Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:25 pm BST

PDB ID	:	6EOD
Title	:	Structure of Reductive Aminase from Aspergillus terreus in complex with NADPH
Authors	:	Sharma, M.; Mangas-Sanchez, J.; Turner, N.J.; Grogan, G.
Deposited on	:	2017-10-09
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

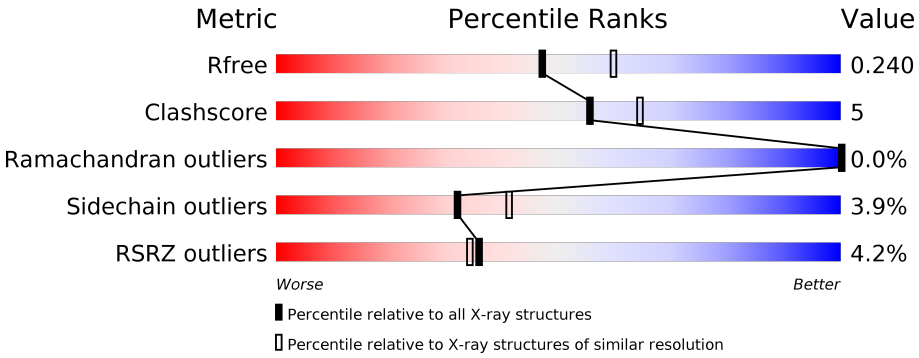
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	298	84% 11% • •
1	B	298	87% 7% • 5%
1	C	298	84% 8% • • 6%
1	D	298	% 81% 11% • • 6%
1	E	298	2% 83% 9% • • 5%
1	F	298	16% 75% 10% • 12%

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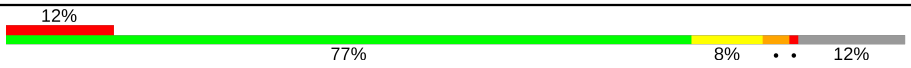
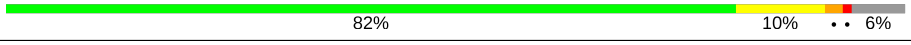
Mol	Chain	Length	Quality of chain
1	G	298	
1	H	298	

2 Entry composition

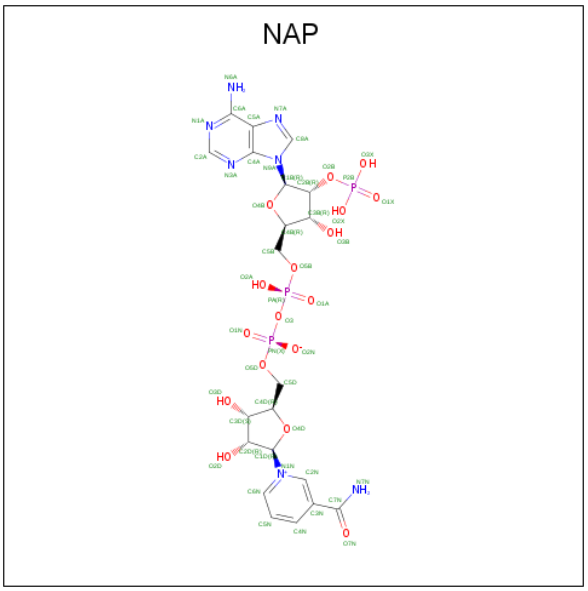
There are 3 unique types of molecules in this entry. The entry contains 16618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Reductive Aminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	1	0
			2064	1308	356	389	11			
1	B	284	Total	C	N	O	S	0	1	0
			2028	1286	352	379	11			
1	C	279	Total	C	N	O	S	0	0	0
			1994	1265	346	373	10			
1	D	279	Total	C	N	O	S	0	0	0
			1983	1258	346	369	10			
1	F	262	Total	C	N	O	S	0	0	0
			1766	1113	310	335	8			
1	G	263	Total	C	N	O	S	0	0	0
			1818	1146	313	349	10			
1	E	283	Total	C	N	O	S	0	1	0
			1987	1263	343	370	11			
1	H	281	Total	C	N	O	S	0	0	0
			2011	1273	347	381	10			

- 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	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

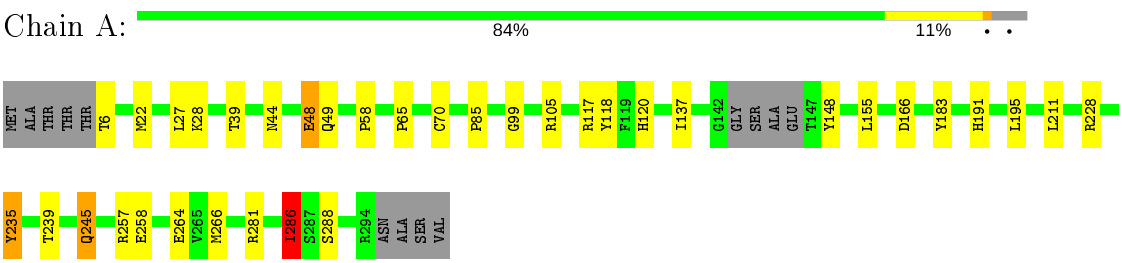
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	96	Total	O	0	0
			96	96		
3	C	97	Total	O	0	0
			97	97		
3	D	92	Total	O	0	0
			92	92		
3	F	81	Total	O	0	0
			81	81		
3	G	65	Total	O	0	0
			65	65		
3	E	77	Total	O	0	0
			77	77		
3	H	147	Total	O	0	0
			147	147		

