Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:45 AM EDT

PDB ID	:	3CH6
Title	:	Crystal Structure of 11beta-HSD1 Double Mutant (L262R, F278E) Complexed with (3,3-dimethylpiperidin-1-yl)(6-(3-fluoro-4-methylphenyl)pyridin-2-yl)methanone
Authors	:	Sheriff, S.
Deposited on	:	2008-03-07
Resolution	:	2.35 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:

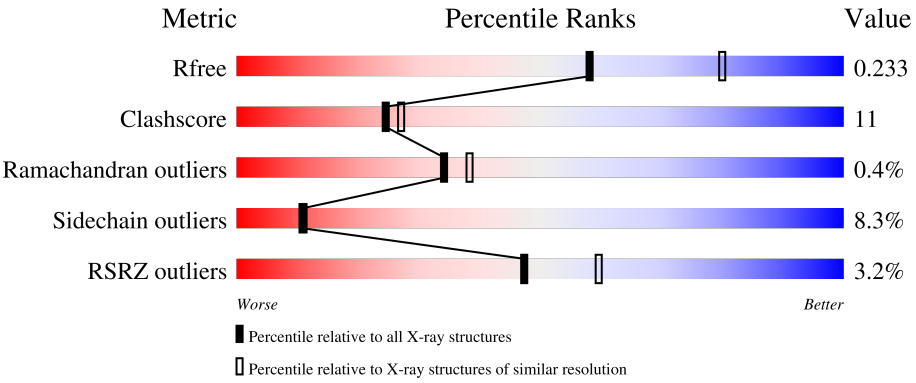
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	286	3% 73% 15% • 8%
1	B	286	3% 76% 17% 5% •
1	D	286	3% 76% 16% • 5%
1	E	286	3% 73% 16% • 8%

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
3	311	E	604	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8775 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	2	0
			2036	1292	351	376	17			
1	B	279	Total	C	N	O	S	0	1	0
			2125	1341	364	400	20			
1	D	273	Total	C	N	O	S	0	1	0
			2072	1312	354	388	18			
1	E	263	Total	C	N	O	S	0	1	0
			2019	1282	343	377	17			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP P28845
A	8	SER	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	MET	-	expression tag	UNP P28845
A	11	ALA	-	expression tag	UNP P28845
A	12	SER	-	expression tag	UNP P28845
A	13	MET	-	expression tag	UNP P28845
A	14	THR	-	expression tag	UNP P28845
A	15	GLY	-	expression tag	UNP P28845
A	16	GLY	-	expression tag	UNP P28845
A	17	GLN	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	MET	-	expression tag	UNP P28845
A	20	GLY	-	expression tag	UNP P28845
A	21	ARG	-	expression tag	UNP P28845
A	22	GLY	-	expression tag	UNP P28845
A	23	SER	-	expression tag	UNP P28845
A	262	ARG	LEU	engineered mutation	UNP P28845
A	278	GLU	PHE	engineered mutation	UNP P28845
B	7	GLY	-	expression tag	UNP P28845
B	8	SER	-	expression tag	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP P28845
B	10	MET	-	expression tag	UNP P28845
B	11	ALA	-	expression tag	UNP P28845
B	12	SER	-	expression tag	UNP P28845
B	13	MET	-	expression tag	UNP P28845
B	14	THR	-	expression tag	UNP P28845
B	15	GLY	-	expression tag	UNP P28845
B	16	GLY	-	expression tag	UNP P28845
B	17	GLN	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	MET	-	expression tag	UNP P28845
B	20	GLY	-	expression tag	UNP P28845
B	21	ARG	-	expression tag	UNP P28845
B	22	GLY	-	expression tag	UNP P28845
B	23	SER	-	expression tag	UNP P28845
B	262	ARG	LEU	engineered mutation	UNP P28845
B	278	GLU	PHE	engineered mutation	UNP P28845
D	7	GLY	-	expression tag	UNP P28845
D	8	SER	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	MET	-	expression tag	UNP P28845
D	11	ALA	-	expression tag	UNP P28845
D	12	SER	-	expression tag	UNP P28845
D	13	MET	-	expression tag	UNP P28845
D	14	THR	-	expression tag	UNP P28845
D	15	GLY	-	expression tag	UNP P28845
D	16	GLY	-	expression tag	UNP P28845
D	17	GLN	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	MET	-	expression tag	UNP P28845
D	20	GLY	-	expression tag	UNP P28845
D	21	ARG	-	expression tag	UNP P28845
D	22	GLY	-	expression tag	UNP P28845
D	23	SER	-	expression tag	UNP P28845
D	262	ARG	LEU	engineered mutation	UNP P28845
D	278	GLU	PHE	engineered mutation	UNP P28845
E	7	GLY	-	expression tag	UNP P28845
E	8	SER	-	expression tag	UNP P28845
E	9	HIS	-	expression tag	UNP P28845
E	10	MET	-	expression tag	UNP P28845
E	11	ALA	-	expression tag	UNP P28845
E	12	SER	-	expression tag	UNP P28845

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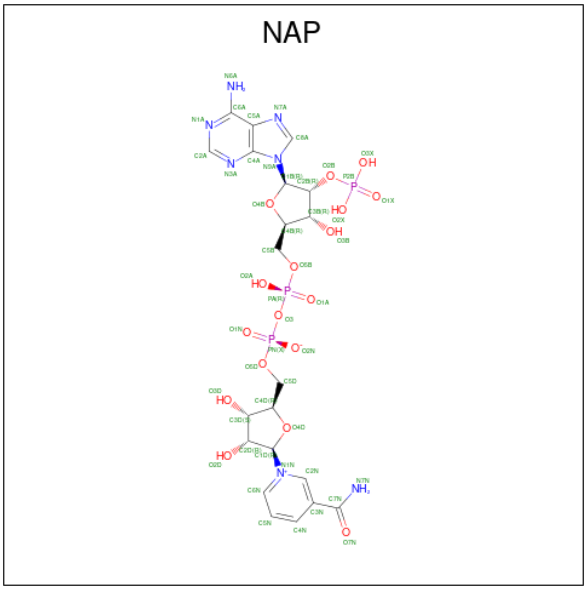
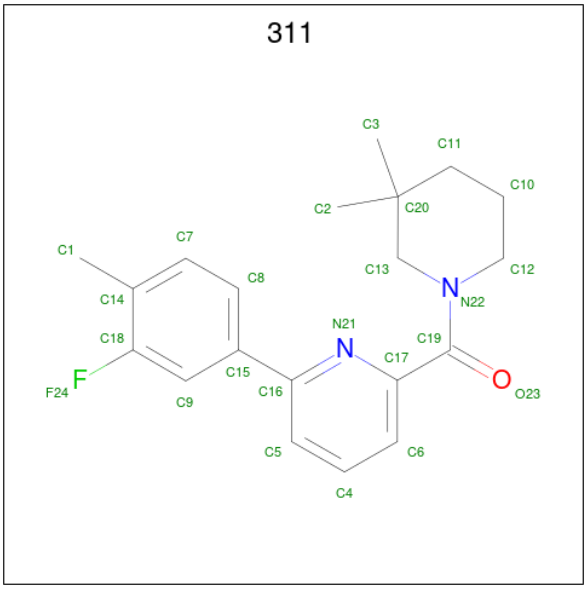
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	MET	-	expression tag	UNP P28845
E	14	THR	-	expression tag	UNP P28845
E	15	GLY	-	expression tag	UNP P28845
E	16	GLY	-	expression tag	UNP P28845
E	17	GLN	-	expression tag	UNP P28845
E	18	GLN	-	expression tag	UNP P28845
E	19	MET	-	expression tag	UNP P28845
E	20	GLY	-	expression tag	UNP P28845
E	21	ARG	-	expression tag	UNP P28845
E	22	GLY	-	expression tag	UNP P28845
E	23	SER	-	expression tag	UNP P28845
E	262	ARG	LEU	engineered mutation	UNP P28845
E	278	GLU	PHE	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (3,3-dimethylpiperidin-1-yl)(6-(3-fluoro-4-methylphenyl)pyridin-2-yl)methanone (three-letter code: 311) (formula: $C_{20}H_{23}FN_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 24 20 1 2 1	0	0
3	B	1	Total C F N O 24 20 1 2 1	0	0
3	D	1	Total C F N O 24 20 1 2 1	0	0
3	E	1	Total C F N O 24 20 1 2 1	0	0

- Molecule 4 is water.

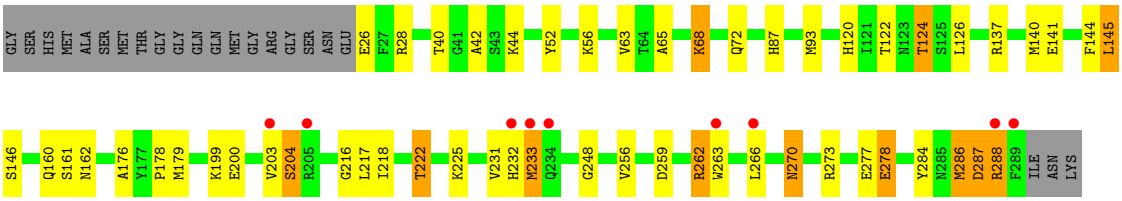
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	65	Total O 65 65	0	0
4	D	60	Total O 60 60	0	0
4	E	55	Total O 55 55	0	0

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.

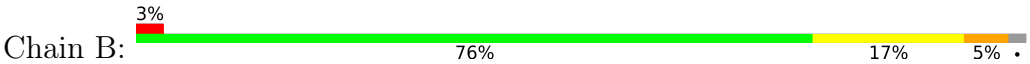
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

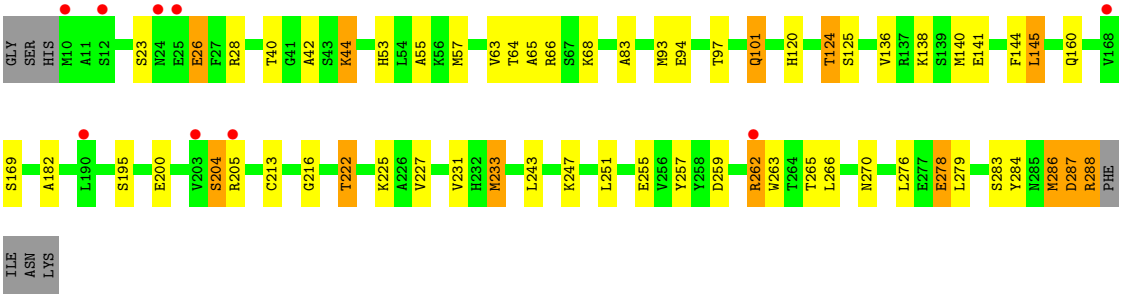
Chain A:



• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

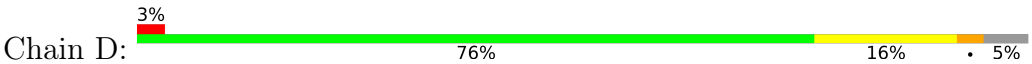
Chain B:

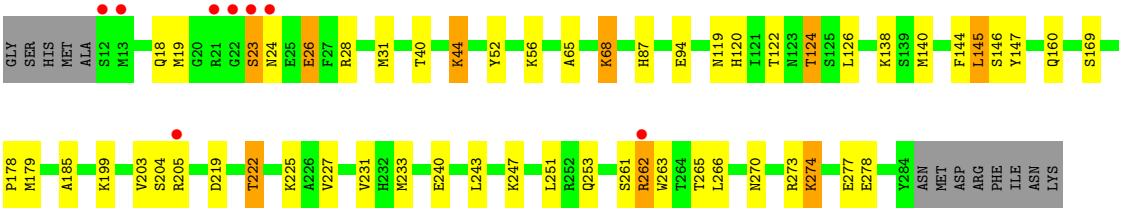




• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

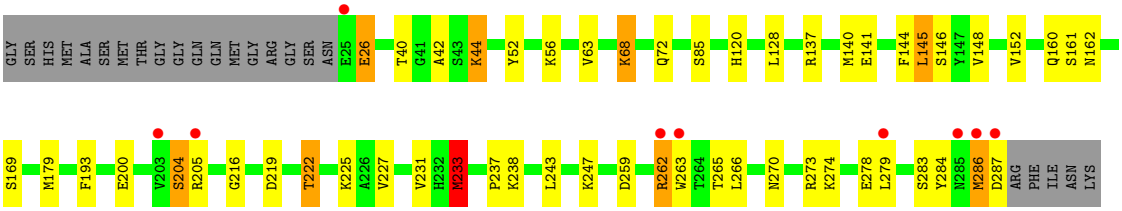
Chain D:





• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain E:


GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER ASN E25 E26 T40 G41 A42 S43 K44 Y52 K56 V63 K68 Q72 S85 H120 L128 R137 M140 E141 F144 L145 S146 Y147 V148 V152 Q160 S161 N162
S169 M179 F193 E200 V203 S204 R205 G216 D219 T222 K225 A226 V227 V231 H232 M233 P237 K238 L243 K247 D259 R262 W263 T264 T265 L266 N270 R273 K274 E278 L279 S283 Y284 N285 M286 D287 ARG PHE ILE ASN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.50Å 94.30Å 167.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 32.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	89.3 (50.00-2.35) 89.2 (32.00-2.34)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.47 (at 2.34Å)	Xtriage
Refinement program	TNT, BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.187 , 0.230 0.187 , 0.233	Depositor DCC
R_{free} test set	1062 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8775	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: NAP, 311

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	0.69	0/2081	0.77	0/2808
1	B	0.70	0/2163	0.76	0/2915
1	D	0.73	0/2110	0.76	0/2846
1	E	0.72	1/2057 (0.0%)	0.78	2/2776 (0.1%)
All	All	0.71	1/8411 (0.0%)	0.77	2/11345 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	233	MET	CG-SD	5.55	1.95	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	273	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	273	ARG	NE-CZ-NH1	6.18	123.39	120.30

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	2036	0	2073	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2125	0	2152	57	0
1	D	2072	0	2099	43	0
1	E	2019	0	2056	49	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
2	D	48	0	25	4	0
2	E	48	0	25	3	0
3	A	24	0	23	1	0
3	B	24	0	23	1	0
3	D	24	0	23	0	0
3	E	24	0	23	2	0
4	A	55	0	0	2	0
4	B	65	0	0	2	0
4	D	60	0	0	2	0
4	E	55	0	0	1	0
All	All	8775	0	8572	186	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 11.

