CYS
2	F	532[B]	CYS
2	F	683	SER
2	F	701	ARG
2	F	717	LEU
2	G	549	GLU
2	G	599	THR
2	G	671	ARG
2	G	717	LEU
2	G	719	ARG
1	H	205	LYS
1	H	218	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	153	GLN
2	F	524	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACP	E	901	4	27,33,33	1.37	5 (18%)	32,52,52	1.55	8 (25%)
5	573	H	904	-	25,29,29	1.46	2 (8%)	23,41,41	2.59	9 (39%)
3	ACP	H	901	4	27,33,33	1.42	5 (18%)	32,52,52	1.43	6 (18%)
5	573	D	903	-	25,29,29	1.49	3 (12%)	23,41,41	2.98	8 (34%)
3	ACP	D	901	4	27,33,33	1.35	4 (14%)	32,52,52	1.47	6 (18%)
5	573	E	903	-	25,29,29	1.54	3 (12%)	23,41,41	3.01	8 (34%)
5	573	H	903	-	25,29,29	1.33	3 (12%)	23,41,41	2.45	7 (30%)
5	573	A	903	-	25,29,29	1.30	2 (8%)	23,41,41	2.36	6 (26%)
3	ACP	A	901	4	27,33,33	1.44	5 (18%)	32,52,52	1.42	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	E	901	4	-	10/15/38/38	0/3/3/3
5	573	H	904	-	-	2/8/14/14	0/3/3/3
3	ACP	H	901	4	-	3/15/38/38	0/3/3/3
5	573	D	903	-	-	3/8/14/14	0/3/3/3
3	ACP	D	901	4	-	4/15/38/38	0/3/3/3
5	573	E	903	-	-	0/8/14/14	0/3/3/3
5	573	H	903	-	-	0/8/14/14	0/3/3/3
5	573	A	903	-	-	0/8/14/14	0/3/3/3
3	ACP	A	901	4	-	1/15/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	903	573	C9-C7	-5.62	1.41	1.49
5	E	903	573	C9-C7	-5.47	1.41	1.49
5	H	903	573	C9-C7	-4.67	1.42	1.49
5	A	903	573	C9-C7	-4.42	1.43	1.49
5	H	904	573	C10-C11	4.24	1.49	1.41
5	H	904	573	C9-C7	-3.45	1.44	1.49
3	H	901	ACP	PG-O2G	3.28	1.62	1.54
3	A	901	ACP	PG-O3G	3.14	1.62	1.54
3	D	901	ACP	PG-O3G	3.08	1.62	1.54
3	H	901	ACP	PG-O3G	3.07	1.61	1.54
3	A	901	ACP	PG-O2G	3.04	1.61	1.54
3	D	901	ACP	PG-O2G	3.03	1.61	1.54
5	E	903	573	C12-C11	-2.98	1.38	1.42
3	E	901	ACP	PG-O3G	2.88	1.61	1.54
5	A	903	573	C10-C11	2.88	1.47	1.41
3	H	901	ACP	PB-O3A	2.87	1.61	1.58
3	E	901	ACP	PB-O3A	2.84	1.61	1.58
5	E	903	573	C10-C11	2.82	1.47	1.41
5	H	903	573	C10-C11	2.76	1.46	1.41
3	A	901	ACP	PB-O3A	2.74	1.61	1.58
5	D	903	573	C10-C11	2.70	1.46	1.41
3	E	901	ACP	PG-O2G	2.70	1.61	1.54
3	A	901	ACP	PB-O2B	2.56	1.62	1.56
5	D	903	573	C12-C11	-2.54	1.39	1.42
3	E	901	ACP	C5-C4	2.53	1.47	1.40
3	D	901	ACP	C5-C4	2.52	1.47	1.40
3	H	901	ACP	C5-C4	2.48	1.47	1.40
3	A	901	ACP	C5-C4	2.40	1.47	1.40
3	D	901	ACP	PB-O2B	2.24	1.61	1.56
5	H	903	573	C12-C11	-2.22	1.39	1.42
3	H	901	ACP	PB-O2B	2.15	1.61	1.56
3	E	901	ACP	PB-O2B	2.01	1.61	1.56

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	903	573	F18-C15-C16	8.07	120.66	117.40
5	D	903	573	F18-C15-C16	7.27	120.34	117.40
5	E	903	573	C12-N13-C14	7.24	123.01	116.87
5	D	903	573	C12-N13-C14	7.18	122.96	116.87
5	D	903	573	C9-C7-N6	6.23	122.71	113.94
5	H	903	573	C12-N13-C14	6.02	121.98	116.87
5	A	903	573	C12-N13-C14	5.89	121.86	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	904	573	C12-N13-C14	5.78	121.77	116.87
5	A	903	573	O5-N6-C7	5.67	125.54	118.57
5	H	903	573	C9-C7-N6	5.61	121.84	113.94
5	H	904	573	F18-C15-C16	5.17	119.49	117.40
5	H	903	573	F18-C15-C16	4.88	119.37	117.40
5	E	903	573	O5-N6-C7	4.60	124.23	118.57
5	D	903	573	C11-C12-N13	-4.18	120.08	124.55
5	E	903	573	C11-C12-N13	-4.13	120.14	124.55
5	H	904	573	O5-N6-C7	4.09	123.60	118.57
5	H	904	573	C9-C7-N6	3.98	119.55	113.94
5	A	903	573	C11-C12-N13	-3.89	120.39	124.55
5	A	903	573	C9-C7-N6	3.86	119.38	113.94
5	H	904	573	C22-C23-C24	-3.85	116.56	121.09
3	D	901	ACP	C3'-C2'-C1'	3.58	106.37	100.98
5	H	904	573	O8-C7-N6	-3.37	118.09	123.03
3	A	901	ACP	C3'-C2'-C1'	3.34	106.00	100.98
3	E	901	ACP	O2G-PG-C3B	3.33	114.47	106.40
5	E	903	573	C9-C7-N6	3.25	118.51	113.94
5	E	903	573	F26-C25-C20	3.24	121.57	117.50
3	H	901	ACP	N3-C2-N1	-3.23	123.63	128.68
3	A	901	ACP	N3-C2-N1	-3.15	123.76	128.68
3	E	901	ACP	N3-C2-N1	-3.05	123.91	128.68
3	D	901	ACP	N3-C2-N1	-3.00	123.99	128.68
3	H	901	ACP	C4-C5-N7	-2.97	106.31	109.40
5	E	903	573	C24-C25-C20	-2.95	120.69	123.50
5	H	903	573	C11-C12-N13	-2.90	121.44	124.55
3	H	901	ACP	PB-O3A-PA	-2.90	123.37	132.56
3	E	901	ACP	PB-O3A-PA	-2.88	123.43	132.56
5	A	903	573	C24-C25-C20	-2.83	120.81	123.50
3	H	901	ACP	C3'-C2'-C1'	2.80	105.19	100.98
3	E	901	ACP	C3'-C2'-C1'	2.72	105.08	100.98
5	A	903	573	F18-C15-C14	2.70	122.91	118.39
3	A	901	ACP	PB-O3A-PA	-2.69	124.02	132.56
5	H	903	573	O8-C7-N6	-2.62	119.18	123.03
5	H	903	573	C24-C25-C20	-2.56	121.07	123.50
5	D	903	573	C22-C23-C24	-2.54	118.10	121.09
3	H	901	ACP	O2G-PG-C3B	2.49	112.43	106.40
5	H	904	573	C24-C25-C20	-2.48	121.14	123.50
5	H	903	573	C21-C20-C25	2.46	119.65	117.17
3	D	901	ACP	O3G-PG-C3B	2.43	112.30	106.40
5	E	903	573	C22-C23-I27	2.40	123.30	119.68
5	D	903	573	O8-C7-C9	-2.36	117.16	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	903	573	C24-C25-C20	-2.28	121.33	123.50
3	D	901	ACP	C4-C5-N7	-2.23	107.07	109.40
3	D	901	ACP	O2B-PB-C3B	2.23	115.71	106.58
3	A	901	ACP	C4-C5-N7	-2.23	107.08	109.40
5	D	903	573	C22-C23-I27	2.23	123.04	119.68
3	D	901	ACP	O1G-PG-C3B	-2.21	106.48	111.24
5	H	904	573	C12-C11-C16	-2.16	116.41	119.34
3	E	901	ACP	C2-N1-C6	2.14	122.42	118.75
5	H	904	573	C15-C14-N13	-2.13	119.47	121.89
3	E	901	ACP	O1G-PG-C3B	-2.10	106.71	111.24
3	H	901	ACP	C2-N1-C6	2.10	122.34	118.75
3	E	901	ACP	C4-C5-N7	-2.04	107.28	109.40
3	E	901	ACP	N6-C6-N1	2.02	122.76	118.57

There are no chirality outliers.