3 Residue-property plots (i)

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

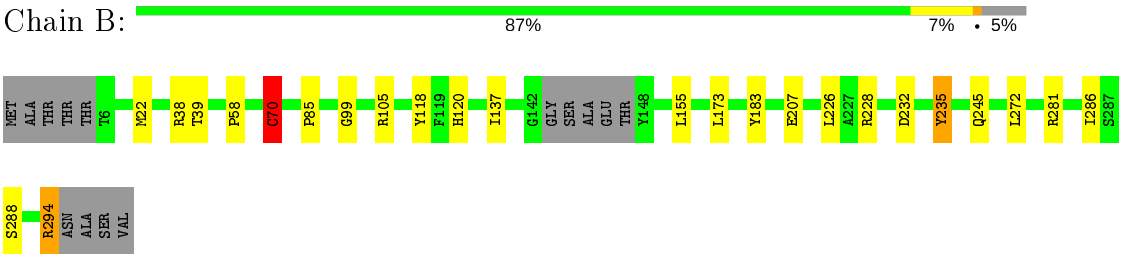
- Molecule 1: Reductive Aminase

Chain A:



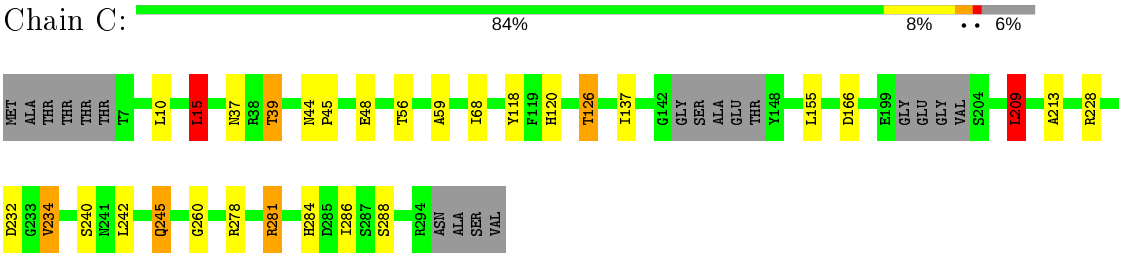
- Molecule 1: Reductive Aminase

Chain B:



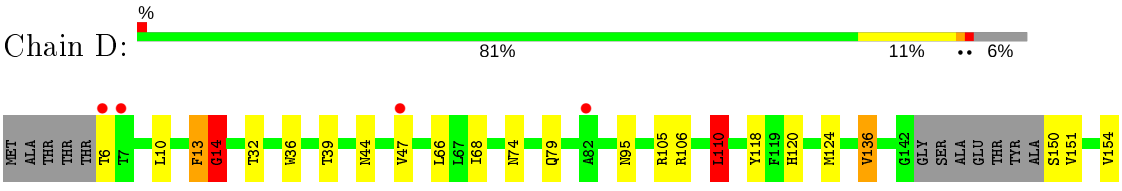
- Molecule 1: Reductive Aminase

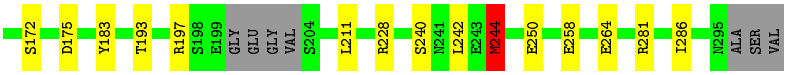
Chain C:



- Molecule 1: Reductive Aminase

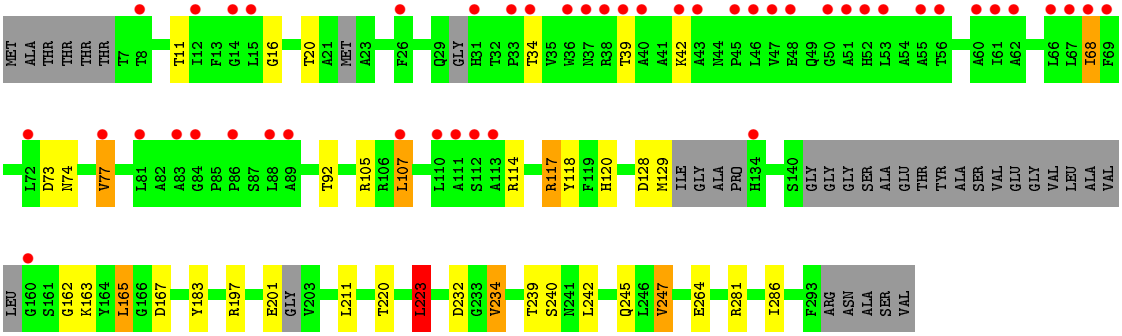
Chain D:





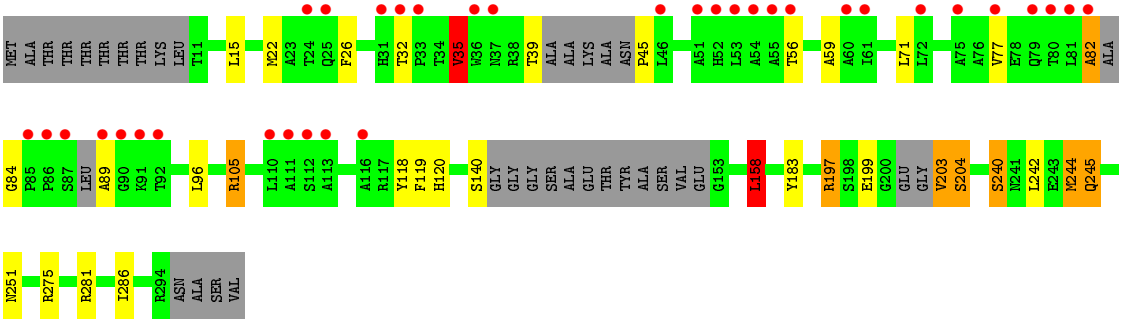
- Molecule 1: Reductive Aminase

Chain F:



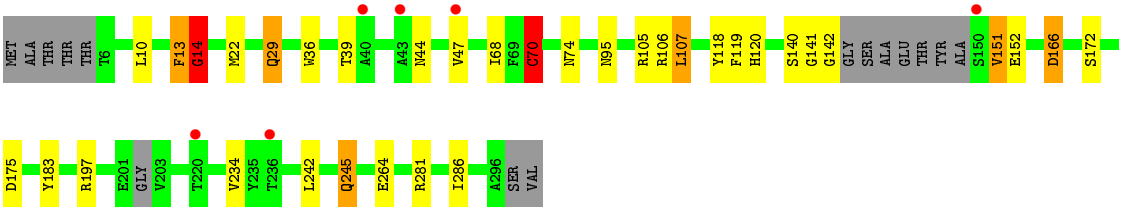
- Molecule 1: Reductive Aminase

Chain G:



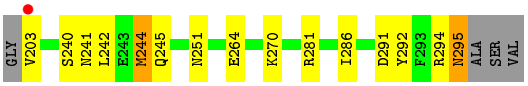
- Molecule 1: Reductive Aminase

Chain E:



- Molecule 1: Reductive Aminase

Chain H:


GLY
V203
S240
N241
L242
E243
M244
Q245
N251
E264
K270
R281
I286
D291
Y292
F293
R294
N295
ALA
SER
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.98Å 85.55Å 355.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	177.71 – 2.20 48.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (177.71-2.20) 100.0 (48.70-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.198 , 0.236 0.204 , 0.240	Depositor DCC
R_{free} test set	5951 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

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	0.85	0/2103	0.96	12/2860 (0.4%)
1	B	0.71	2/2066 (0.1%)	0.86	8/2813 (0.3%)
1	C	0.73	1/2028 (0.0%)	0.87	6/2760 (0.2%)
1	D	0.83	4/2017 (0.2%)	0.88	10/2746 (0.4%)
1	E	0.81	4/2024 (0.2%)	0.87	9/2760 (0.3%)
1	F	0.75	0/1789	0.89	10/2436 (0.4%)
1	G	0.70	0/1844	0.86	8/2508 (0.3%)
1	H	0.84	1/2044 (0.0%)	0.96	12/2784 (0.4%)
All	All	0.78	12/15915 (0.1%)	0.89	75/21667 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
1	E	0	4
1	G	0	1
1	H	0	2
All	All	0	10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	258	GLU	CD-OE1	13.57	1.40	1.25
1	E	14	GLY	N-CA	-12.40	1.27	1.46
1	D	14	GLY	N-CA	-12.24	1.27	1.46
1	H	70	CYS	CB-SG	-10.02	1.65	1.82
1	C	126	THR	CB-CG2	-8.20	1.25	1.52
1	E	70[A]	CYS	CB-SG	-7.43	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	70[B]	CYS	CB-SG	-7.43	1.69	1.82
1	B	70[A]	CYS	CB-SG	-6.13	1.71	1.82
1	B	70[B]	CYS	CB-SG	-6.13	1.71	1.82
1	D	172	SER	CB-OG	6.10	1.50	1.42
1	D	258	GLU	CG-CD	5.86	1.60	1.51
1	E	172	SER	CB-OG	5.43	1.49	1.42

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	TYR	CB-CG-CD1	10.53	127.32	121.00
1	B	272	LEU	CB-CG-CD1	9.99	127.99	111.00
1	A	235	TYR	CB-CG-CD2	-9.95	115.03	121.00
1	E	13	PHE	O-C-N	-9.68	106.74	123.20
1	D	13	PHE	O-C-N	-9.17	107.61	123.20
1	B	235	TYR	CB-CG-CD1	8.52	126.11	121.00
1	C	15	LEU	CB-CG-CD1	8.34	125.18	111.00
1	F	223	LEU	CB-CG-CD1	8.33	125.16	111.00
1	B	235	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	A	286	ILE	CA-CB-CG2	8.01	126.93	110.90
1	D	13	PHE	CA-C-N	7.95	132.09	116.20
1	E	13	PHE	CA-C-N	7.75	131.71	116.20
1	G	244	MET	CG-SD-CE	7.54	112.26	100.20
1	H	281	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	H	291	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	228	ARG	CG-CD-NE	-6.95	97.20	111.80
1	C	278	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	E	175	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	D	110	LEU	CB-CG-CD1	6.81	122.57	111.00
1	H	159	LEU	CB-CG-CD1	6.80	122.56	111.00
1	F	117	ARG	CA-CB-CG	6.76	128.28	113.40
1	H	244	MET	CG-SD-CE	6.75	111.00	100.20
1	G	35	VAL	CG1-CB-CG2	6.75	121.70	110.90
1	H	175	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	H	38	ARG	CA-CB-CG	6.65	128.03	113.40
1	A	166	ASP	CB-CG-OD1	6.36	124.03	118.30
1	E	166	ASP	CB-CG-OD1	6.33	124.00	118.30
1	E	281	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	281	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	F	281	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	G	281	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	258	GLU	CA-CB-CG	6.10	126.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	244	MET	CA-CB-CG	6.09	123.65	113.30
1	F	77	VAL	CA-CB-CG2	6.07	120.00	110.90
1	H	167(A)	ASP	CB-CG-OD1	6.04	123.74	118.30
1	G	158	LEU	CB-CG-CD1	5.98	121.16	111.00
1	H	197	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	C	166	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	281	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	258	GLU	CG-CD-OE1	5.83	129.97	118.30
1	F	247	VAL	CA-CB-CG2	5.80	119.60	110.90
1	A	228	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	281	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	G	275	ARG	CG-CD-NE	5.71	123.80	111.80
1	G	82	ALA	N-CA-C	5.71	126.42	111.00
1	D	175	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	E	107	LEU	CB-CG-CD1	5.61	120.53	111.00
1	C	126	THR	OG1-CB-CG2	5.59	122.87	110.00
1	G	281	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	48	GLU	OE1-CD-OE2	5.47	129.87	123.30
1	B	281	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	29	GLN	CA-CB-CG	5.47	125.43	113.40
1	A	28	LYS	CA-CB-CG	5.44	125.36	113.40
1	F	107	LEU	CB-CG-CD1	5.39	120.17	111.00
1	A	105	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	175	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	272	LEU	CB-CG-CD2	-5.30	102.00	111.00
1	B	232	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	165	LEU	CB-CG-CD1	5.28	119.97	111.00
1	E	105	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	105	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	294	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	F	165	LEU	CB-CG-CD1	5.23	119.90	111.00
1	F	197	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	117	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	209	LEU	CB-CG-CD2	5.18	119.80	111.00
1	F	247	VAL	CA-CB-CG1	5.17	118.66	110.90
1	B	105	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	13	PHE	C-N-CA	5.14	133.09	122.30
1	H	295	ASN	N-CA-CB	5.08	119.75	110.60
1	E	106	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	D	244	MET	CA-CB-CG	5.06	121.90	113.30
1	A	257	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	F	105	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	105	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	13	PHE	Peptide
1	D	14	GLY	Mainchain,Peptide
1	E	13	PHE	Peptide
1	E	14	GLY	Mainchain,Peptide
1	E	140	SER	Peptide
1	G	203	VAL	Peptide
1	H	200	GLY	Peptide
1	H	292	TYR	Mainchain