All (186) 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:B:262:ARG:HB2	1:B:262:ARG:HH11	1.05	1.12
1:E:262:ARG:HB2	1:E:262:ARG:HH11	1.14	1.08
1:D:231:VAL:HG12	1:D:233:MET:HG2	1.40	0.98
1:D:19:MET:HE3	1:D:23:SER:HB2	1.47	0.96
1:B:284:TYR:CD2	1:B:286:MET:HE1	2.07	0.89
1:D:122:THR:O	1:D:124:THR:HG22	1.76	0.86
1:B:262:ARG:HH11	1:B:262:ARG:CB	1.89	0.85
1:D:262:ARG:HH11	1:D:262:ARG:HA	1.44	0.83
1:B:262:ARG:HB2	1:B:262:ARG:NH1	1.91	0.83
1:E:262:ARG:HH11	1:E:262:ARG:CB	1.93	0.80
1:E:284:TYR:CD2	1:E:286:MET:HE1	2.15	0.80
1:A:68:LYS:O	1:A:72:GLN:HG3	1.82	0.80
1:E:231:VAL:HG12	1:E:233:MET:HG2	1.64	0.79
1:D:231:VAL:CG1	1:D:233:MET:HG2	2.15	0.76
1:B:44:LYS:HG3	2:B:502:NAP:H3B	1.68	0.75
1:B:124:THR:HG21	4:B:858:HOH:O	1.86	0.75
1:A:137:ARG:NH2	1:B:145:LEU:HD22	2.04	0.73
1:A:140:MET:HE3	1:A:140:MET:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HG2	1:A:72:GLN:HE21	1.57	0.70
1:E:284:TYR:CE2	1:E:286:MET:HE1	2.27	0.70
1:E:26:GLU:HA	1:E:26:GLU:OE1	1.93	0.68
1:A:126:LEU:HD23	1:A:126:LEU:N	2.08	0.68
1:E:231:VAL:HG12	1:E:233:MET:CG	2.24	0.68
1:D:262:ARG:HH11	1:D:262:ARG:CA	2.06	0.67
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.78	0.67
1:A:124:THR:HG21	4:A:975:HOH:O	1.94	0.66
1:A:231:VAL:HG12	1:A:233:MET:HG2	1.78	0.66
1:A:262:ARG:HH11	1:A:262:ARG:CB	2.10	0.64
1:A:68:LYS:HG2	1:A:72:GLN:NE2	2.13	0.64
1:E:222:THR:HG21	2:E:504:NAP:O2A	1.98	0.64
1:A:262:ARG:HB2	1:A:262:ARG:NH1	2.12	0.64
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.79	0.64
1:B:26:GLU:HA	1:B:26:GLU:OE1	1.97	0.63
1:B:222:THR:HG21	2:B:502:NAP:O2A	1.98	0.63
1:B:263:TRP:CH2	1:E:279:LEU:HD21	2.34	0.63
1:A:262:ARG:HH11	1:A:262:ARG:HB2	1.63	0.63
1:A:284:TYR:CE2	1:A:286:MET:HE1	2.34	0.63
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.33	0.63
1:E:243:LEU:HG	1:E:247:LYS:HE3	1.80	0.63
1:B:284:TYR:HD2	1:B:286:MET:HE1	1.62	0.61
1:A:26:GLU:HA	1:A:26:GLU:OE1	2.00	0.61
1:A:262:ARG:HH11	1:A:262:ARG:HA	1.65	0.60
1:E:169:SER:O	2:E:504:NAP:H6N	2.01	0.60
1:D:262:ARG:HH11	1:D:262:ARG:CB	2.14	0.60
1:B:263:TRP:HH2	1:E:279:LEU:CD2	2.15	0.60
1:D:87:HIS:HD2	4:D:916:HOH:O	1.84	0.59
1:E:179:MET:HE3	3:E:604:311:H1B	1.84	0.59
1:B:243:LEU:HG	1:B:247:LYS:HE3	1.85	0.59
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.86	0.58
1:E:44:LYS:HG3	2:E:504:NAP:H3B	1.85	0.58
1:E:140:MET:HA	1:E:140:MET:HE3	1.86	0.58
1:A:222:THR:HG21	2:A:501:NAP:O2A	2.04	0.57
1:B:284:TYR:CE2	1:B:286:MET:HE1	2.39	0.57
1:B:263:TRP:HH2	1:E:279:LEU:HD21	1.68	0.57
1:B:279:LEU:HD21	1:E:263:TRP:CH2	2.39	0.57
1:B:279:LEU:CD2	1:E:263:TRP:HH2	2.18	0.57
1:A:263:TRP:CD1	1:A:263:TRP:N	2.69	0.57
1:D:273:ARG:O	1:D:277:GLU:HG3	2.05	0.57
1:B:94:GLU:OE1	1:B:138:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:TYR:CD2	1:E:286:MET:CE	2.89	0.56
1:A:288:ARG:O	1:A:288:ARG:HG2	2.06	0.56
1:E:262:ARG:HB2	1:E:262:ARG:NH1	2.00	0.56
1:A:178:PRO:O	1:A:179:MET:HB2	2.06	0.56
1:D:263:TRP:N	1:D:263:TRP:CD1	2.72	0.56
1:E:243:LEU:O	1:E:247:LYS:HG3	2.06	0.56
1:A:120:HIS:HE1	1:A:146:SER:OG	1.89	0.55
1:B:23:SER:O	1:B:251:LEU:HD22	2.06	0.55
1:A:87:HIS:HD2	4:A:1025:HOH:O	1.88	0.55
1:E:274:LYS:HD3	4:E:1003:HOH:O	2.06	0.55
1:B:140:MET:HE3	1:B:140:MET:HA	1.88	0.55
1:A:68:LYS:CG	1:A:72:GLN:HE21	2.19	0.55
1:D:262:ARG:HB2	1:D:262:ARG:NH1	2.21	0.55
1:E:140:MET:HE3	1:E:144:PHE:HB3	1.89	0.54
1:A:231:VAL:HG12	1:A:233:MET:CG	2.38	0.54
1:D:145:LEU:HD22	1:E:137:ARG:NH2	2.23	0.54
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.91	0.54
1:D:222:THR:HG21	2:D:503:NAP:O2A	2.08	0.54
1:A:262:ARG:HH11	1:A:262:ARG:CA	2.20	0.53
1:B:243:LEU:O	1:B:247:LYS:HG3	2.08	0.53
1:E:200:GLU:O	1:E:204:SER:OG	2.26	0.53
1:B:255:GLU:OE2	1:B:257:TYR:OH	2.22	0.53
1:D:119:ASN:ND2	2:D:503:NAP:H4D	2.25	0.52
1:D:126:LEU:HD23	1:D:126:LEU:N	2.24	0.52
1:D:140:MET:HA	1:D:140:MET:HE3	1.91	0.52
1:E:219:ASP:OD2	1:E:238:LYS:HG2	2.10	0.52
1:B:169:SER:O	2:B:502:NAP:H6N	2.09	0.51
1:B:55:ALA:HA	1:B:83:ALA:HB2	1.93	0.51
1:D:18:GLN:O	1:D:28:ARG:NH2	2.44	0.51
1:A:270:ASN:HD22	1:A:270:ASN:C	2.13	0.51
1:D:23:SER:O	1:D:251:LEU:HD22	2.10	0.51
1:D:26:GLU:OE1	1:D:26:GLU:HA	2.11	0.50
1:E:231:VAL:CG1	1:E:233:MET:HG2	2.37	0.50
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.93	0.50
1:B:97:THR:O	1:B:101:GLN:HG3	2.11	0.50
1:D:140:MET:HE3	1:D:144:PHE:HB3	1.93	0.50
1:D:68:LYS:HB3	4:D:941:HOH:O	2.10	0.50
1:D:243:LEU:O	1:D:247:LYS:HG3	2.11	0.50
1:A:122:THR:O	1:A:124:THR:HG22	2.12	0.50
1:A:179:MET:CE	1:B:286:MET:SD	3.00	0.50
1:B:200:GLU:O	1:B:204:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HG3	2:D:503:NAP:H3B	1.94	0.49
1:A:140:MET:HE3	1:A:140:MET:CA	2.39	0.49
1:E:120:HIS:HE1	1:E:146:SER:OG	1.96	0.49
1:A:278:GLU:HG2	1:D:266:LEU:HD21	1.95	0.48
1:B:227:VAL:HB	1:B:231:VAL:HB	1.95	0.48
1:B:231:VAL:HG12	1:B:233:MET:CG	2.44	0.48
1:D:261:SER:O	1:D:265:THR:HG23	2.13	0.48
1:B:279:LEU:HD21	1:E:263:TRP:HH2	1.77	0.48
1:E:216:GLY:HA3	1:E:259:ASP:OD2	2.13	0.48
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.96	0.48
1:E:262:ARG:O	1:E:262:ARG:HG3	2.14	0.48
1:B:216:GLY:HA3	1:B:259:ASP:OD2	2.13	0.48
1:D:233:MET:CE	1:E:283:SER:HB2	2.44	0.48
1:A:68:LYS:HD3	1:A:72:GLN:NE2	2.28	0.48
1:D:231:VAL:HG12	1:D:233:MET:CG	2.29	0.47
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.49	0.47
1:B:279:LEU:CD2	1:E:263:TRP:CH2	2.97	0.47
1:A:263:TRP:N	1:A:263:TRP:HD1	2.13	0.47
1:B:53:HIS:O	1:B:57:MET:HG3	2.14	0.47
1:B:136:VAL:HG22	1:B:182:ALA:HB2	1.97	0.47
1:D:169:SER:O	2:D:503:NAP:H6N	2.14	0.47
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.97	0.47
1:A:233:MET:CE	1:B:283:SER:HB2	2.45	0.46
1:A:217:LEU:O	1:A:218:ILE:HD13	2.16	0.46
1:B:64:THR:O	1:B:65:ALA:HB2	2.15	0.46
1:D:120:HIS:HE1	1:D:146:SER:OG	1.97	0.46
1:B:263:TRP:CD1	1:B:263:TRP:N	2.80	0.46
1:E:52:TYR:O	1:E:56:LYS:HG3	2.16	0.46
1:E:141:GLU:HA	1:E:145:LEU:HB2	1.97	0.46
1:A:126:LEU:N	1:A:126:LEU:CD2	2.77	0.46
1:A:137:ARG:NH2	1:B:145:LEU:CD2	2.76	0.46
1:B:287:ASP:OD2	1:B:287:ASP:N	2.38	0.46
1:A:52:TYR:O	1:A:56:LYS:HG3	2.16	0.46
1:E:179:MET:CE	3:E:604:311:H1B	2.45	0.46
1:E:227:VAL:HB	1:E:231:VAL:HB	1.98	0.46
1:D:178:PRO:O	1:D:179:MET:HB2	2.15	0.45
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.16	0.45
1:B:284:TYR:HD2	1:B:286:MET:CE	2.26	0.45
3:B:602:311:H10	3:B:602:311:H2A	1.64	0.45
1:B:141:GLU:HA	1:B:145:LEU:HB2	1.98	0.45
1:B:231:VAL:HG12	1:B:233:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:THR:CB	1:E:120:HIS:HD2	2.29	0.45
1:B:136:VAL:HA	1:B:182:ALA:HB1	1.99	0.45
1:B:262:ARG:O	1:B:262:ARG:HG3	2.15	0.44
1:D:94:GLU:OE1	1:D:138:LYS:HE2	2.16	0.44
1:D:274:LYS:H	1:D:274:LYS:HG2	1.61	0.44
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.83	0.44
1:E:68:LYS:HD2	1:E:72:GLN:NE2	2.32	0.44
1:B:66:ARG:HB2	2:B:502:NAP:O2X	2.17	0.44
1:A:140:MET:O	1:A:144:PHE:HB3	2.17	0.44
1:D:199:LYS:O	1:D:203:VAL:HG13	2.17	0.44
1:B:278:GLU:HG2	1:E:263:TRP:HZ2	1.82	0.43
1:A:200:GLU:O	1:A:204:SER:OG	2.36	0.43
1:E:231:VAL:CG1	1:E:233:MET:CG	2.95	0.43
1:D:227:VAL:HB	1:D:231:VAL:HB	2.01	0.43
1:D:262:ARG:HH11	1:D:262:ARG:HB2	1.77	0.43
1:A:140:MET:HE3	1:A:144:PHE:HB3	2.00	0.42
1:A:284:TYR:CD2	1:A:286:MET:HE1	2.54	0.42
1:B:287:ASP:O	1:B:288:ARG:CB	2.67	0.42
1:D:19:MET:SD	1:D:31:MET:CE	3.08	0.42
1:E:219:ASP:OD1	1:E:237:PRO:HA	2.19	0.42
1:A:248:GLY:HA3	1:A:256:VAL:HG21	2.02	0.42
1:D:144:PHE:O	1:D:147:TYR:HB2	2.20	0.42
1:E:284:TYR:HD2	1:E:286:MET:CE	2.32	0.42
1:B:40:THR:CB	1:B:120:HIS:HD2	2.32	0.42
1:B:125:SER:HB2	4:B:926:HOH:O	2.19	0.42
1:A:273:ARG:O	1:A:277:GLU:HG3	2.21	0.41
1:E:161:SER:O	1:E:162:ASN:HB2	2.20	0.41
1:E:42:ALA:HB3	1:E:63:VAL:HB	2.03	0.41
1:A:176:ALA:HB2	1:B:195:SER:HB3	2.02	0.41
1:B:169:SER:N	1:B:213:CYS:O	2.45	0.41
1:A:140:MET:HA	1:A:140:MET:CE	2.47	0.41
1:A:161:SER:O	1:A:162:ASN:HB2	2.20	0.41
1:A:199:LYS:O	1:A:203:VAL:HG13	2.21	0.41
1:B:287:ASP:O	1:B:288:ARG:HB3	2.20	0.41
1:A:287:ASP:OD2	1:A:287:ASP:N	2.54	0.41
3:A:601:311:H10	3:A:601:311:H2A	1.82	0.41
1:B:140:MET:HE3	1:B:144:PHE:HB3	2.03	0.41
1:D:263:TRP:N	1:D:263:TRP:HD1	2.19	0.41
1:E:148:VAL:O	1:E:152:VAL:HG23	2.21	0.41
1:E:286:MET:HE3	1:E:286:MET:HB2	1.79	0.41
1:A:120:HIS:CE1	1:A:146:SER:OG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD12	1:D:253:GLN:HE21	1.86	0.41
1:D:52:TYR:O	1:D:56:LYS:HG3	2.21	0.40
1:A:141:GLU:HA	1:A:145:LEU:HB2	2.03	0.40
1:D:185:ALA:HB2	1:E:193:PHE:HB2	2.03	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	264/286 (92%)	253 (96%)	9 (3%)	2 (1%)	19 20
1	B	278/286 (97%)	265 (95%)	13 (5%)	0	100 100
1	D	272/286 (95%)	261 (96%)	9 (3%)	2 (1%)	22 23
1	E	262/286 (92%)	252 (96%)	10 (4%)	0	100 100
All	All	1076/1144 (94%)	1031 (96%)	41 (4%)	4 (0%)	34 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ARG
1	D	219	ASP
1	A	65	ALA
1	D	65	ALA