All (23) torsion outliers are listed below:

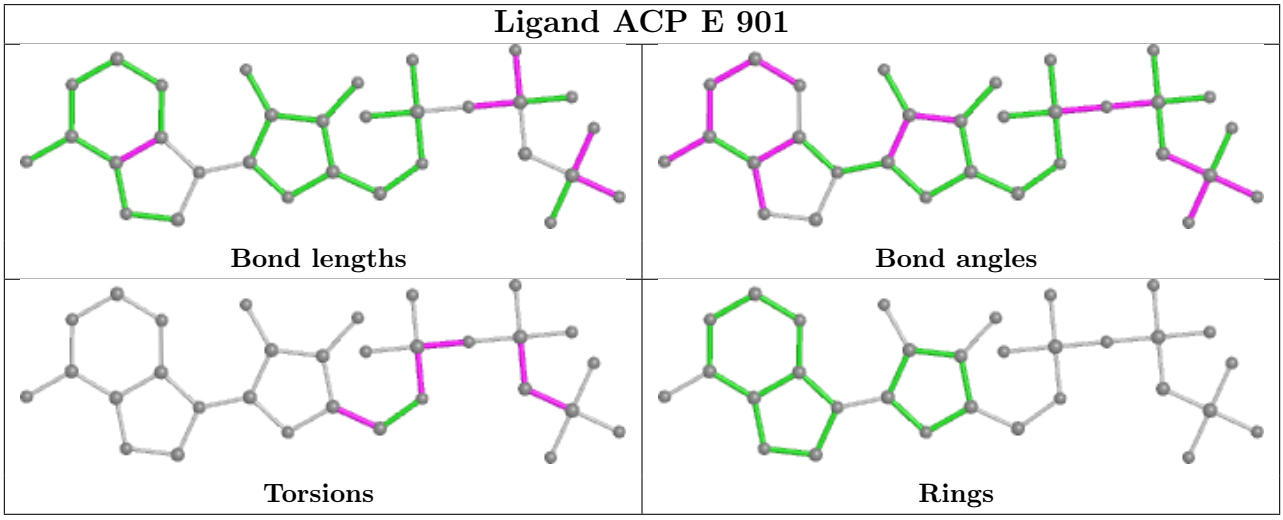
Mol	Chain	Res	Type	Atoms
3	D	901	ACP	C5'-O5'-PA-O3A
3	E	901	ACP	PB-C3B-PG-O1G
3	E	901	ACP	PB-C3B-PG-O2G
3	E	901	ACP	PB-C3B-PG-O3G
3	E	901	ACP	PG-C3B-PB-O1B
3	E	901	ACP	PG-C3B-PB-O2B
3	E	901	ACP	PG-C3B-PB-O3A
3	E	901	ACP	PB-O3A-PA-O5'
3	E	901	ACP	C5'-O5'-PA-O1A
5	D	903	573	O28-C2-C4-O5
3	E	901	ACP	O4'-C4'-C5'-O5'
5	D	903	573	C1-C2-C4-O5
5	H	904	573	C1-C2-C4-O5
3	H	901	ACP	PB-O3A-PA-O5'
3	D	901	ACP	C5'-O5'-PA-O1A
5	D	903	573	C7-N6-O5-C4
3	A	901	ACP	PB-C3B-PG-O1G
3	D	901	ACP	PB-C3B-PG-O1G
5	H	904	573	C2-C4-O5-N6
3	H	901	ACP	C3'-C4'-C5'-O5'
3	D	901	ACP	PB-O3A-PA-O1A
3	E	901	ACP	C5'-O5'-PA-O3A
3	H	901	ACP	O4'-C4'-C5'-O5'

There are no ring outliers.

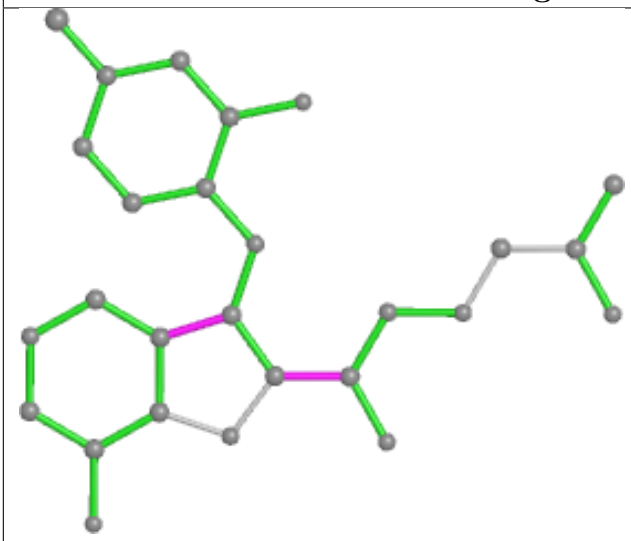
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	901	ACP	1	0
5	H	904	573	3	0
3	D	901	ACP	1	0
5	E	903	573	1	0
5	H	903	573	3	0
5	A	903	573	2	0

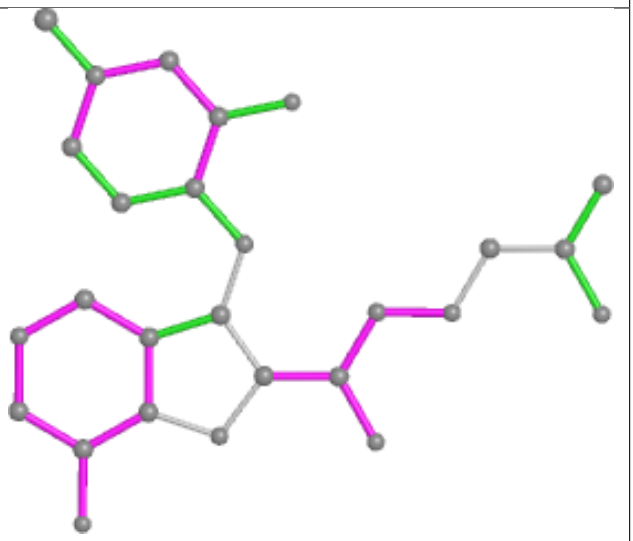
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