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	2064	0	2076	24	0
1	B	2028	0	2020	16	0
1	C	1994	0	1985	17	0
1	D	1983	0	1971	25	0
1	E	1987	0	1948	19	0
1	F	1766	0	1625	27	0
1	G	1818	0	1724	26	0
1	H	2011	0	1999	25	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	6	0
3	A	168	0	0	4	0
3	B	96	0	0	0	0
3	C	97	0	0	4	0
3	D	92	0	0	6	0
3	E	77	0	0	2	0
3	F	81	0	0	9	0
3	G	65	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	147	0	0	10	0
All	All	16618	0	15423	159	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 5.

All (159) 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:244:MET:HB3	3:H:390:HOH:O	1.48	1.09
1:G:140:SER:C	3:G:313:HOH:O	1.97	1.03
1:F:39:THR:O	3:F:301:HOH:O	1.84	0.95
1:H:70:CYS:HB3	3:H:424:HOH:O	1.66	0.94
1:G:15:LEU:HD21	1:G:35:VAL:HG22	1.53	0.88
1:A:22:MET:HE1	1:A:70[B]:CYS:SG	2.19	0.83
1:F:42:LYS:CB	3:F:301:HOH:O	2.27	0.82
1:D:150:SER:N	3:D:301:HOH:O	2.13	0.82
1:B:22:MET:HE1	1:B:70[A]:CYS:SG	2.20	0.81
1:E:141:GLY:HA3	1:E:166:ASP:HA	1.62	0.80
1:A:22:MET:CE	1:A:70[B]:CYS:SG	2.69	0.80
1:D:250:GLU:HG2	3:D:383:HOH:O	1.81	0.80
1:E:22:MET:CE	1:E:70[A]:CYS:SG	2.71	0.79
1:G:197:ARG:HD2	3:G:319:HOH:O	1.82	0.79
1:B:22:MET:CE	1:B:70[A]:CYS:SG	2.71	0.79
2:C:301:NAP:H2D	1:D:244:MET:HE1	1.63	0.78
1:B:173:LEU:CD2	1:G:199:GLU:HG2	2.12	0.78
1:H:241:ASN:H	1:H:244:MET:HE3	1.48	0.78
1:C:56:THR:HG21	3:C:493:HOH:O	1.85	0.76
2:C:301:NAP:C2D	1:D:244:MET:HE1	2.15	0.76
1:H:22:MET:CE	1:H:70:CYS:SG	2.74	0.76
1:B:183:TYR:OH	1:G:245:GLN:NE2	2.21	0.74
1:E:22:MET:HE1	1:E:70[A]:CYS:SG	2.29	0.71
1:G:45:PRO:N	3:G:301:HOH:O	2.24	0.70
1:A:258:GLU:OE2	3:A:401:HOH:O	2.09	0.70
1:C:39:THR:HG23	2:C:301:NAP:O2X	1.91	0.70
1:F:167:ASP:CB	3:F:360:HOH:O	2.40	0.70
1:H:22:MET:HE1	1:H:70:CYS:SG	2.33	0.69
1:F:74:ASN:HA	1:F:77:VAL:HG13	1.75	0.69
1:A:48:GLU:HG2	1:F:163:LYS:HA	1.75	0.69
1:A:183:TYR:OH	1:H:245:GLN:NE2	2.24	0.69
1:F:92:THR:HG23	1:F:117:ARG:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:NAP:H2D	1:D:244:MET:CE	2.24	0.67
1:A:264:GLU:HG2	3:A:559:HOH:O	1.94	0.66
1:G:82:ALA:O	1:G:84:GLY:N	2.29	0.66
1:C:245:GLN:NE2	1:D:183:TYR:OH	2.29	0.66
1:G:203:VAL:O	1:G:204:SER:HB3	1.94	0.66
1:A:6:THR:HG21	1:A:65:PRO:HD3	1.77	0.66
1:D:79:GLN:CB	3:D:374:HOH:O	2.44	0.65
1:A:245:GLN:NE2	1:H:183:TYR:OH	2.29	0.65
1:F:220:THR:HA	1:F:223:LEU:HD22	1.78	0.65
1:D:124:MET:HB2	1:D:136:VAL:HG13	1.79	0.65
1:F:73:ASP:OD1	1:F:74:ASN:N	2.30	0.64
1:F:239:THR:OG1	3:F:302:HOH:O	2.15	0.64
1:A:48:GLU:HG2	1:F:162:GLY:O	1.98	0.64
1:F:129:MET:CB	3:F:311:HOH:O	2.46	0.63
1:B:173:LEU:HD21	1:G:199:GLU:HG2	1.80	0.63
2:A:301:NAP:O1N	1:H:244:MET:SD	2.58	0.62