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	222/237 (94%)	205 (92%)	17 (8%)	13 12
1	B	230/237 (97%)	209 (91%)	21 (9%)	9 8
1	D	223/237 (94%)	206 (92%)	17 (8%)	13 13
1	E	220/237 (93%)	201 (91%)	19 (9%)	10 9
All	All	895/948 (94%)	821 (92%)	74 (8%)	11 11

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	44	LYS
1	A	68	LYS
1	A	124	THR
1	A	145	LEU
1	A	160	GLN
1	A	204	SER
1	A	222	THR
1	A	225	LYS
1	A	232	HIS
1	A	233	MET
1	A	262	ARG
1	A	266	LEU
1	A	270	ASN
1	A	278	GLU
1	A	286	MET
1	A	287	ASP
1	B	26	GLU
1	B	28	ARG
1	B	44	LYS
1	B	68	LYS
1	B	101	GLN
1	B	124	THR
1	B	145	LEU
1	B	160	GLN
1	B	204	SER
1	B	205	ARG
1	B	222	THR
1	B	225	LYS
1	B	233	MET

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Mol	Chain	Res	Type
1	B	262	ARG
1	B	265	THR
1	B	266	LEU
1	B	270	ASN
1	B	278	GLU
1	B	286	MET
1	B	287	ASP
1	B	288	ARG
1	D	23	SER
1	D	24	ASN
1	D	26	GLU
1	D	44	LYS
1	D	68	LYS
1	D	124	THR
1	D	145	LEU
1	D	160	GLN
1	D	204	SER
1	D	205	ARG
1	D	222	THR
1	D	225	LYS
1	D	240	GLU
1	D	262	ARG
1	D	270	ASN
1	D	274	LYS
1	D	278	GLU
1	E	26	GLU
1	E	44	LYS
1	E	68	LYS
1	E	85	SER
1	E	128	LEU
1	E	145	LEU
1	E	160	GLN
1	E	204	SER
1	E	205	ARG
1	E	222	THR
1	E	225	LYS
1	E	233	MET
1	E	262	ARG
1	E	265	THR
1	E	266	LEU
1	E	270	ASN
1	E	278	GLU

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Mol	Chain	Res	Type
1	E	286	MET
1	E	287	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	270	ASN
1	D	24	ASN
1	D	87	HIS
1	D	119	ASN
1	D	120	HIS
1	D	253	GLN
1	D	270	ASN
1	E	119	ASN
1	E	120	HIS
1	E	270	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 monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	311	B	602	-	26,26,26	2.19	8 (30%)	38,38,38	2.05	14 (36%)
2	NAP	D	503	-	45,52,52	0.89	1 (2%)	56,80,80	0.99	3 (5%)
2	NAP	B	502	-	45,52,52	1.25	3 (6%)	56,80,80	0.94	1 (1%)
2	NAP	A	501	-	45,52,52	1.19	5 (11%)	56,80,80	1.07	4 (7%)
3	311	E	604	-	26,26,26	2.56	16 (61%)	38,38,38	2.97	21 (55%)
2	NAP	E	504	-	45,52,52	1.08	2 (4%)	56,80,80	1.15	3 (5%)
3	311	D	603	-	26,26,26	2.20	9 (34%)	38,38,38	2.47	13 (34%)
3	311	A	601	-	26,26,26	2.01	10 (38%)	38,38,38	2.41	15 (39%)

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	311	B	602	-	-	0/12/24/24	0/3/3/3
2	NAP	D	503	-	-	3/31/67/67	0/5/5/5
2	NAP	B	502	-	-	4/31/67/67	0/5/5/5
2	NAP	A	501	-	-	2/31/67/67	0/5/5/5
3	311	E	604	-	-	1/12/24/24	0/3/3/3
2	NAP	E	504	-	-	4/31/67/67	0/5/5/5
3	311	D	603	-	-	0/12/24/24	0/3/3/3
3	311	A	601	-	-	0/12/24/24	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	604	311	C7-C14	5.23	1.51	1.39
3	B	602	311	C2-C20	4.99	1.63	1.53
2	B	502	NAP	O4B-C1B	4.95	1.48	1.41
3	D	603	311	C11-C20	4.85	1.61	1.53
3	A	601	311	C17-N21	4.56	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	311	C11-C10	4.45	1.63	1.52
2	A	501	NAP	O4B-C1B	4.17	1.46	1.41
3	E	604	311	C8-C7	4.06	1.46	1.38
3	D	603	311	C12-N22	3.93	1.54	1.47
3	A	601	311	C8-C7	3.81	1.45	1.38
3	D	603	311	C6-C17	3.76	1.46	1.39
3	E	604	311	C13-C20	3.72	1.60	1.52
3	E	604	311	C16-N21	3.58	1.40	1.34
3	E	604	311	C8-C15	3.45	1.46	1.39
3	D	603	311	C13-N22	3.44	1.50	1.46
3	B	602	311	C19-N22	3.33	1.42	1.34
3	B	602	311	C14-C18	3.30	1.41	1.37
3	E	604	311	C11-C20	3.27	1.59	1.53
3	D	603	311	C3-C20	3.26	1.59	1.53
2	A	501	NAP	C7N-N7N	3.14	1.39	1.33
3	E	604	311	C12-N22	3.08	1.52	1.47
3	A	601	311	C8-C15	3.03	1.45	1.39
2	E	504	NAP	O4B-C1B	3.00	1.45	1.41
2	D	503	NAP	O4B-C1B	2.98	1.45	1.41
3	A	601	311	C15-C16	2.94	1.53	1.48
3	B	602	311	C9-C18	2.94	1.42	1.37
3	A	601	311	C12-N22	2.91	1.52	1.47
3	A	601	311	C13-N22	2.91	1.49	1.46
3	D	603	311	C15-C16	-2.88	1.44	1.48
3	E	604	311	C6-C17	-2.83	1.33	1.39
3	E	604	311	C17-N21	2.83	1.38	1.34
3	B	602	311	C13-C20	2.77	1.58	1.52
3	E	604	311	C2-C20	2.74	1.58	1.53
3	E	604	311	C4-C6	-2.64	1.33	1.38
3	A	601	311	F24-C18	-2.49	1.29	1.35
3	D	603	311	C8-C7	2.48	1.43	1.38
3	E	604	311	C15-C16	2.48	1.52	1.48
3	A	601	311	O23-C19	2.46	1.27	1.22
3	E	604	311	C1-C14	2.43	1.55	1.51
3	D	603	311	C9-C18	2.43	1.41	1.37
3	B	602	311	C3-C20	2.38	1.58	1.53
3	B	602	311	C13-N22	2.37	1.49	1.46
3	D	603	311	C2-C20	2.33	1.58	1.53
3	E	604	311	O23-C19	2.28	1.27	1.22
2	B	502	NAP	O4D-C1D	2.20	1.44	1.41
3	E	604	311	C9-C15	2.18	1.43	1.39
3	E	604	311	C11-C10	2.14	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	NAP	C7N-N7N	2.13	1.37	1.33
2	E	504	NAP	P2B-O2B	2.11	1.63	1.59
2	A	501	NAP	P2B-O2B	2.10	1.63	1.59
2	A	501	NAP	C2A-N3A	2.04	1.35	1.32
2	A	501	NAP	C3D-C4D	2.02	1.58	1.53
3	A	601	311	C13-C20	2.01	1.56	1.52
3	A	601	311	C4-C6	2.01	1.43	1.38