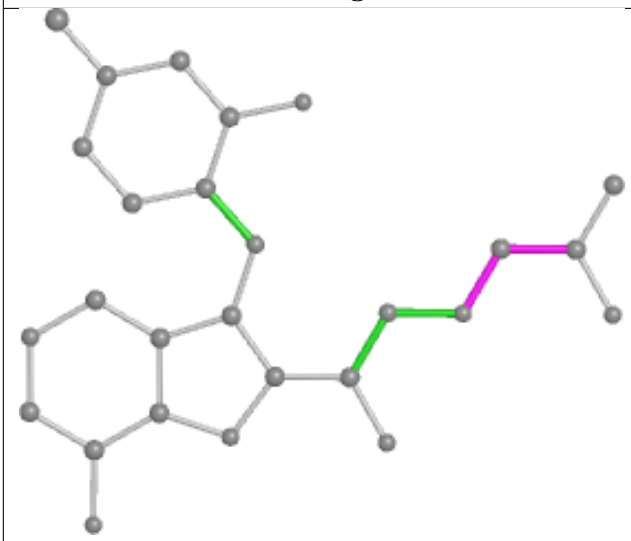
Ligand 573 H 904



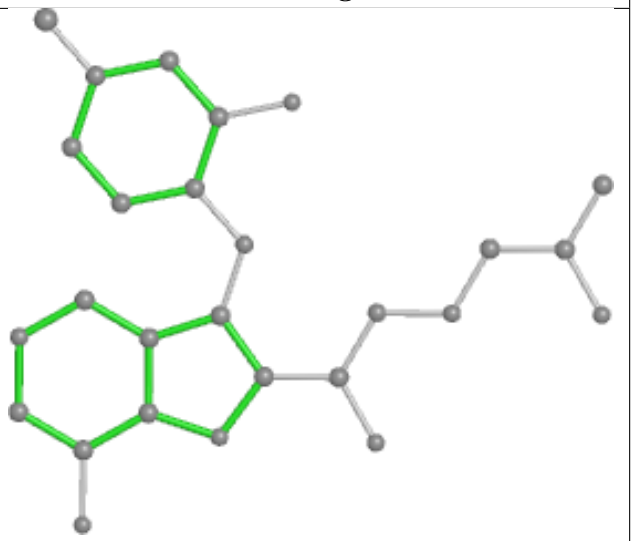
Bond lengths



Bond angles

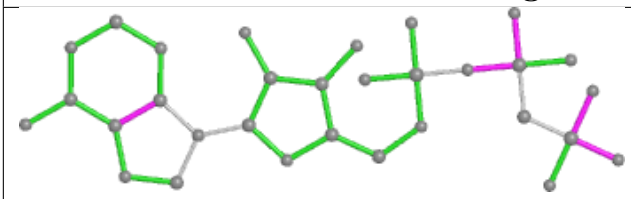


Torsions

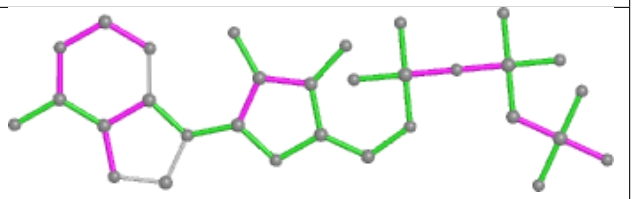


Rings

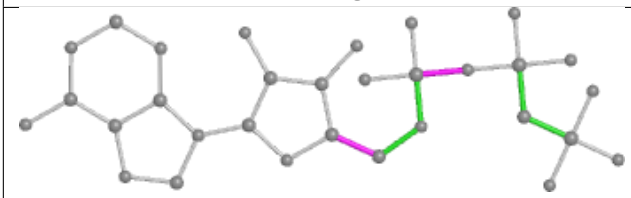
Ligand ACP H 901



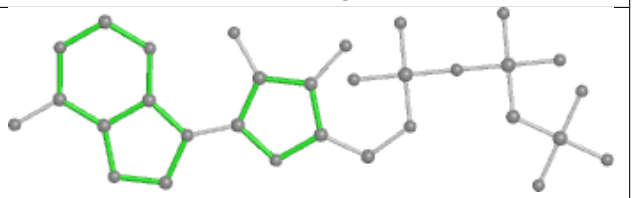
Bond lengths



Bond angles

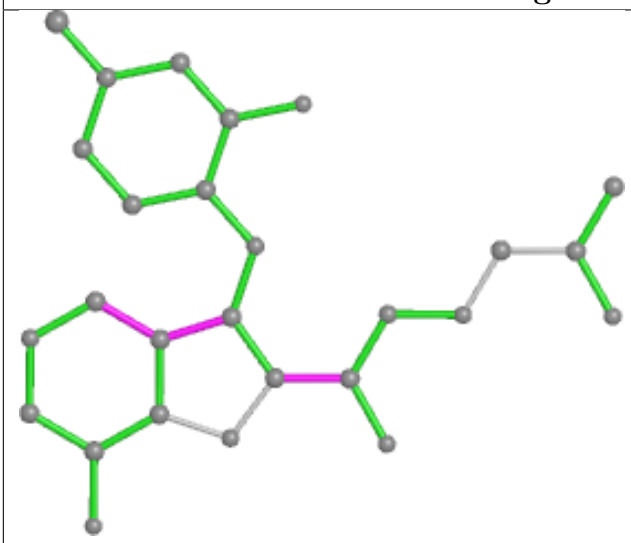


Torsions

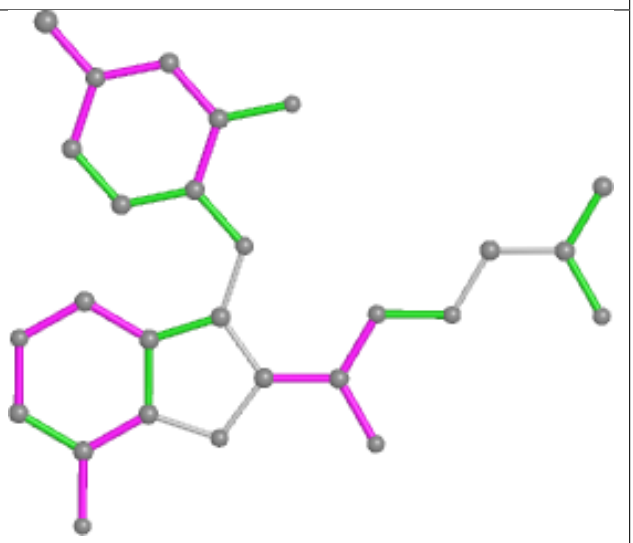


Rings

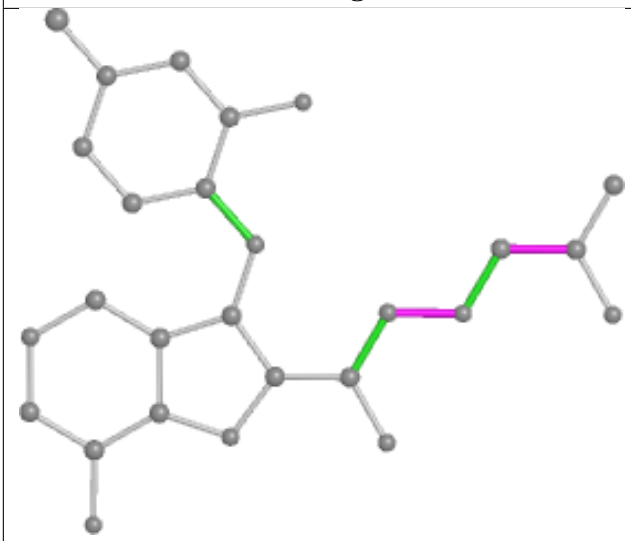
Ligand 573 D 903



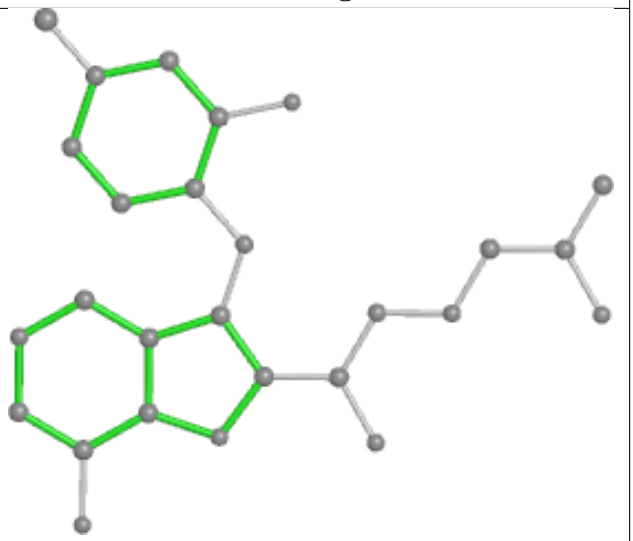
Bond lengths



Bond angles