1:H:56:THR:HG23	1:H:59:ALA:H	1.64	0.62
1:G:119:PHE:CB	3:G:362:HOH:O	2.46	0.62
1:G:15:LEU:HD21	1:G:35:VAL:CG2	2.30	0.62
1:G:56:THR:HG23	1:G:59:ALA:H	1.64	0.61
1:C:209:LEU:HD22	1:C:213:ALA:HB2	1.82	0.61
1:G:71:LEU:HD22	1:G:71:LEU:N	2.16	0.61
1:B:245:GLN:NE2	1:G:183:TYR:OH	2.34	0.60
1:C:56:THR:HG23	1:C:59:ALA:H	1.66	0.60
1:F:92:THR:OG1	1:F:117:ARG:HG2	2.00	0.59
2:C:301:NAP:O2D	1:D:244:MET:HE1	2.02	0.59
1:D:44:ASN:O	1:D:47:VAL:HG22	2.03	0.59
1:E:264:GLU:CB	3:E:377:HOH:O	2.51	0.57
1:E:44:ASN:O	1:E:47:VAL:HG22	2.04	0.57
1:C:15:LEU:HD22	1:C:37:ASN:HB2	1.87	0.57
1:B:207:GLU:CB	3:C:491:HOH:O	2.52	0.56
1:F:11:THR:CB	1:F:34:THR:HG23	2.35	0.56
1:A:48:GLU:CG	1:F:163:LYS:HA	2.35	0.56
1:C:48:GLU:CB	3:C:473:HOH:O	2.52	0.56
1:F:11:THR:CB	1:F:34:THR:CG2	2.84	0.56
1:F:114:ARG:CB	3:F:346:HOH:O	2.54	0.55
1:A:49:GLN:NE2	3:A:403:HOH:O	2.25	0.53
1:A:191:HIS:HE1	1:A:266:MET:CE	2.21	0.53
1:C:232:ASP:HB2	1:C:234:VAL:HG12	1.92	0.52
1:D:14:GLY:HA2	1:D:36:TRP:O	2.09	0.52
1:G:89:ALA:N	3:G:305:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ASN:HA	1:E:47:VAL:HG22	1.92	0.52
1:F:128:ASP:CB	3:F:315:HOH:O	2.59	0.51
1:D:118:TYR:OH	1:D:120:HIS:HD2	1.93	0.51
1:D:151:VAL:HA	1:D:154:VAL:HG22	1.92	0.51
1:H:264:GLU:HG2	3:H:336:HOH:O	2.09	0.51
1:D:44:ASN:HA	1:D:47:VAL:HG22	1.91	0.51
1:D:6:THR:N	3:D:306:HOH:O	2.44	0.51
1:E:119:PHE:CZ	1:E:142:GLY:HA3	2.46	0.50
1:E:118:TYR:OH	1:E:120:HIS:HD2	1.93	0.50
1:A:118:TYR:OH	1:A:120:HIS:HD2	1.93	0.50
1:G:118:TYR:OH	1:G:120:HIS:HD2	1.94	0.50
1:H:118:TYR:OH	1:H:120:HIS:HD2	1.94	0.50
1:C:118:TYR:OH	1:C:120:HIS:HD2	1.94	0.50
1:F:118:TYR:OH	1:F:120:HIS:HD2	1.94	0.50
1:B:118:TYR:OH	1:B:120:HIS:HD2	1.94	0.50
1:D:66:LEU:HD21	1:D:154:VAL:HG21	1.92	0.50
1:F:245:GLN:NE2	1:E:183:TYR:OH	2.37	0.50
1:A:44:ASN:O	1:A:48:GLU:OE2	2.30	0.49
1:D:197:ARG:NH2	3:D:302:HOH:O	2.13	0.49
1:A:195:LEU:HD22	1:H:173:LEU:HD11	1.94	0.49
1:E:14:GLY:HA2	1:E:36:TRP:O	2.13	0.49
1:G:71:LEU:HD23	1:G:77:VAL:HG22	1.93	0.49
1:H:74:ASN:ND2	1:H:95:ASN:HD21	2.11	0.48
1:A:6:THR:N	3:A:410:HOH:O	2.46	0.48
1:D:74:ASN:ND2	1:D:95:ASN:HD21	2.12	0.48
1:G:203:VAL:O	1:G:204:SER:CB	2.58	0.48
1:A:286:ILE:HD12	1:H:190:LEU:HD11	1.96	0.48
1:A:58:PRO:HB3	1:B:85:PRO:HG3	1.96	0.47
1:E:74:ASN:ND2	1:E:95:ASN:HD21	2.12	0.47
1:F:11:THR:HA	1:F:34:THR:CG2	2.45	0.47
1:H:270:LYS:HE3	3:H:419:HOH:O	2.14	0.47
1:C:137:ILE:HG21	1:C:155:LEU:HD22	1.96	0.46
1:A:137:ILE:HG21	1:A:155:LEU:HD22	1.98	0.46
1:E:119:PHE:CE2	1:E:151:VAL:HG11	2.51	0.46
1:D:264:GLU:HB3	3:D:386:HOH:O	2.14	0.46
1:D:242:LEU:HD21	1:D:286:ILE:HA	1.98	0.46
1:B:235:TYR:HB3	1:B:288:SER:HB2	1.98	0.46