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	603	311	C20-C13-N22	-7.23	105.16	111.69
3	D	603	311	C11-C20-C13	6.60	111.80	108.26
3	E	604	311	C20-C13-N22	-6.58	105.75	111.69
3	E	604	311	C8-C15-C16	6.21	131.09	121.28
3	E	604	311	C8-C7-C14	-5.79	113.17	121.97
3	A	601	311	C9-C18-C14	5.62	127.99	124.39
3	A	601	311	C8-C15-C16	5.04	129.25	121.28
3	A	601	311	C8-C7-C14	-4.91	114.52	121.97
3	E	604	311	C9-C15-C16	-4.82	113.61	120.59
3	E	604	311	C1-C14-C18	-4.71	116.27	121.75
3	E	604	311	C5-C16-N21	-4.70	115.88	121.97
3	D	603	311	C6-C17-C19	4.54	127.60	119.21
3	B	602	311	C10-C11-C20	-4.50	107.13	113.00
3	A	601	311	C1-C14-C18	-4.45	116.56	121.75
3	E	604	311	C12-N22-C13	4.40	121.39	114.27
3	B	602	311	C11-C20-C13	-4.21	106.00	108.26
3	A	601	311	C20-C13-N22	-4.14	107.95	111.69
3	B	602	311	C6-C17-C19	4.01	126.63	119.21
3	B	602	311	C1-C14-C18	-3.90	117.21	121.75
3	E	604	311	C10-C12-N22	-3.86	103.03	110.66
3	D	603	311	C1-C14-C18	-3.75	117.38	121.75
3	E	604	311	C3-C20-C2	-3.71	102.59	109.36
3	D	603	311	C19-C17-N21	-3.55	109.57	117.38
3	E	604	311	C6-C4-C5	3.45	125.14	120.25
3	E	604	311	C7-C8-C15	3.36	125.97	121.13
3	E	604	311	C3-C20-C13	3.34	117.09	109.54
3	A	601	311	C10-C11-C20	-3.26	108.75	113.00
2	A	501	NAP	C5A-C6A-N6A	3.19	125.21	120.35
3	D	603	311	C10-C11-C20	-3.19	108.85	113.00
3	A	601	311	C7-C8-C15	3.15	125.67	121.13
2	E	504	NAP	C5A-C6A-N6A	3.14	125.12	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	NAP	C5A-C6A-N6A	3.12	125.10	120.35
3	A	601	311	C8-C15-C9	-2.99	113.94	118.16
3	B	602	311	C11-C10-C12	-2.93	105.74	110.69
3	D	603	311	C9-C15-C16	-2.84	116.47	120.59
2	E	504	NAP	O7N-C7N-N7N	-2.84	118.55	122.58
3	E	604	311	F24-C18-C9	-2.83	112.98	118.61
3	D	603	311	C1-C14-C7	2.77	125.72	120.31
3	A	601	311	C1-C14-C7	2.76	125.69	120.31
3	D	603	311	C15-C16-N21	-2.75	112.11	116.02
2	A	501	NAP	O4D-C4D-C5D	-2.75	100.34	109.37
3	D	603	311	C8-C15-C16	2.70	125.54	121.28
3	A	601	311	C9-C15-C16	-2.62	116.79	120.59
3	D	603	311	C3-C20-C11	-2.58	106.17	110.05
3	D	603	311	C2-C20-C11	2.57	113.91	110.05
3	A	601	311	C5-C16-C15	2.57	126.94	121.93
3	B	602	311	O23-C19-N22	2.56	126.57	122.34
3	B	602	311	C5-C16-N21	-2.55	118.66	121.97
3	A	601	311	C4-C6-C17	-2.54	115.56	118.63
3	B	602	311	C2-C20-C11	-2.54	106.23	110.05
3	E	604	311	C9-C18-C14	2.51	126.00	124.39
2	A	501	NAP	O2B-P2B-O1X	-2.48	99.82	109.39
3	E	604	311	O23-C19-N22	-2.42	118.34	122.34
3	D	603	311	O23-C19-C17	-2.39	114.38	119.00
2	E	504	NAP	O2N-PN-O1N	2.37	123.97	112.24
3	A	601	311	C5-C16-N21	-2.27	119.03	121.97
3	A	601	311	C4-C5-C16	2.27	121.99	118.90
3	B	602	311	C1-C14-C7	2.26	124.72	120.31
3	B	602	311	C6-C17-N21	-2.24	120.30	122.92
3	E	604	311	C4-C6-C17	-2.21	115.96	118.63
3	B	602	311	C19-C17-N21	-2.18	112.58	117.38
3	B	602	311	O23-C19-C17	-2.18	114.80	119.00
3	E	604	311	C3-C20-C11	-2.16	106.80	110.05
2	D	503	NAP	C5A-C6A-N6A	2.15	123.62	120.35
3	B	602	311	C9-C15-C16	-2.13	117.51	120.59
3	B	602	311	C3-C20-C13	2.12	114.31	109.54
3	E	604	311	F24-C18-C14	2.11	120.99	117.84
3	E	604	311	C1-C14-C7	2.11	124.43	120.31
2	D	503	NAP	O2B-C2B-C3B	-2.10	104.06	111.68
2	D	503	NAP	O3B-C3B-C2B	-2.09	105.22	111.17
3	E	604	311	C8-C15-C9	-2.05	115.26	118.16
3	E	604	311	C13-N22-C19	-2.04	114.32	120.94
3	A	601	311	O23-C19-C17	-2.01	115.11	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	O2N-PN-O1N	2.00	122.14	112.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	NAP	C2B-O2B-P2B-O2X
2	E	504	NAP	C3B-C2B-O2B-P2B
3	E	604	311	O23-C19-N22-C13
2	E	504	NAP	C1B-C2B-O2B-P2B
2	B	502	NAP	C2B-O2B-P2B-O1X
2	D	503	NAP	O4B-C4B-C5B-O5B
2	D	503	NAP	C3B-C2B-O2B-P2B
2	B	502	NAP	O4B-C4B-C5B-O5B
2	A	501	NAP	C2B-O2B-P2B-O2X
2	D	503	NAP	C5D-O5D-PN-O3
2	E	504	NAP	O4B-C4B-C5B-O5B
2	B	502	NAP	PN-O3-PA-O1A
2	E	504	NAP	PN-O3-PA-O2A
2	A	501	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

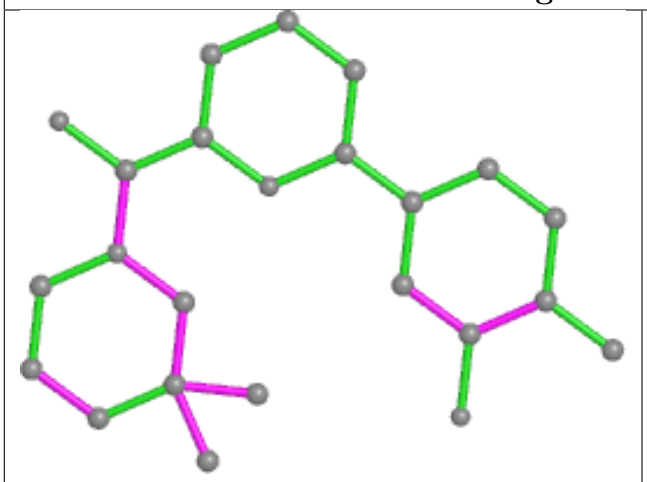
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	311	1	0
2	D	503	NAP	4	0
2	B	502	NAP	4	0
2	A	501	NAP	1	0
3	E	604	311	2	0
2	E	504	NAP	3	0
3	A	601	311	1	0

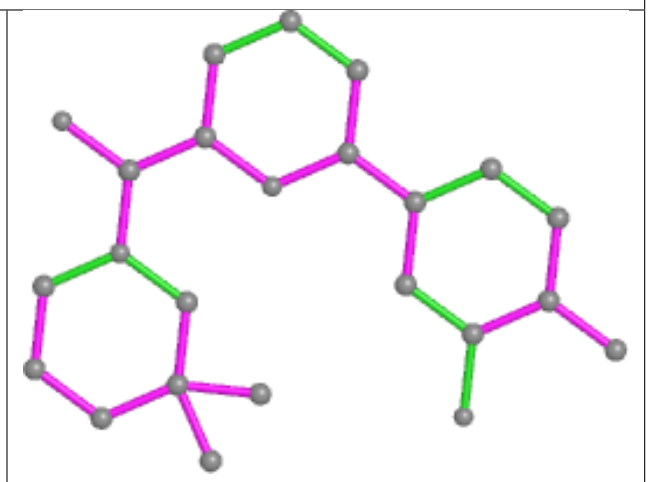
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

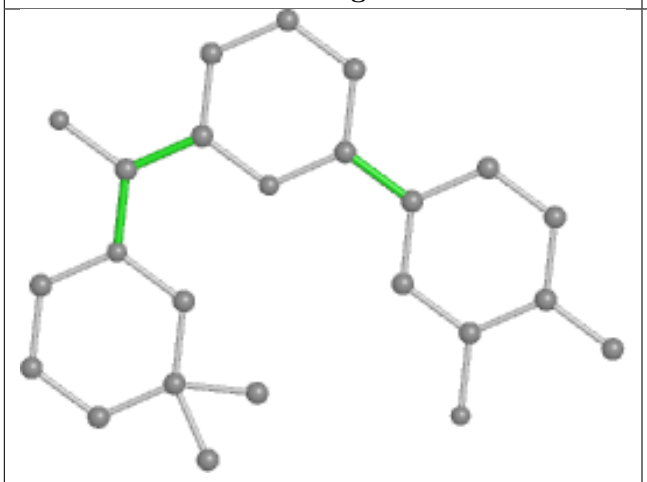
Ligand 311 B 602



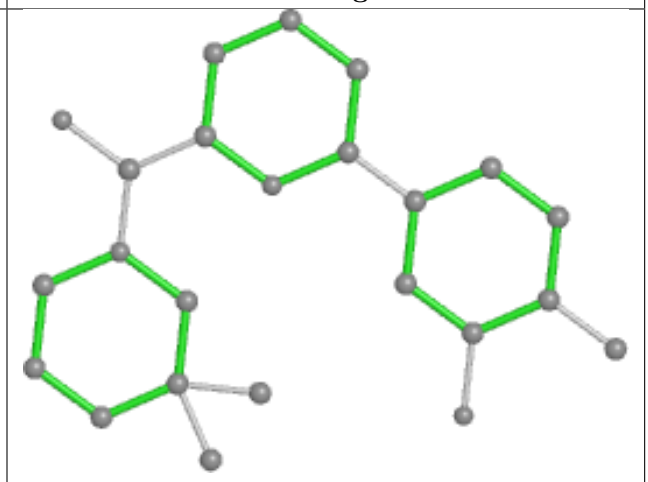
Bond lengths



Bond angles

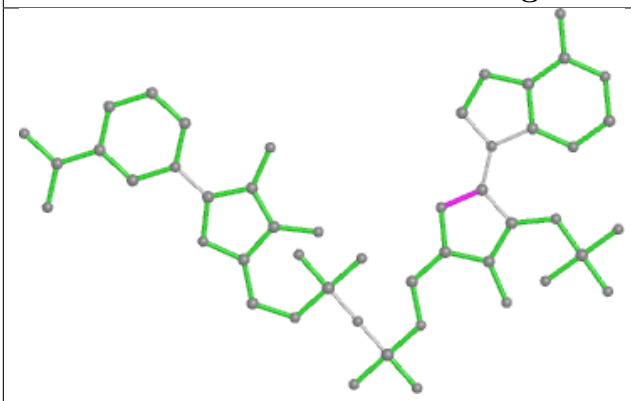


Torsions

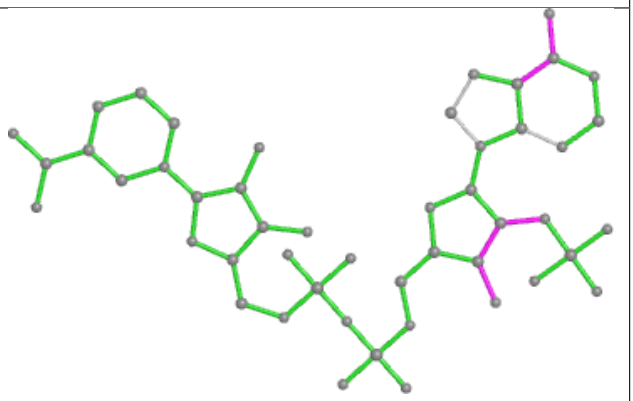


Rings

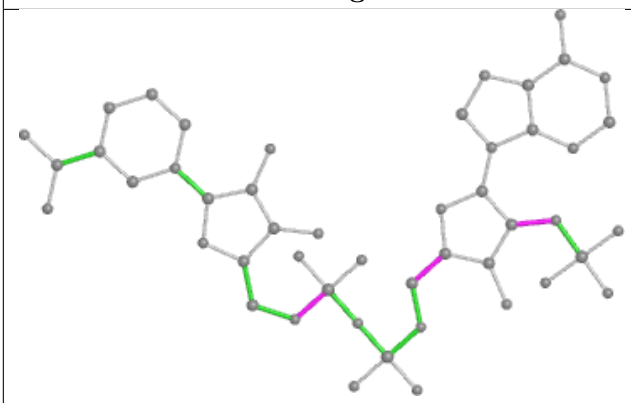
Ligand NAP D 503



Bond lengths



Bond angles



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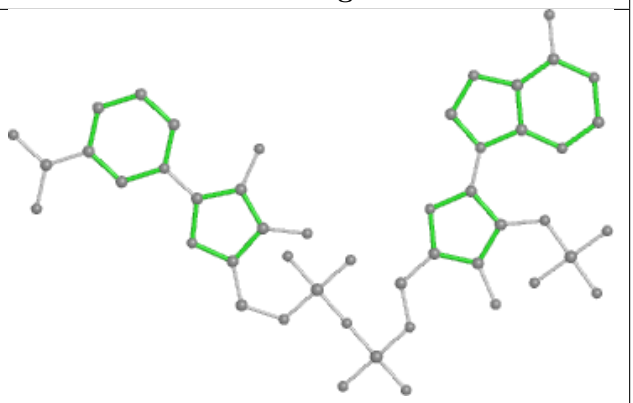
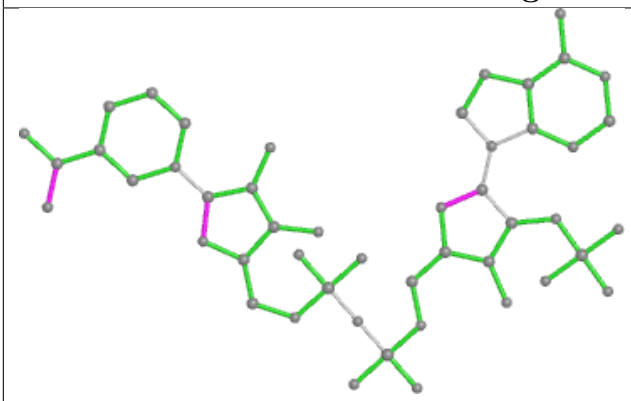
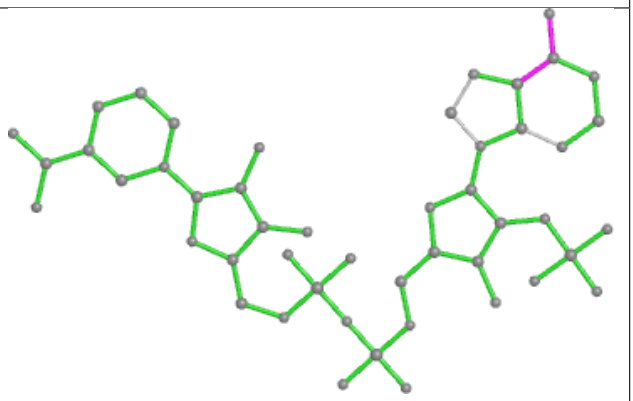