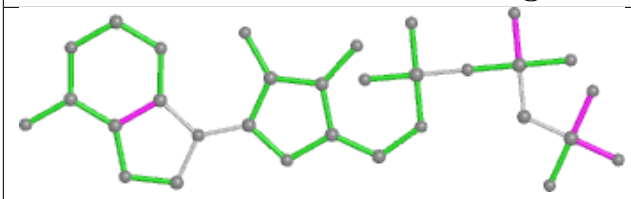


Torsions

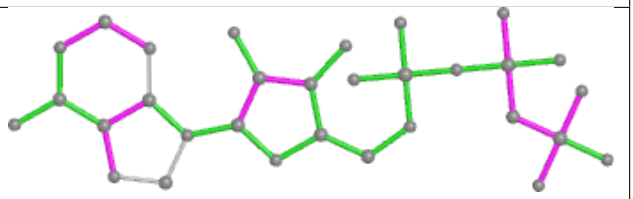


Rings

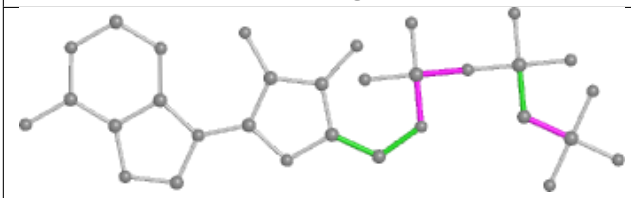
Ligand ACP D 901



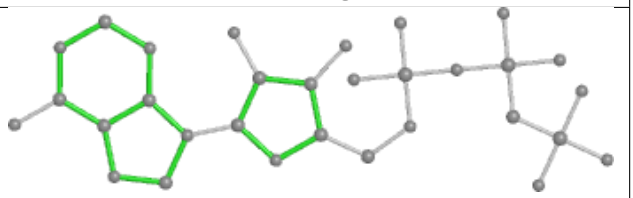
Bond lengths



Bond angles

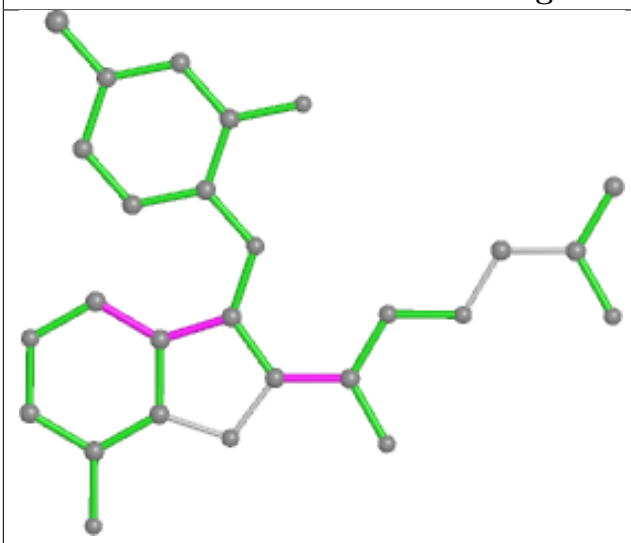


Torsions

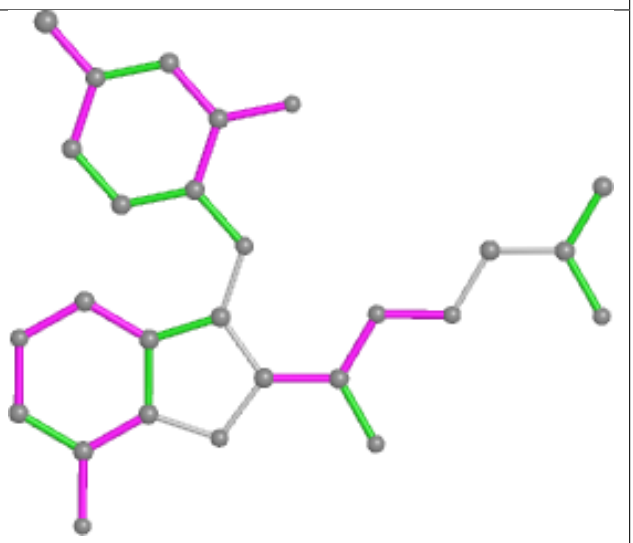


Rings

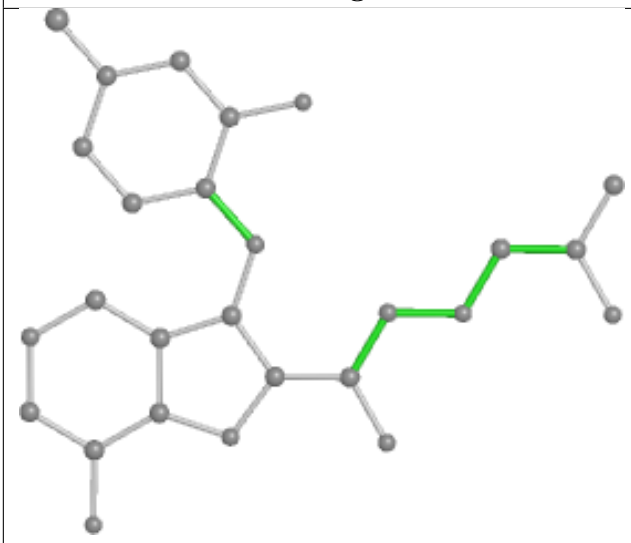
Ligand 573 E 903



Bond lengths



Bond angles



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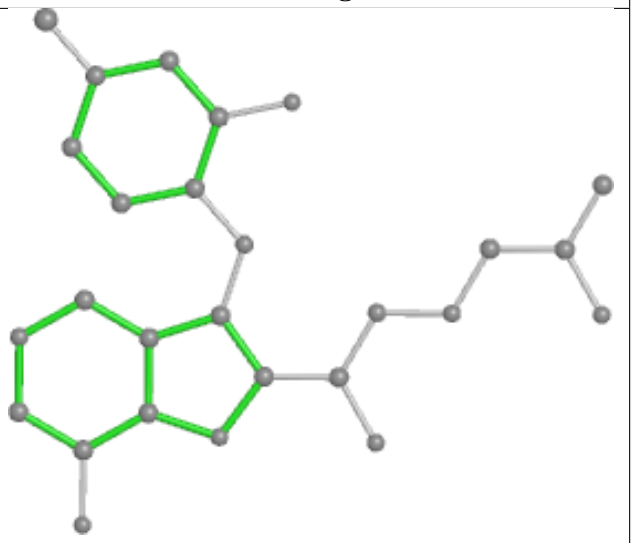
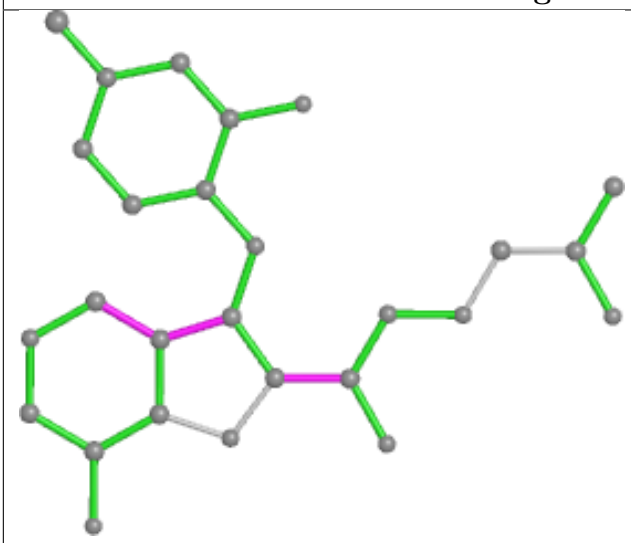
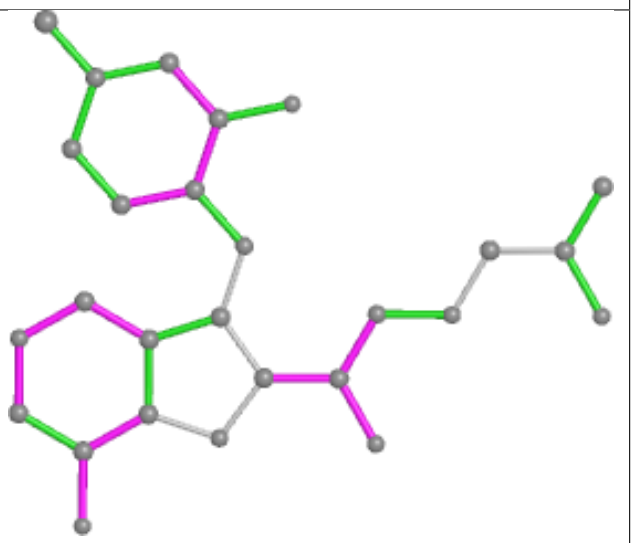