1:D:106:ARG:O	1:D:110:LEU:HD13	2.15	0.46
1:G:242:LEU:HD21	1:G:286:ILE:HA	1.98	0.45
1:A:85:PRO:HG3	1:B:58:PRO:HB3	1.99	0.45
1:B:38:ARG:HB3	2:B:301:NAP:O2X	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:HG21	1:B:155:LEU:HD22	1.99	0.45
1:B:99:GLY:HA2	1:G:251:ASN:ND2	2.32	0.45
1:B:173:LEU:CD2	1:G:199:GLU:CG	2.91	0.45
1:E:242:LEU:HD21	1:E:286:ILE:HA	1.99	0.45
1:F:183:TYR:OH	1:E:245:GLN:NE2	2.50	0.45
1:A:27:LEU:HD13	1:A:49:GLN:HB2	1.98	0.45
1:E:197:ARG:NH1	3:E:301:HOH:O	2.24	0.44
1:E:44:ASN:O	1:E:47:VAL:CG2	2.66	0.44
1:F:264:GLU:HG2	3:F:377:HOH:O	2.17	0.44
1:A:191:HIS:HE1	1:A:266:MET:HE1	1.83	0.44
1:F:232:ASP:HB2	1:F:234:VAL:HG12	1.99	0.44
1:H:294:ARG:O	1:H:295:ASN:CB	2.65	0.44
1:D:44:ASN:O	1:D:47:VAL:CG2	2.66	0.44
1:E:234:VAL:O	1:E:234:VAL:HG13	2.17	0.44
1:H:70:CYS:CB	3:H:424:HOH:O	2.45	0.44
1:A:235:TYR:HB3	1:A:288:SER:HB2	2.00	0.44
1:F:16:GLY:O	1:F:20:THR:HG23	2.18	0.44
1:B:173:LEU:HD22	1:G:199:GLU:HG2	1.95	0.43
1:E:10:LEU:HD13	1:E:68:ILE:HD12	1.99	0.43
1:G:22:MET:HE1	1:G:96:LEU:HD13	2.00	0.43
1:H:242:LEU:HD21	1:H:286:ILE:HA	1.99	0.43
1:C:39:THR:CG2	2:C:301:NAP:O2X	2.65	0.43
1:D:10:LEU:HD13	1:D:68:ILE:HD12	2.00	0.43
1:F:201:GLU:HA	3:F:307:HOH:O	2.18	0.43
1:E:119:PHE:CZ	1:E:151:VAL:HG11	2.53	0.42
1:C:10:LEU:HD13	1:C:68:ILE:HD12	2.01	0.42
1:F:11:THR:O	1:F:68:ILE:HG23	2.20	0.42
1:H:203:VAL:HG13	3:H:350:HOH:O	2.19	0.42
1:C:242:LEU:HD21	1:C:286:ILE:HA	2.01	0.41
1:D:193:THR:HG22	1:D:197:ARG:HD3	2.01	0.41
1:C:260:GLY:HA2	3:C:434:HOH:O	2.20	0.41
2:B:301:NAP:C7N	1:G:240:SER:HB3	2.50	0.41
1:H:244:MET:CB	3:H:390:HOH:O	2.33	0.41
1:C:284:HIS:HD2	1:C:288:SER:OG	2.04	0.41
1:H:119:PHE:CZ	1:H:152:VAL:HG11	2.55	0.41
1:H:47:VAL:HG13	3:H:323:HOH:O	2.21	0.40
1:D:32:THR:HG23	1:D:32:THR:O	2.21	0.40
1:G:26:PHE:CE2	1:G:158:LEU:HD11	2.56	0.40
1:H:38:ARG:HG3	3:H:441:HOH:O	2.19	0.40
1:F:242:LEU:HD21	1:F:286:ILE:HA	2.03	0.40
1:H:152:VAL:HG12	3:H:404:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ARG:HD3	1:C:288:SER:HG	1.85	0.40
1:C:44:ASN:HB2	1:C:45:PRO:HD3	2.03	0.40
1:G:105:ARG:HD2	3:G:343:HOH:O	2.20	0.40
1:A:99:GLY:HA2	1:H:251:ASN:ND2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/298 (95%)	277 (98%)	5 (2%)	0	100	100
1	B	281/298 (94%)	278 (99%)	3 (1%)	0	100	100
1	C	273/298 (92%)	270 (99%)	3 (1%)	0	100	100
1	D	273/298 (92%)	269 (98%)	4 (2%)	0	100	100
1	E	278/298 (93%)	273 (98%)	5 (2%)	0	100	100
1	F	250/298 (84%)	244 (98%)	6 (2%)	0	100	100
1	G	251/298 (84%)	246 (98%)	4 (2%)	1 (0%)	34	37
1	H	275/298 (92%)	272 (99%)	3 (1%)	0	100	100
All	All	2163/2384 (91%)	2129 (98%)	33 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	204	SER