Rings

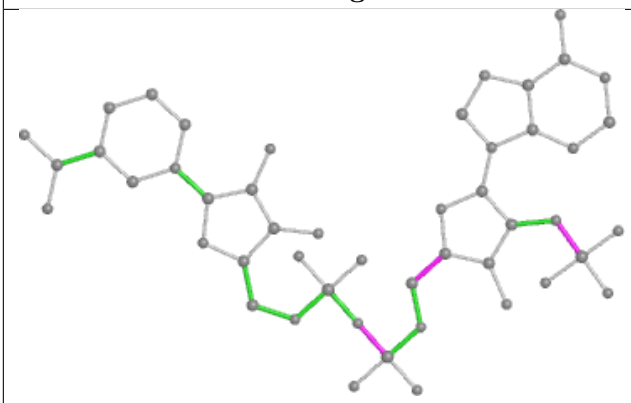
Ligand NAP B 502



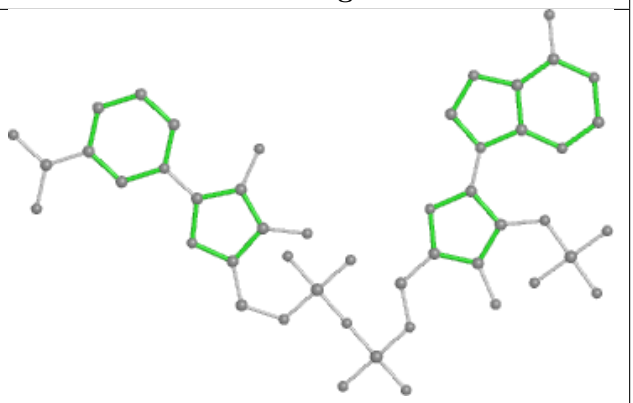
Bond lengths



Bond angles

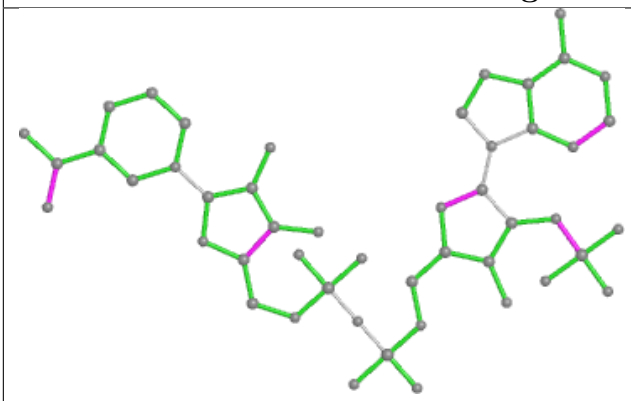


Torsions

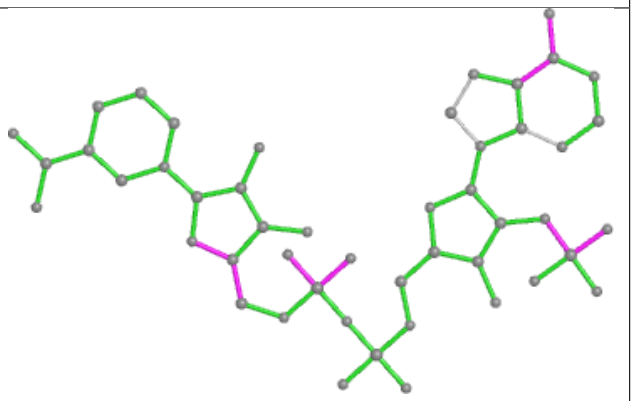


Rings

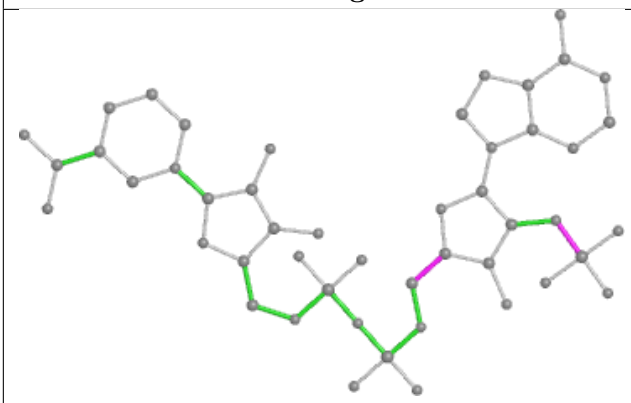
Ligand NAP A 501



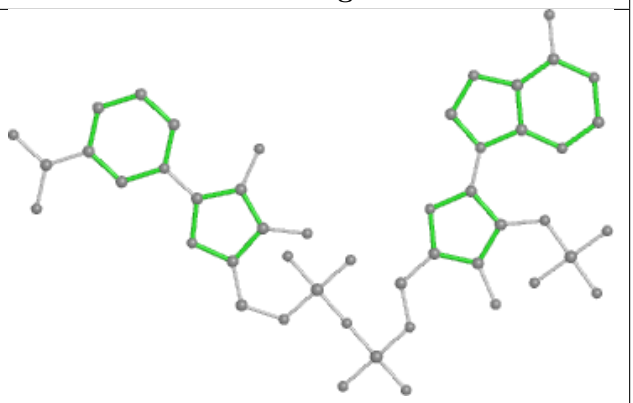
Bond lengths



Bond angles

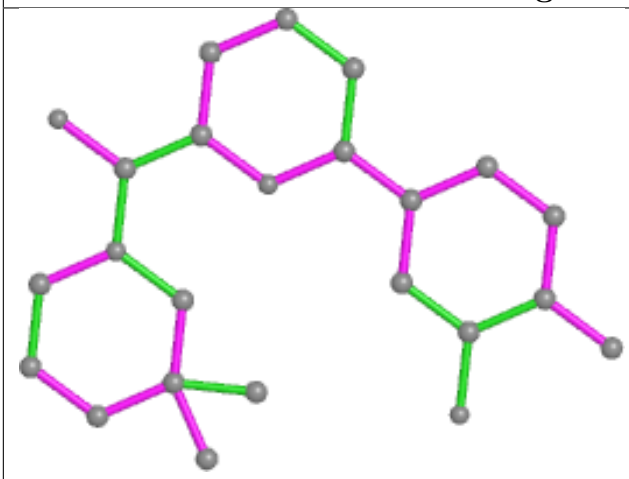


Torsions

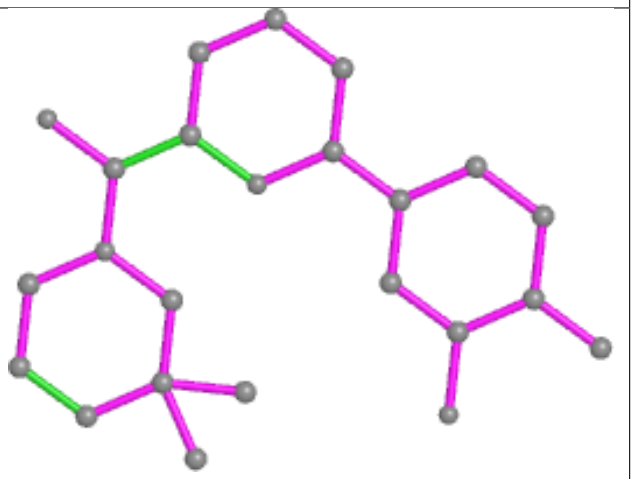


Rings

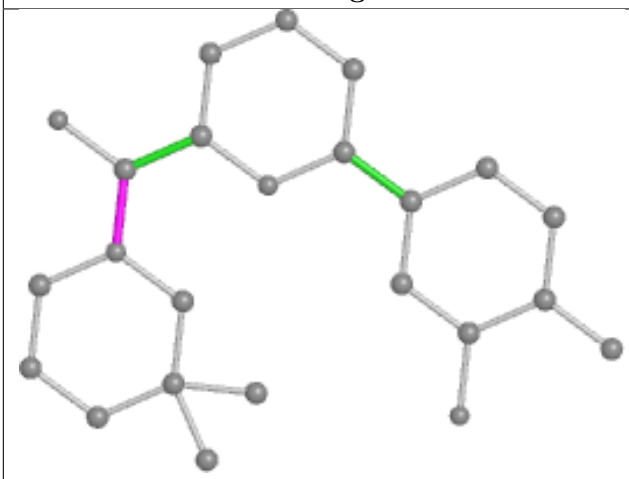
Ligand 311 E 604



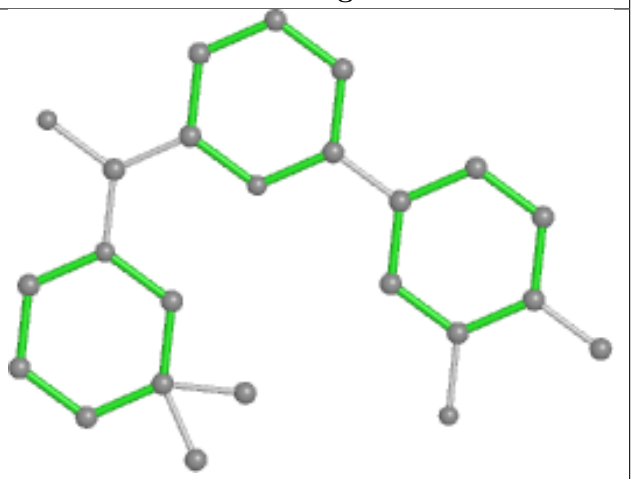
Bond lengths



Bond angles

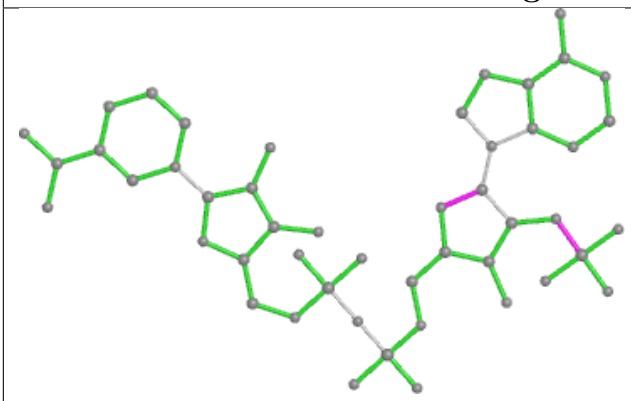


Torsions

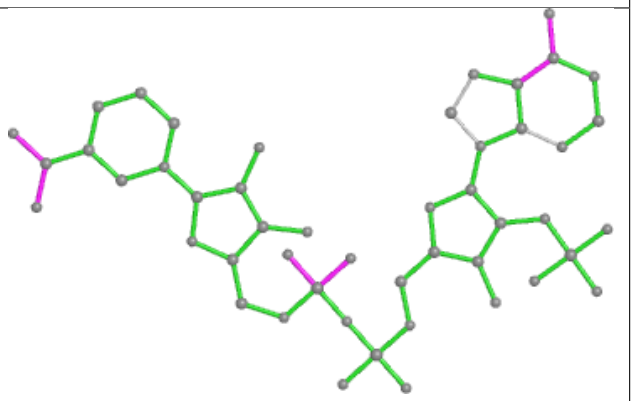


Rings

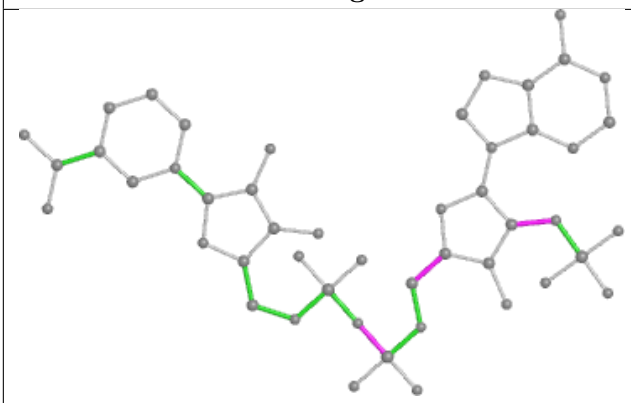
Ligand NAP E 504



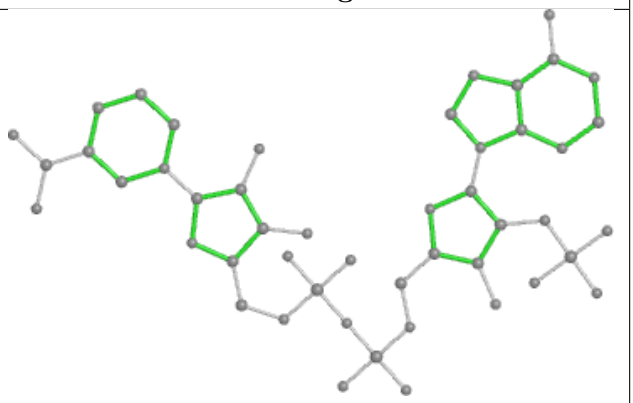
Bond lengths



Bond angles

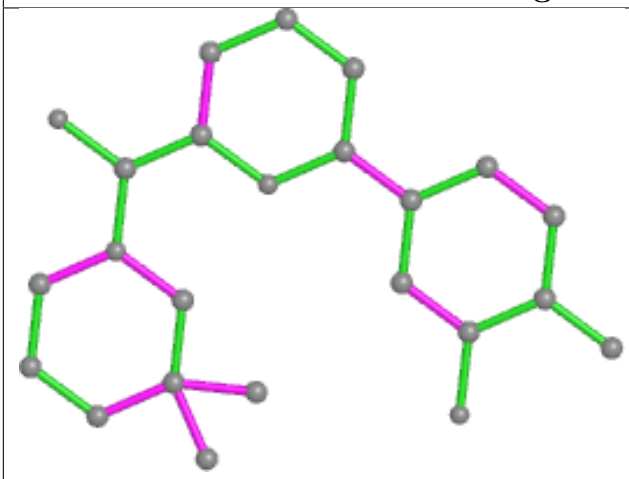


Torsions

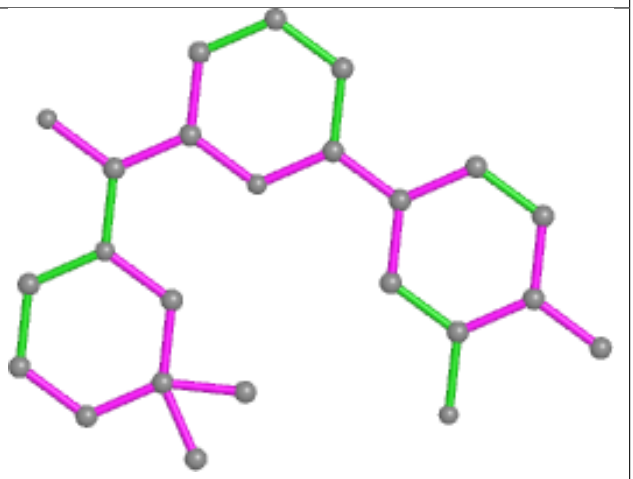


Rings

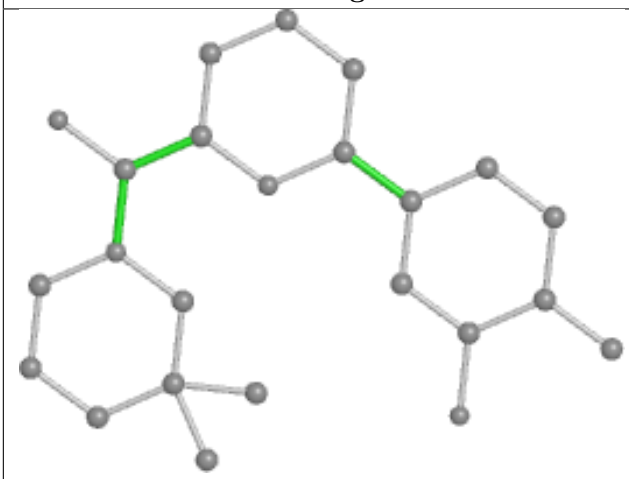
Ligand 311 D 603



Bond lengths



Bond angles



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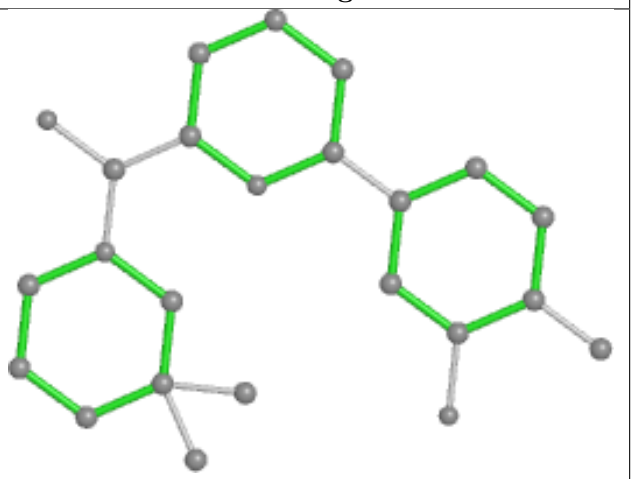
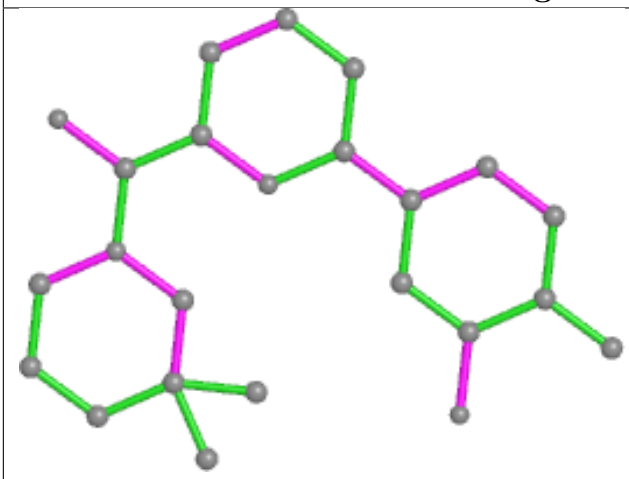
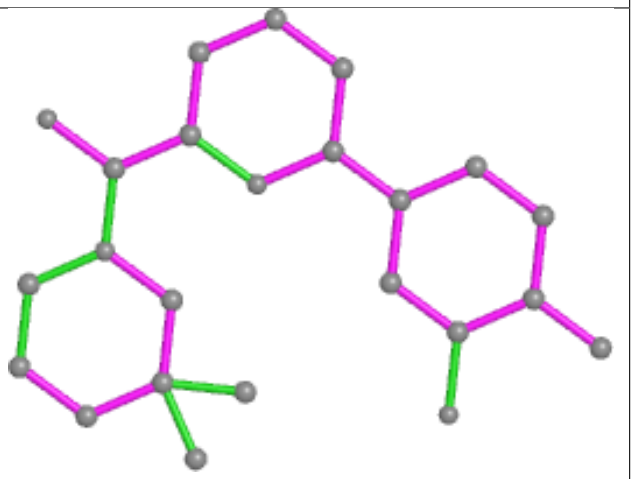


Rings

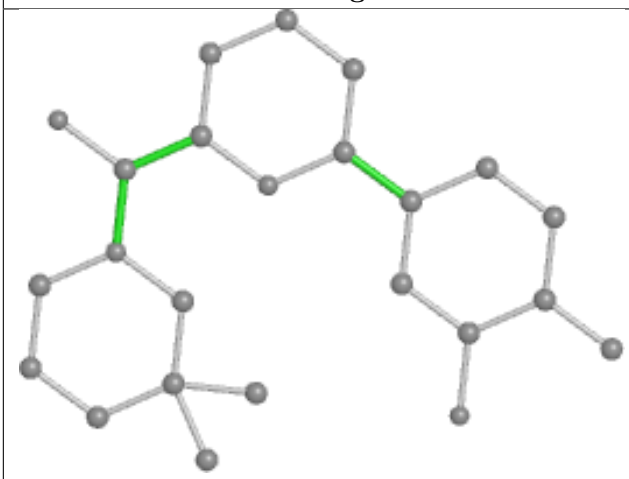
Ligand 311 A 601



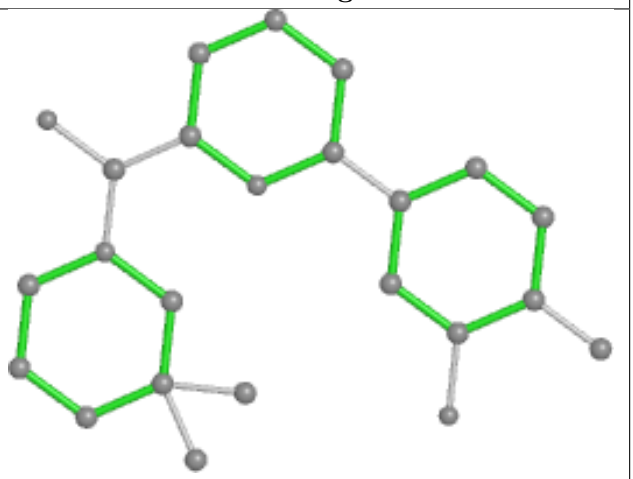
Bond lengths



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	264/286 (92%)	-0.15	9 (3%)	45	57	17, 29, 56, 100	0