Rings

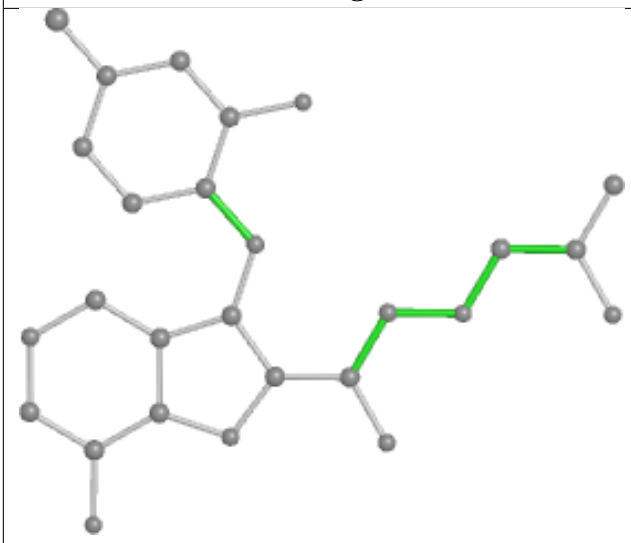
Ligand 573 H 903



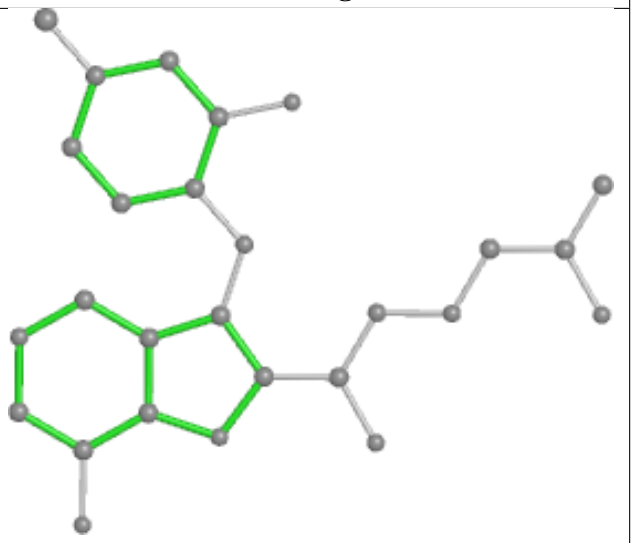
Bond lengths



Bond angles

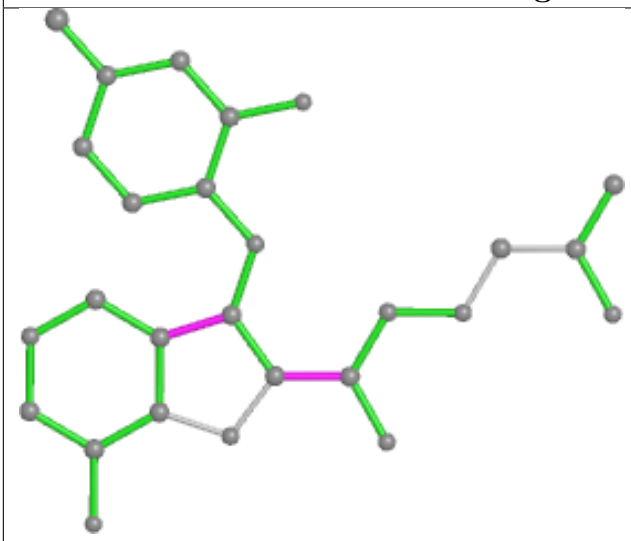


Torsions

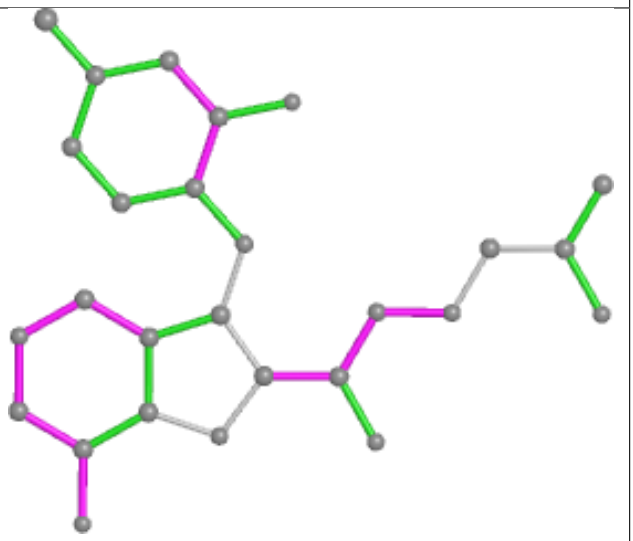


Rings

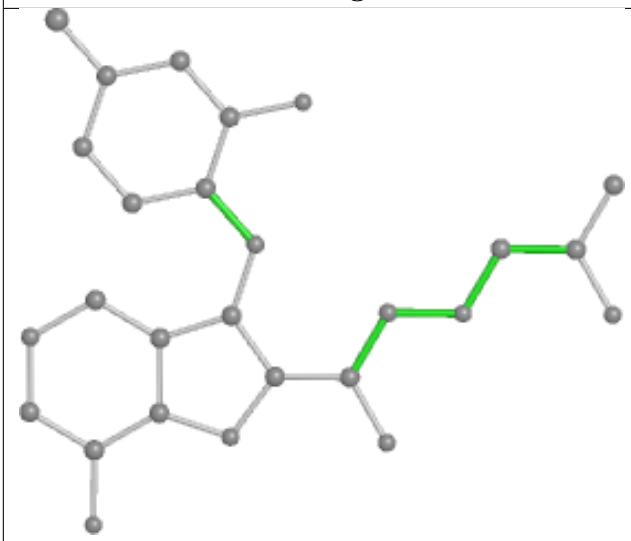
Ligand 573 A 903



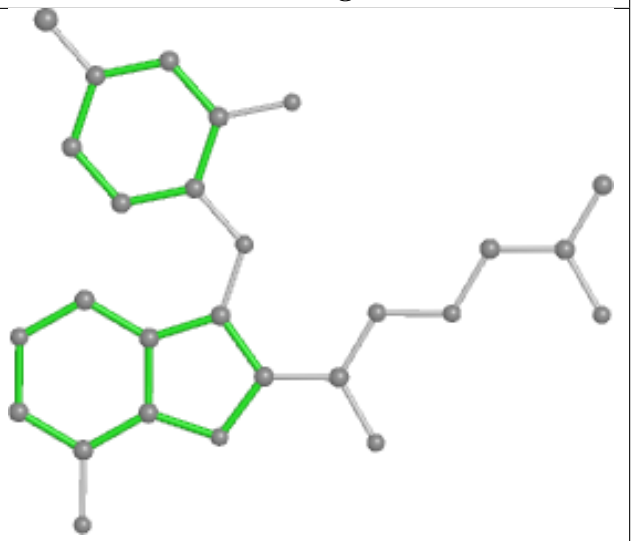
Bond lengths



Bond angles

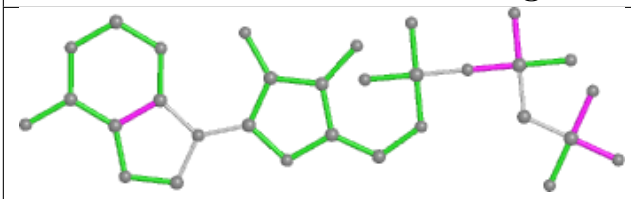


Torsions

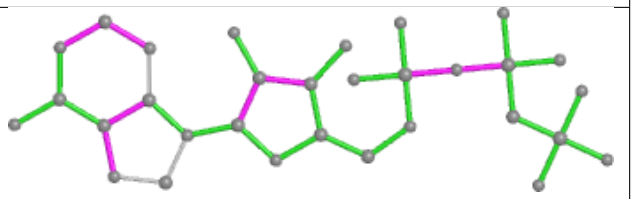


Rings

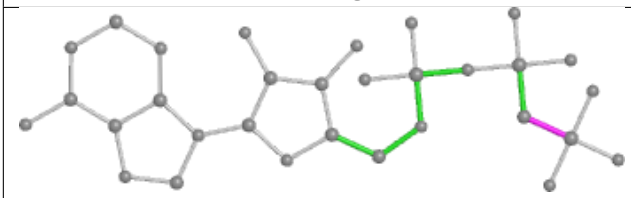
Ligand ACP A 901



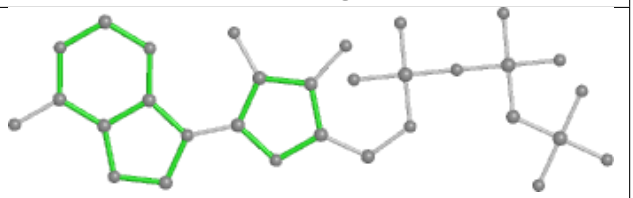
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	286/341 (83%)	-0.36	4 (1%)	75	71	24, 45, 78, 127	0
1	D	285/341 (83%)	-0.48	3 (1%)	80	78	24, 41, 83, 139	0
1	E	286/341 (83%)	-0.33	5 (1%)	70	66	25, 49, 89, 143	0
1	H	275/341 (80%)	-0.31	2 (0%)	87	86	29, 54, 89, 146	0
2	B	270/308 (87%)	-0.50	1 (0%)	92	91	16, 33, 85, 143	0
2	C	260/308 (84%)	-0.46	1 (0%)	92	91	22, 39, 80, 129	0
2	F	258/308 (83%)	-0.48	2 (0%)	86	85	18, 37, 84, 137	0
2	G	259/308 (84%)	-0.52	2 (0%)	86	85	20, 40, 84, 125	0
All	All	2179/2596 (83%)	-0.43	20 (0%)	84	83	16, 43, 87, 146	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	LYS	4.7
1	H	266	PRO	4.6
2	F	486	ASN	4.1