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	205/216 (95%)	199 (97%)	6 (3%)	42	54
1	B	196/216 (91%)	189 (96%)	7 (4%)	35	45
1	C	193/216 (89%)	185 (96%)	8 (4%)	30	39
1	D	191/216 (88%)	184 (96%)	7 (4%)	34	43
1	E	187/216 (87%)	179 (96%)	8 (4%)	29	36
1	F	147/216 (68%)	139 (95%)	8 (5%)	22	26
1	G	166/216 (77%)	158 (95%)	8 (5%)	25	32
1	H	197/216 (91%)	189 (96%)	8 (4%)	30	39
All	All	1482/1728 (86%)	1422 (96%)	60 (4%)	32	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	148	TYR
1	A	211	LEU
1	A	239	THR
1	A	245	GLN
1	A	286	ILE
1	B	39	THR
1	B	70[A]	CYS
1	B	70[B]	CYS
1	B	226	LEU
1	B	228	ARG
1	B	286	ILE
1	B	294	ARG
1	C	15	LEU
1	C	39	THR
1	C	126	THR
1	C	209	LEU
1	C	228	ARG
1	C	234	VAL

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Mol	Chain	Res	Type
1	C	240	SER
1	C	245	GLN
1	D	39	THR
1	D	110	LEU
1	D	136	VAL
1	D	211	LEU
1	D	228	ARG
1	D	240	SER
1	D	244	MET
1	F	68	ILE
1	F	107	LEU
1	F	165	LEU
1	F	211	LEU
1	F	223	LEU
1	F	234	VAL
1	F	240	SER
1	F	247	VAL
1	G	32	THR
1	G	35	VAL
1	G	39	THR
1	G	158	LEU
1	G	197	ARG
1	G	240	SER
1	G	244	MET
1	G	245	GLN
1	E	29	GLN
1	E	39	THR
1	E	70[A]	CYS
1	E	70[B]	CYS
1	E	107	LEU
1	E	151	VAL
1	E	152	GLU
1	E	245	GLN
1	H	10	LEU
1	H	38	ARG
1	H	39	THR
1	H	70	CYS
1	H	152	VAL
1	H	159	LEU
1	H	165	LEU
1	H	240	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	120	HIS
1	A	245	GLN
1	A	259	GLN
1	B	25	GLN
1	B	120	HIS
1	B	245	GLN
1	C	120	HIS
1	C	245	GLN
1	C	259	GLN
1	C	284	HIS
1	D	25	GLN
1	D	74	ASN
1	D	120	HIS
1	D	238	GLN
1	D	259	GLN
1	F	120	HIS
1	F	238	GLN
1	F	245	GLN
1	G	120	HIS
1	G	245	GLN
1	G	259	GLN
1	E	74	ASN
1	E	120	HIS
1	E	245	GLN
1	E	259	GLN
1	H	74	ASN
1	H	120	HIS
1	H	238	GLN
1	H	245	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	B	301	-	45,52,52	1.05	3 (6%)	56,80,80	1.31	8 (14%)
2	NAP	A	301	-	45,52,52	1.18	3 (6%)	56,80,80	1.48	8 (14%)
2	NAP	C	301	-	45,52,52	1.01	3 (6%)	56,80,80	1.66	10 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	301	-	-	6/31/67/67	0/5/5/5
2	NAP	A	301	-	-	8/31/67/67	0/5/5/5
2	NAP	C	301	-	-	2/31/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C5A-C4A	3.32	1.49	1.40
2	C	301	NAP	C5A-C4A	2.57	1.47	1.40
2	A	301	NAP	P2B-O2B	2.56	1.64	1.59
2	B	301	NAP	C5A-C4A	2.46	1.47	1.40
2	B	301	NAP	C2N-C3N	2.27	1.42	1.39
2	B	301	NAP	C2A-N3A	2.12	1.35	1.32
2	C	301	NAP	C2A-N3A	2.11	1.35	1.32
2	C	301	NAP	P2B-O2B	2.10	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	O4B-C1B	2.09	1.44	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	O4D-C1D-C2D	-4.78	99.94	106.93
2	A	301	NAP	C3N-C7N-N7N	4.60	123.27	117.75
2	A	301	NAP	O7N-C7N-C3N	-4.24	114.55	119.63
2	B	301	NAP	C3N-C7N-N7N	3.72	122.22	117.75
2	C	301	NAP	C3N-C7N-N7N	3.59	122.06	117.75
2	C	301	NAP	C3D-C2D-C1D	3.53	106.30	100.98
2	C	301	NAP	N6A-C6A-N1A	3.45	125.74	118.57
2	C	301	NAP	PN-O3-PA	-3.44	121.04	132.83
2	C	301	NAP	C5A-C6A-N6A	-3.09	115.66	120.35
2	B	301	NAP	C1B-N9A-C4A	-3.07	121.24	126.64
2	C	301	NAP	O7N-C7N-C3N	-3.07	115.96	119.63
2	C	301	NAP	N3A-C2A-N1A	-3.07	123.89	128.68
2	B	301	NAP	N3A-C2A-N1A	-3.05	123.92	128.68
2	A	301	NAP	C2A-N1A-C6A	3.04	123.95	118.75
2	A	301	NAP	N3A-C2A-N1A	-2.90	124.14	128.68
2	A	301	NAP	O2A-PA-O1A	2.86	126.36	112.24
2	A	301	NAP	O2D-C2D-C3D	2.79	120.86	111.82
2	A	301	NAP	N6A-C6A-N1A	2.74	124.27	118.57
2	B	301	NAP	PN-O3-PA	-2.54	124.10	132.83
2	B	301	NAP	O3X-P2B-O1X	2.52	120.54	110.68
2	C	301	NAP	C6N-N1N-C2N	-2.45	119.74	121.97
2	A	301	NAP	C1B-N9A-C4A	-2.40	122.42	126.64
2	B	301	NAP	O2B-P2B-O1X	-2.33	100.40	109.39
2	B	301	NAP	O2A-PA-O1A	2.17	122.98	112.24
2	C	301	NAP	C3B-C2B-C1B	-2.08	98.99	102.89
2	B	301	NAP	O7N-C7N-N7N	-2.03	119.69	122.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C1B-C2B-O2B-P2B
2	A	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	O4B-C4B-C5B-O5B

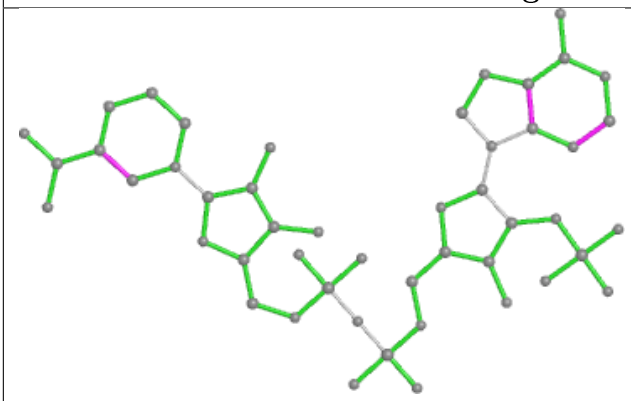
There are no ring outliers.