1	B	279/286 (97%)	-0.14	9 (3%)	47	59	18, 30, 60, 100	0
1	D	273/286 (95%)	-0.21	8 (2%)	51	62	14, 26, 66, 86	0
1	E	263/286 (91%)	0.03	9 (3%)	45	57	18, 31, 58, 86	0
All	All	1079/1144 (94%)	-0.12	35 (3%)	47	59	14, 29, 60, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	SER	5.1
1	D	23	SER	5.1
1	E	263	TRP	4.9
1	E	25	GLU	4.3
1	D	262	ARG	4.0
1	D	13	MET	3.9
1	E	285	ASN	3.6
1	A	288	ARG	3.6
1	E	205	ARG	3.4
1	D	24	ASN	3.4
1	E	286	MET	3.3
1	D	22	GLY	3.1
1	B	262	ARG	3.1
1	B	24	ASN	3.0
1	E	203	VAL	3.0
1	A	266	LEU	2.9
1	A	232	HIS	2.9
1	D	205	ARG	2.8
1	B	168	VAL	2.7
1	E	287	ASP	2.7
1	A	234	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	25	GLU	2.6
1	B	203	VAL	2.6
1	B	10	MET	2.6
1	A	233	MET	2.4
1	B	205	ARG	2.4
1	B	12	SER	2.4
1	E	262	ARG	2.4
1	B	190	LEU	2.4
1	E	279	LEU	2.4
1	A	205	ARG	2.3
1	A	263	TRP	2.2
1	D	21	ARG	2.1
1	A	203	VAL	2.1
1	A	289	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

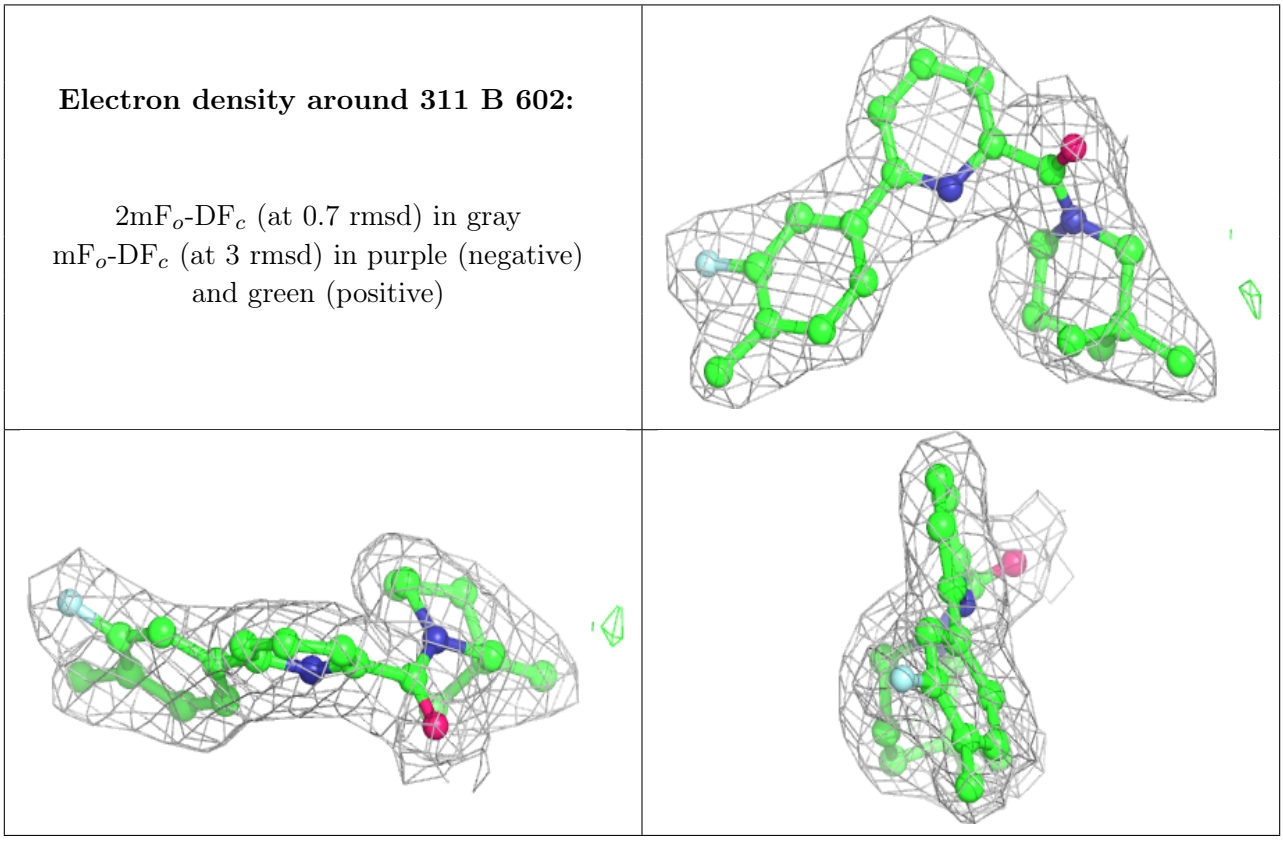
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	311	B	602	24/24	0.95	0.12	12,21,26,27	0
3	311	A	601	24/24	0.96	0.11	18,25,37,38	0
2	NAP	E	504	48/48	0.97	0.10	24,25,29,30	0
2	NAP	A	501	48/48	0.97	0.09	22,23,26,28	0
2	NAP	B	502	48/48	0.97	0.10	20,23,27,28	0
3	311	D	603	24/24	0.97	0.10	11,18,27,28	0
3	311	E	604	24/24	0.97	0.09	16,22,30,43	0
2	NAP	D	503	48/48	0.98	0.09	18,20,24,26	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.