2	C	610	PHE	3.6
1	E	271	LEU	3.5
2	F	485	LEU	3.4
1	E	274	MET	3.2
1	D	382	ASN	2.8
2	G	486	ASN	2.7
1	E	268	ALA	2.6
1	E	269	LYS	2.5
2	B	469	GLY	2.5
1	A	379	ILE	2.5
1	D	273	LEU	2.4
2	G	461	GLN	2.3
1	E	273	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	357	VAL	2.1
1	A	273	LEU	2.0
1	A	87	HIS	2.0
1	H	326	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

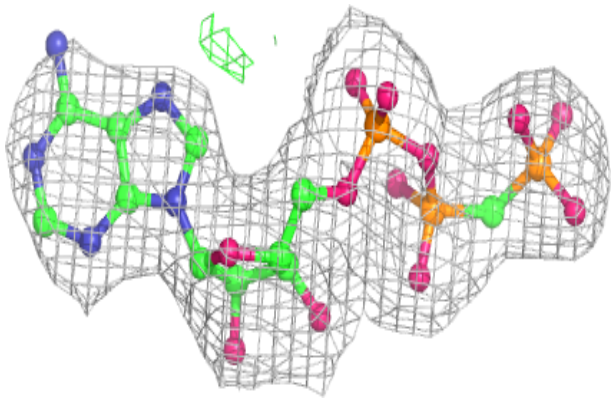
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

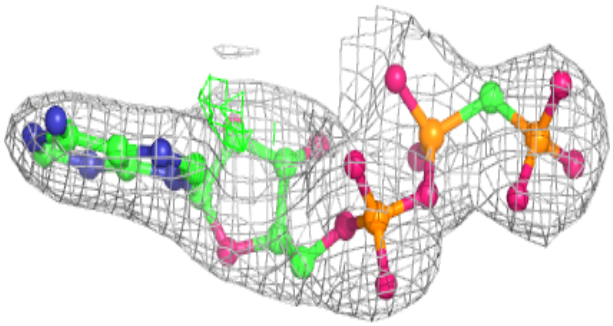
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	F	801	1/1	0.66	0.41	71,71,71,71	0
3	ACP	E	901	31/31	0.95	0.17	34,46,57,64	0
4	MG	H	902	1/1	0.96	0.17	52,52,52,52	0
3	ACP	A	901	31/31	0.97	0.16	31,44,50,51	0
5	573	H	904	27/27	0.97	0.22	41,54,74,83	0
3	ACP	H	901	31/31	0.97	0.16	41,49,56,58	0
4	MG	E	902	1/1	0.98	0.18	68,68,68,68	0
3	ACP	D	901	31/31	0.98	0.12	33,38,43,46	0
5	573	E	903	27/27	0.98	0.15	42,47,58,61	0
4	MG	A	902	1/1	0.98	0.18	45,45,45,45	0
4	MG	D	902	1/1	0.98	0.11	47,47,47,47	0
5	573	H	903	27/27	0.99	0.18	36,42,49,51	0
5	573	D	903	27/27	0.99	0.15	33,39,47,51	0
5	573	A	903	27/27	0.99	0.15	35,39,45,51	0

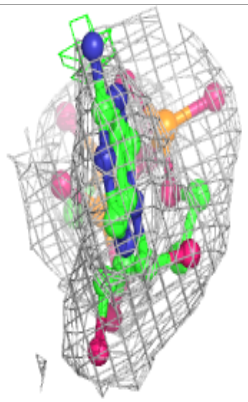
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP E 901:

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

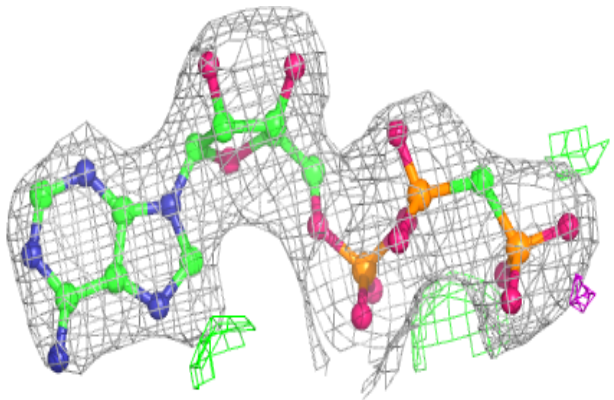


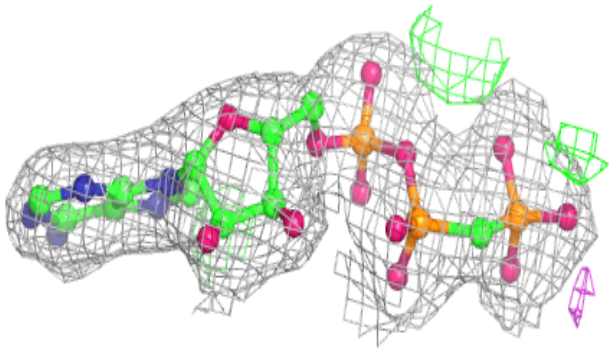


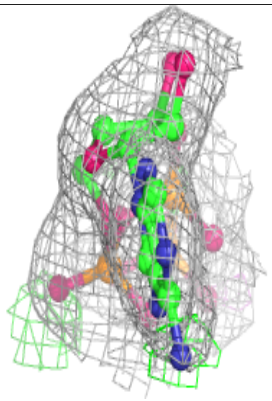


Electron density around ACP A 901:

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

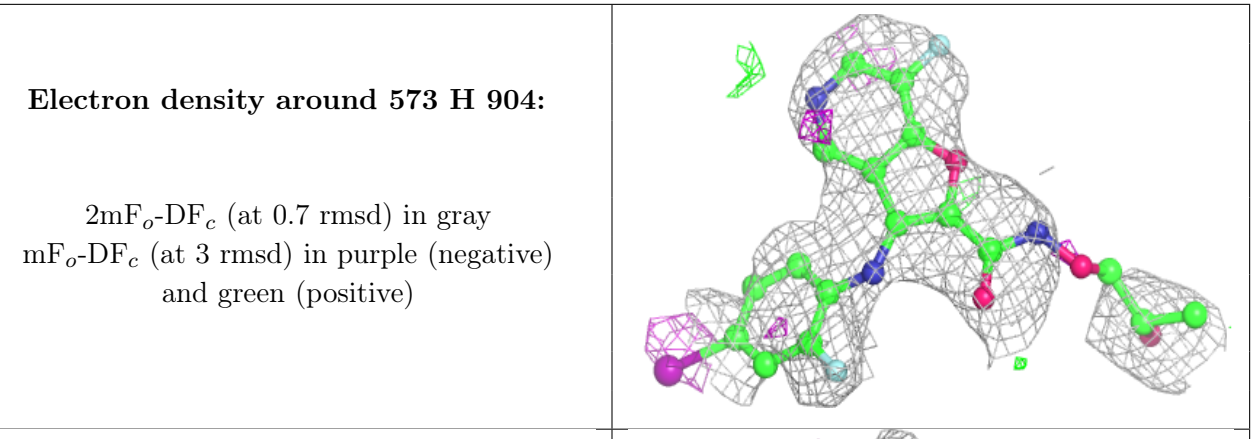






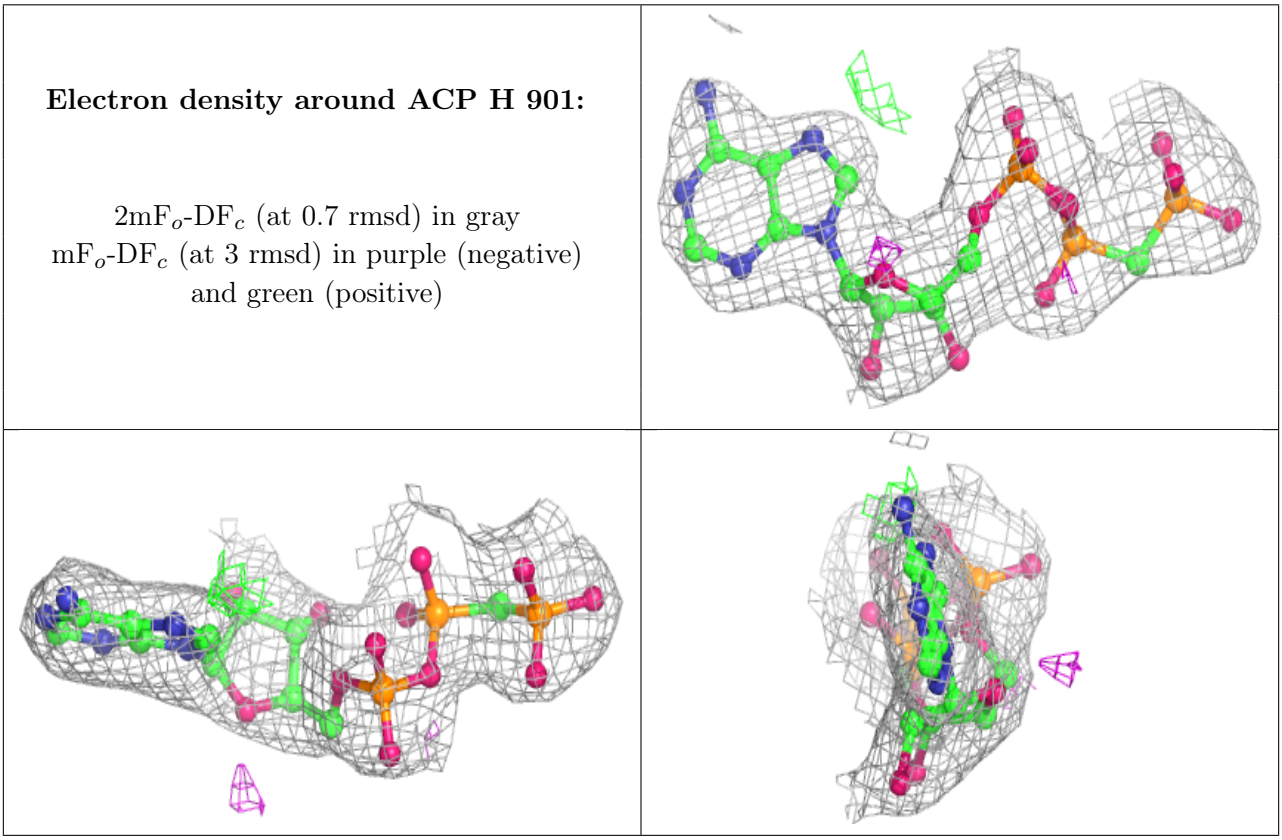
Electron density around 573 H 904:

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



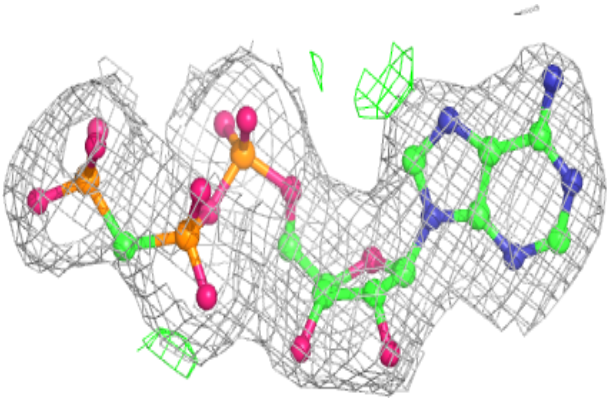
Electron density around ACP H 901:

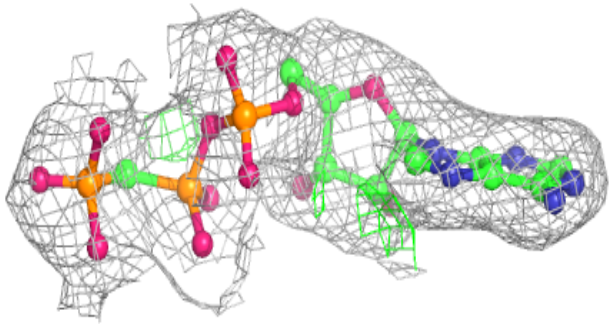
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