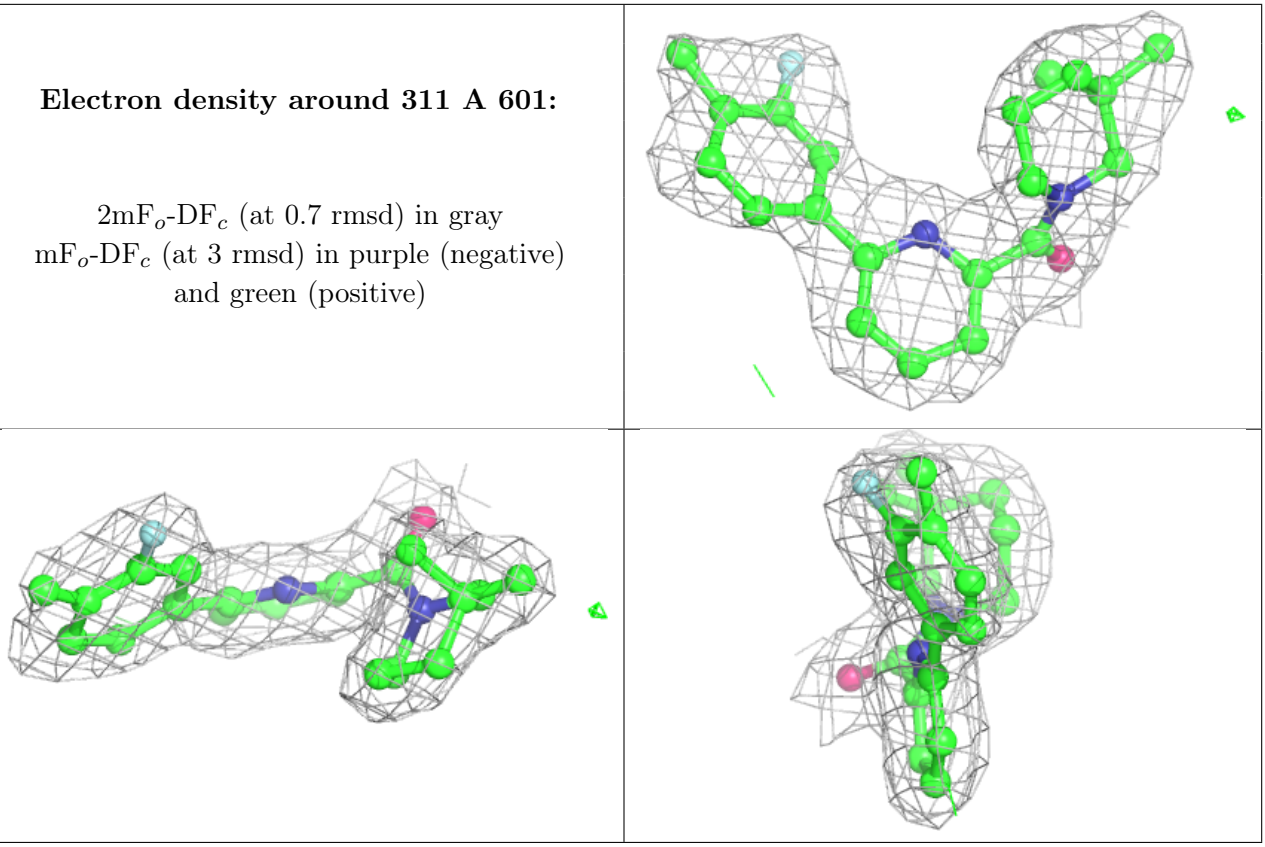
Electron density around 311 B 602:

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



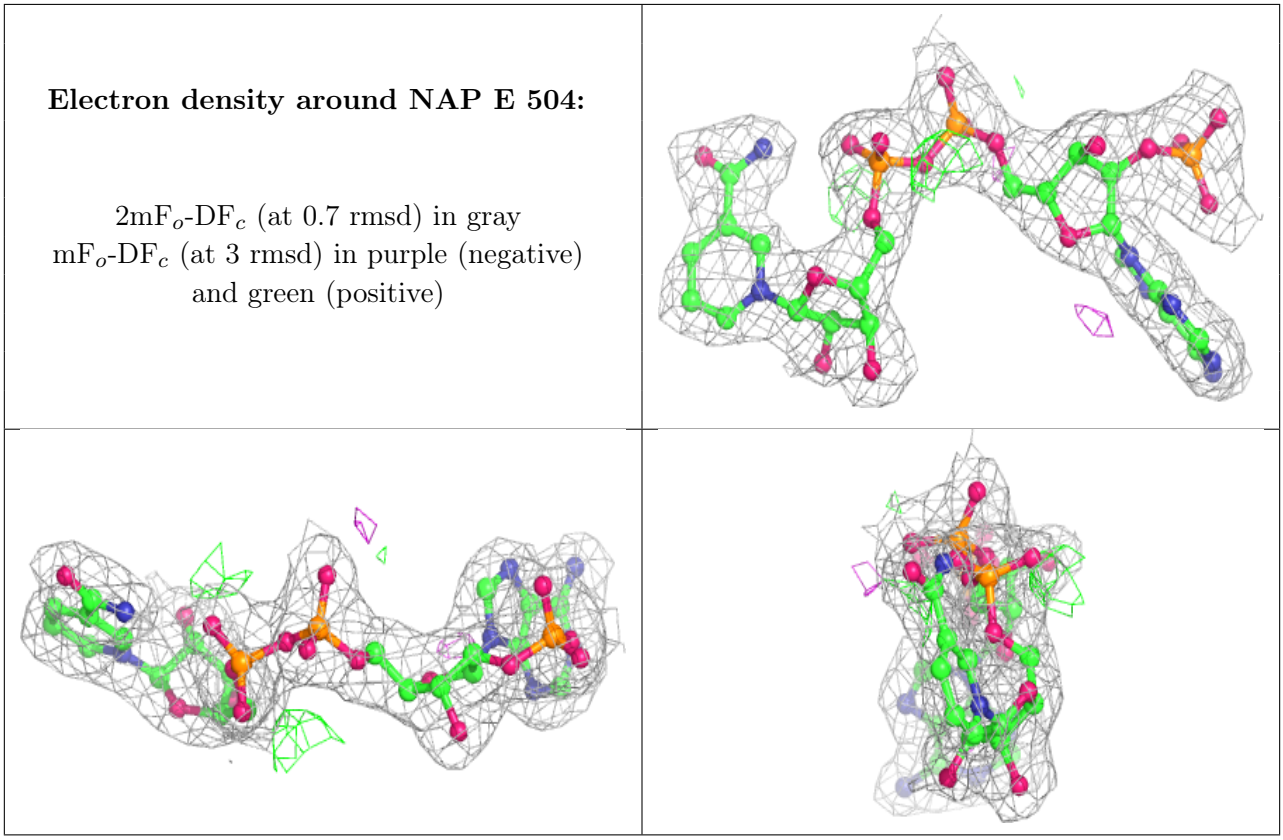
Electron density around 311 A 601:

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



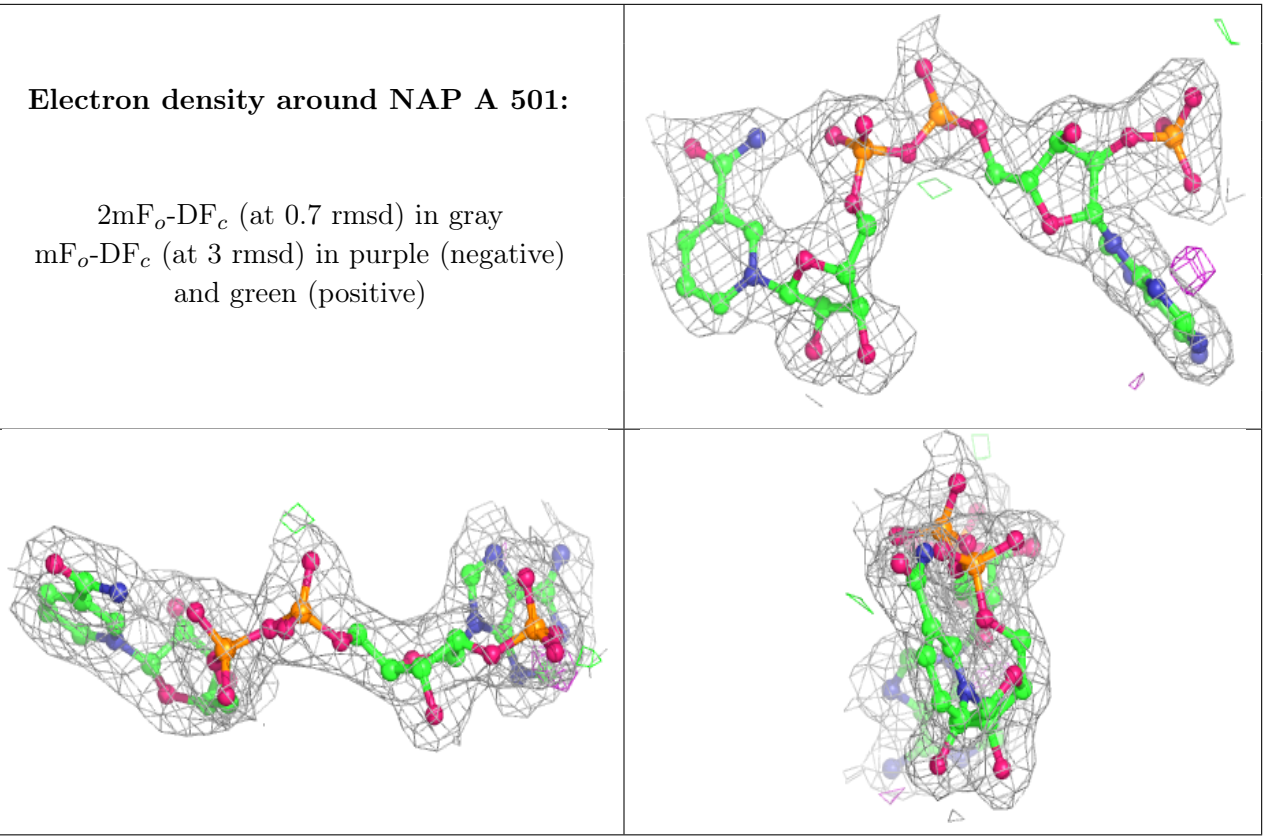
Electron density around NAP E 504:

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



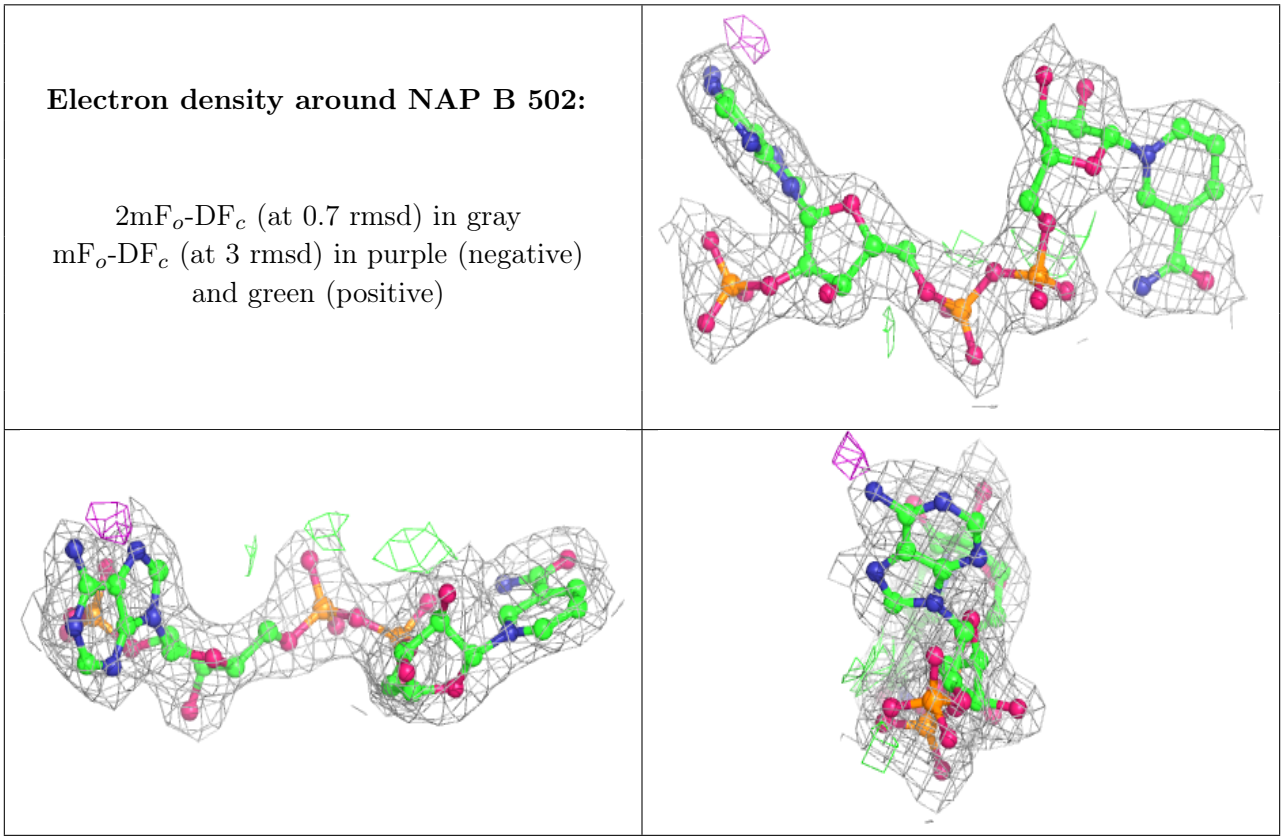
Electron density around NAP A 501:

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



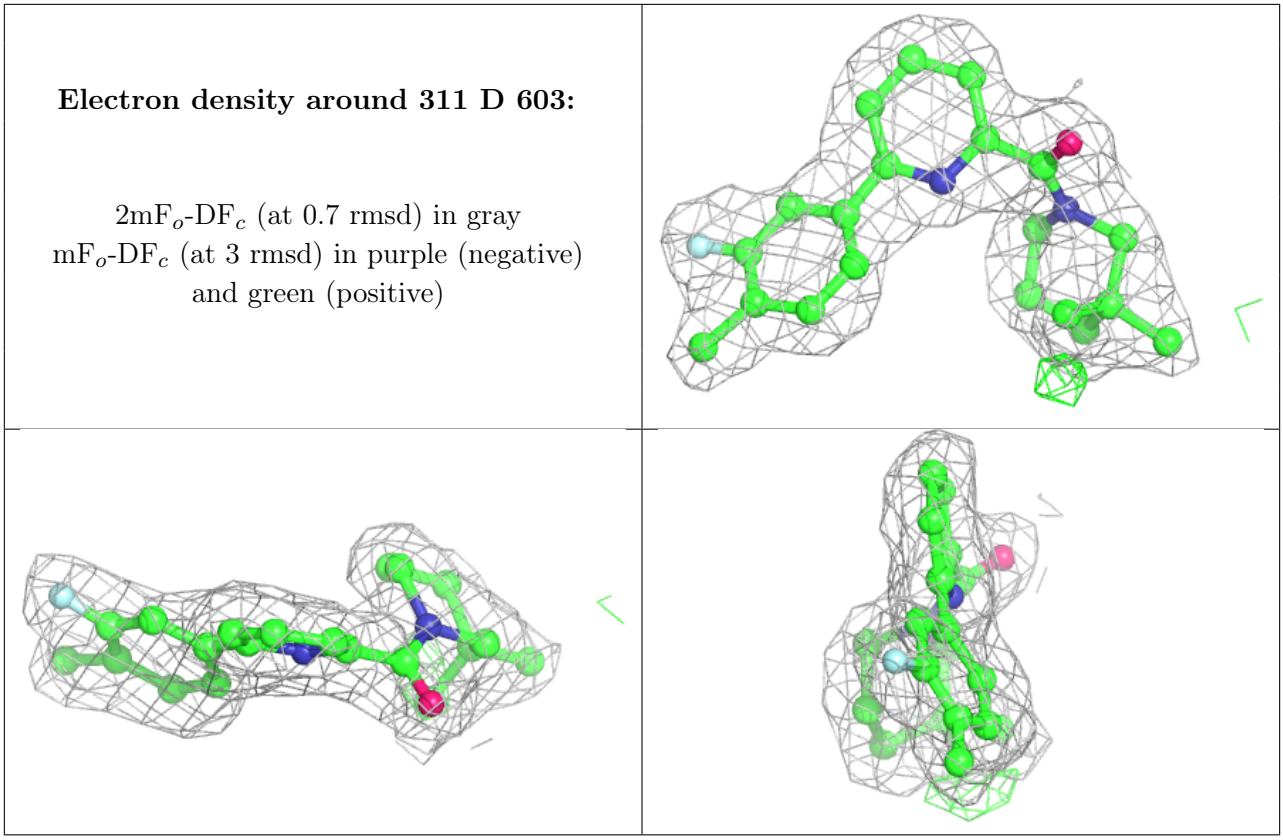
Electron density around NAP B 502:

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



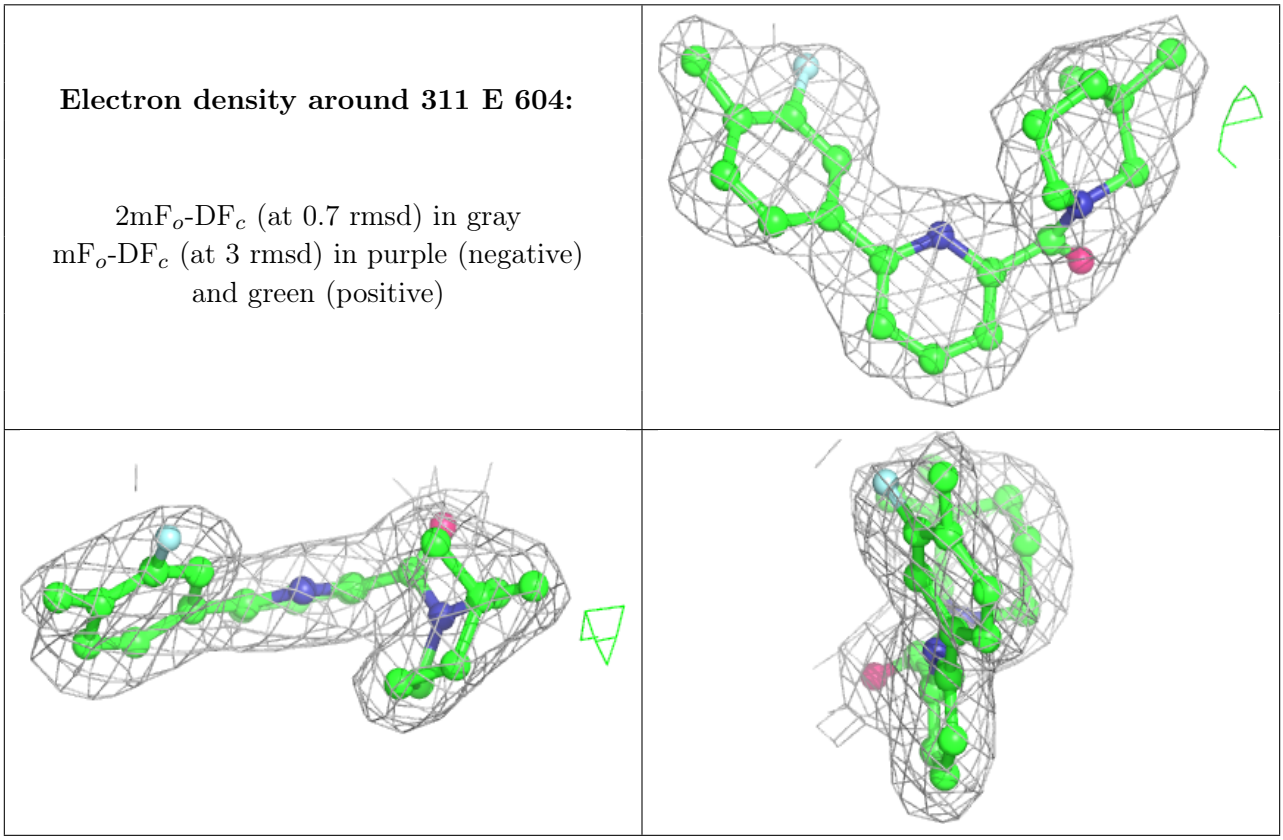
Electron density around 311 D 603:

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



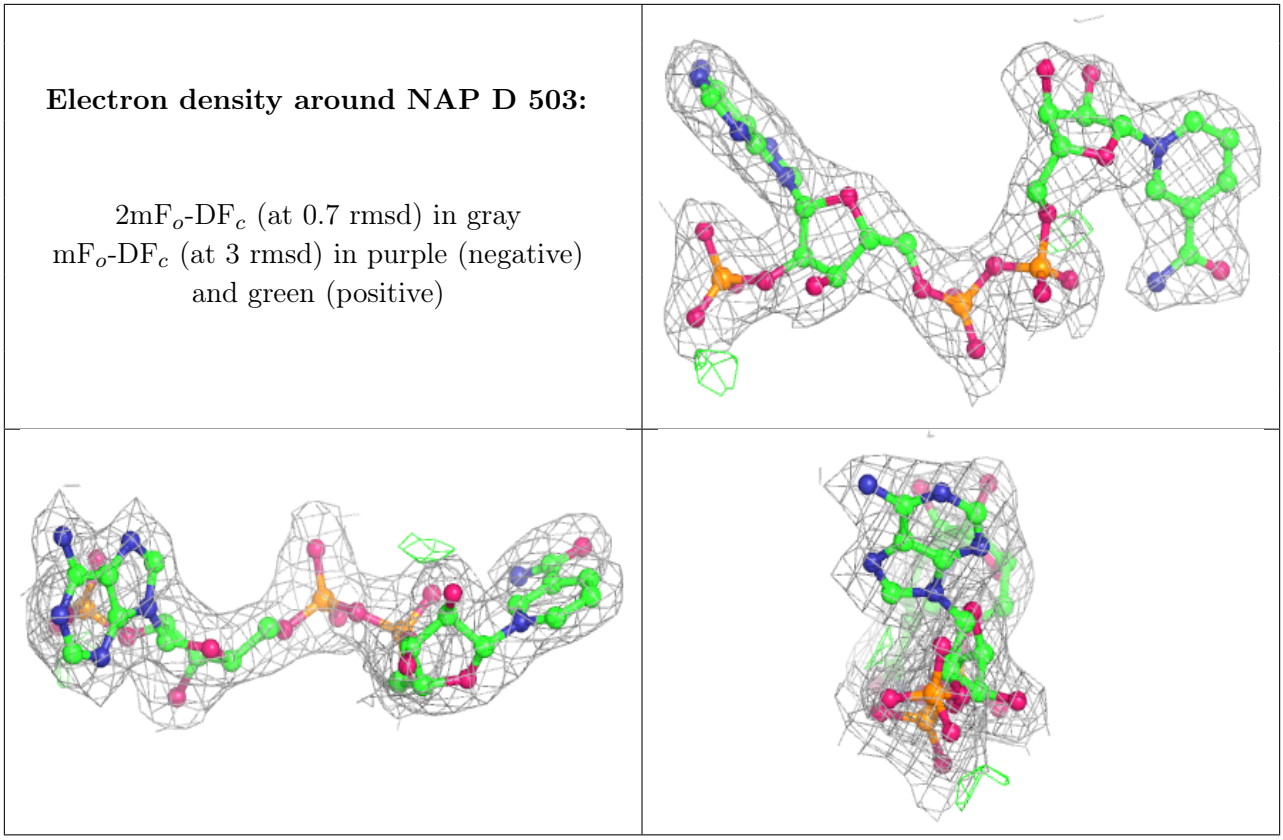
Electron density around 311 E 604:

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



Electron density around NAP D 503:

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



6.5 Other polymers (i)

There are no such residues in this entry.