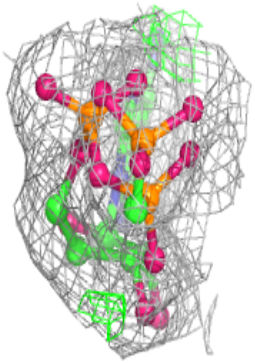


Electron density around ACP D 901:

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







Electron density around 573 E 903:

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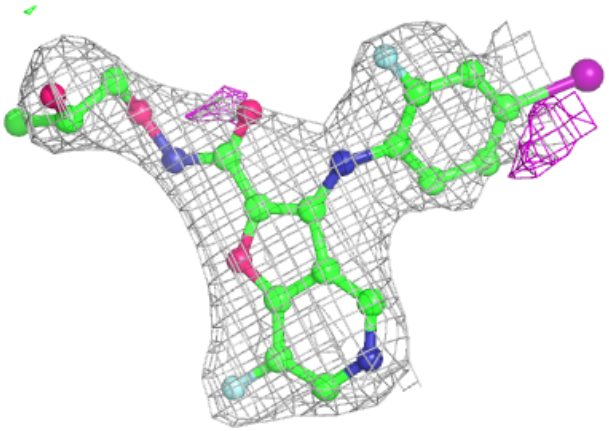
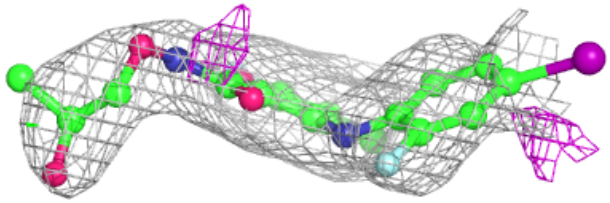
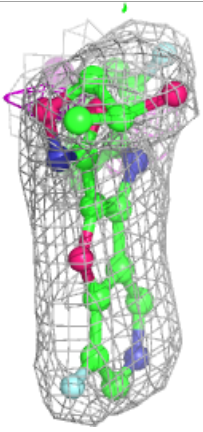
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

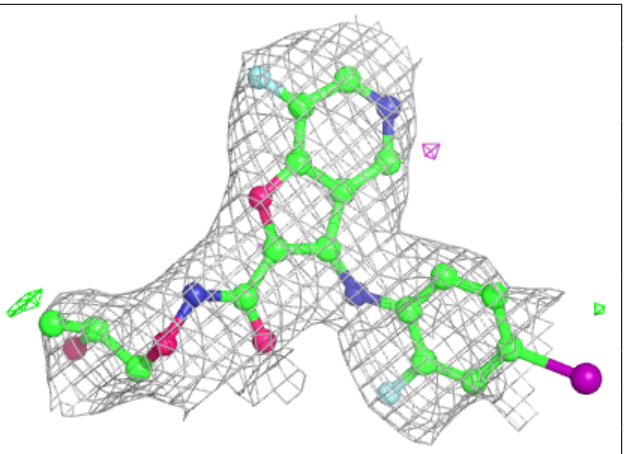


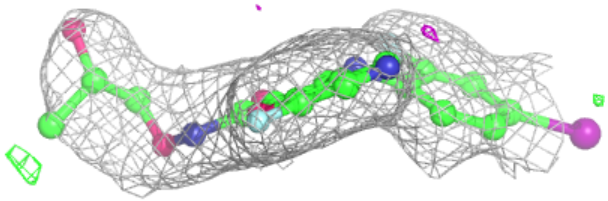


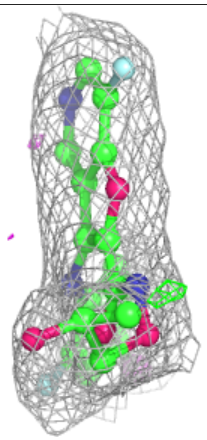


Electron density around 573 H 903:

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

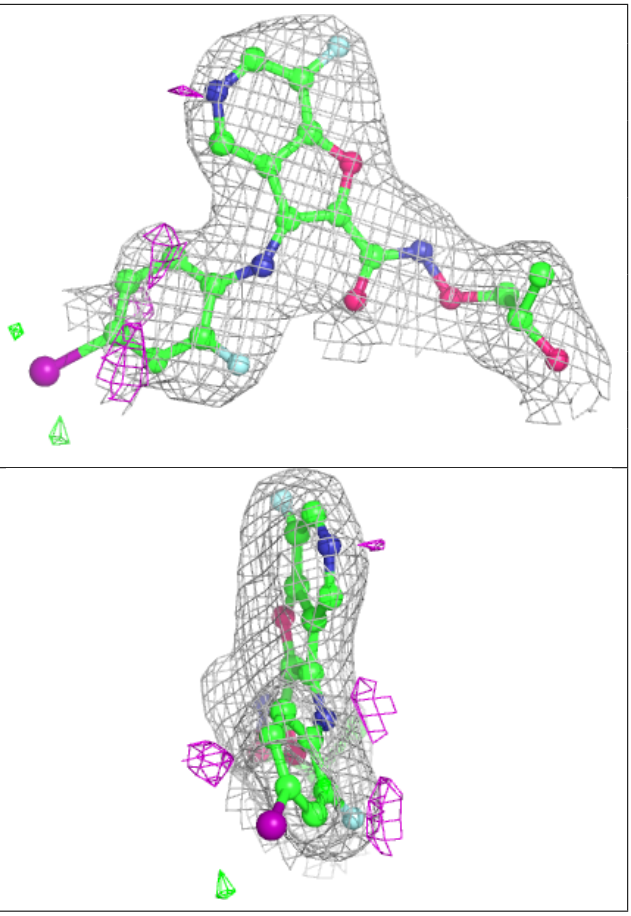


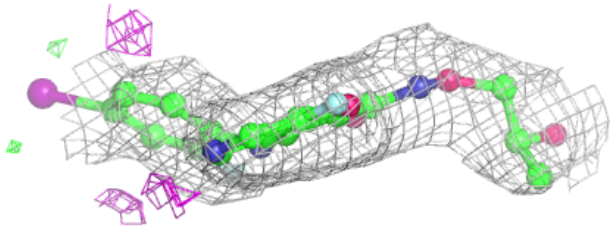




Electron density around 573 D 903:

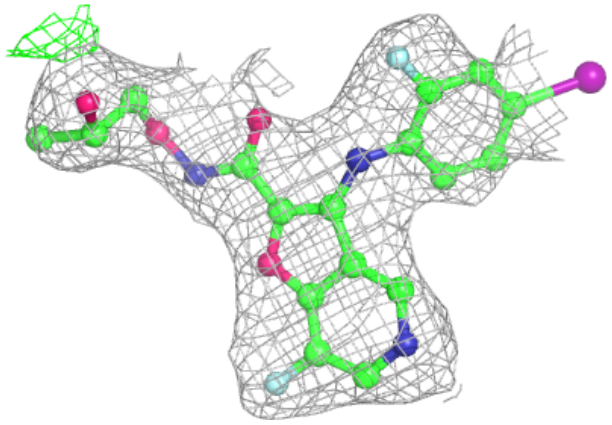
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

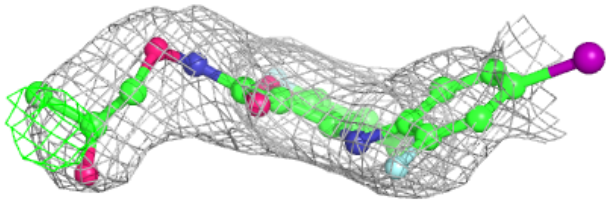


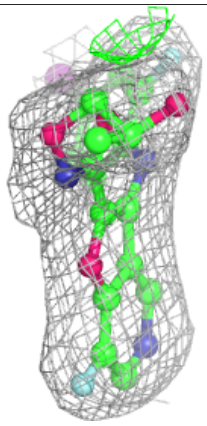


Electron density around 573 A 903:

$2mF_o$-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.