3 monomers are involved in 9 short contacts:

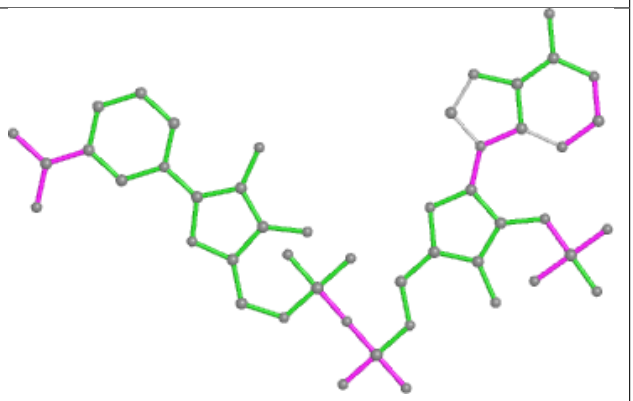
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	2	0
2	A	301	NAP	1	0
2	C	301	NAP	6	0

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.

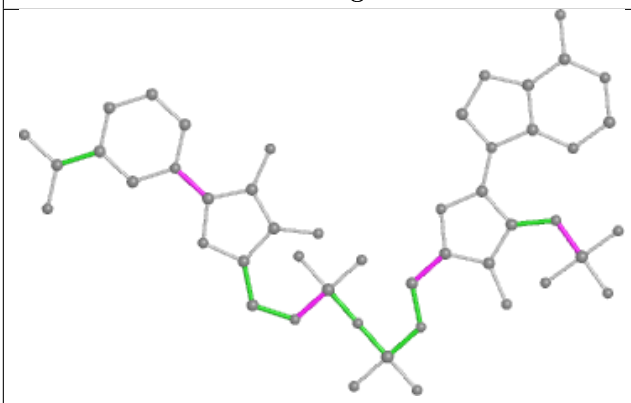
Ligand NAP B 301



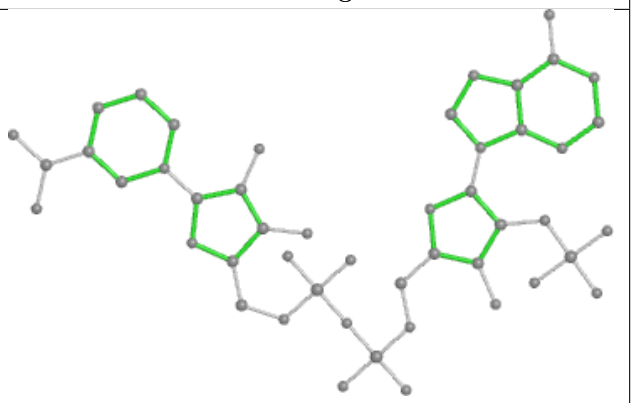
Bond lengths



Bond angles

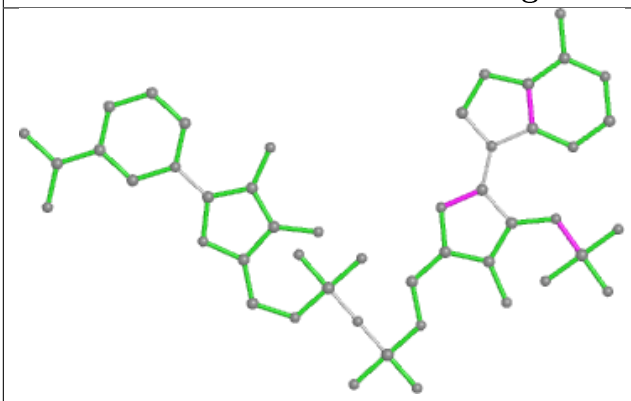


Torsions

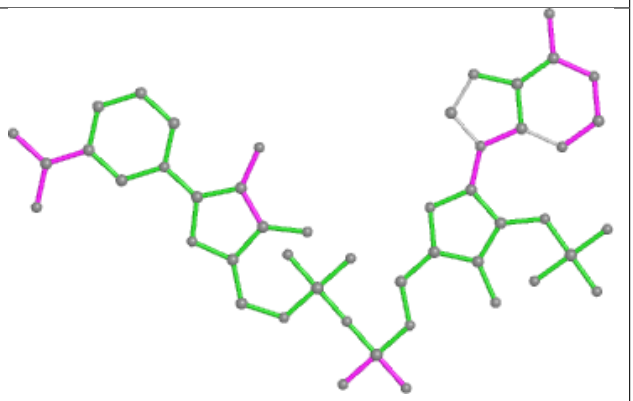


Rings

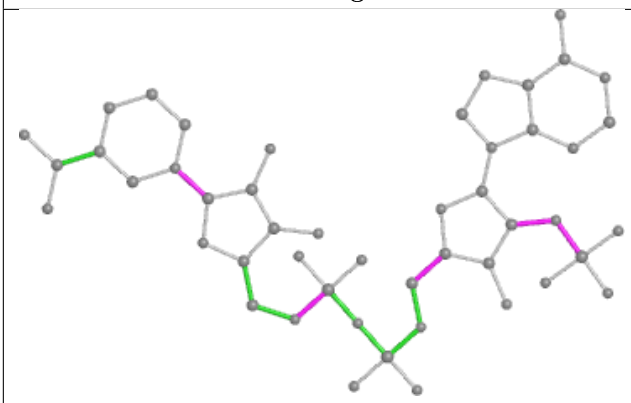
Ligand NAP A 301



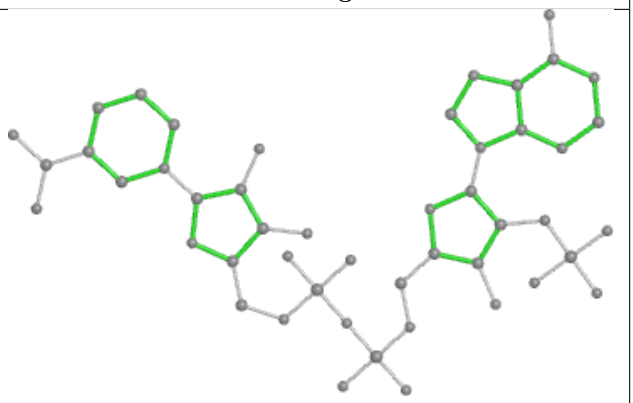
Bond lengths



Bond angles

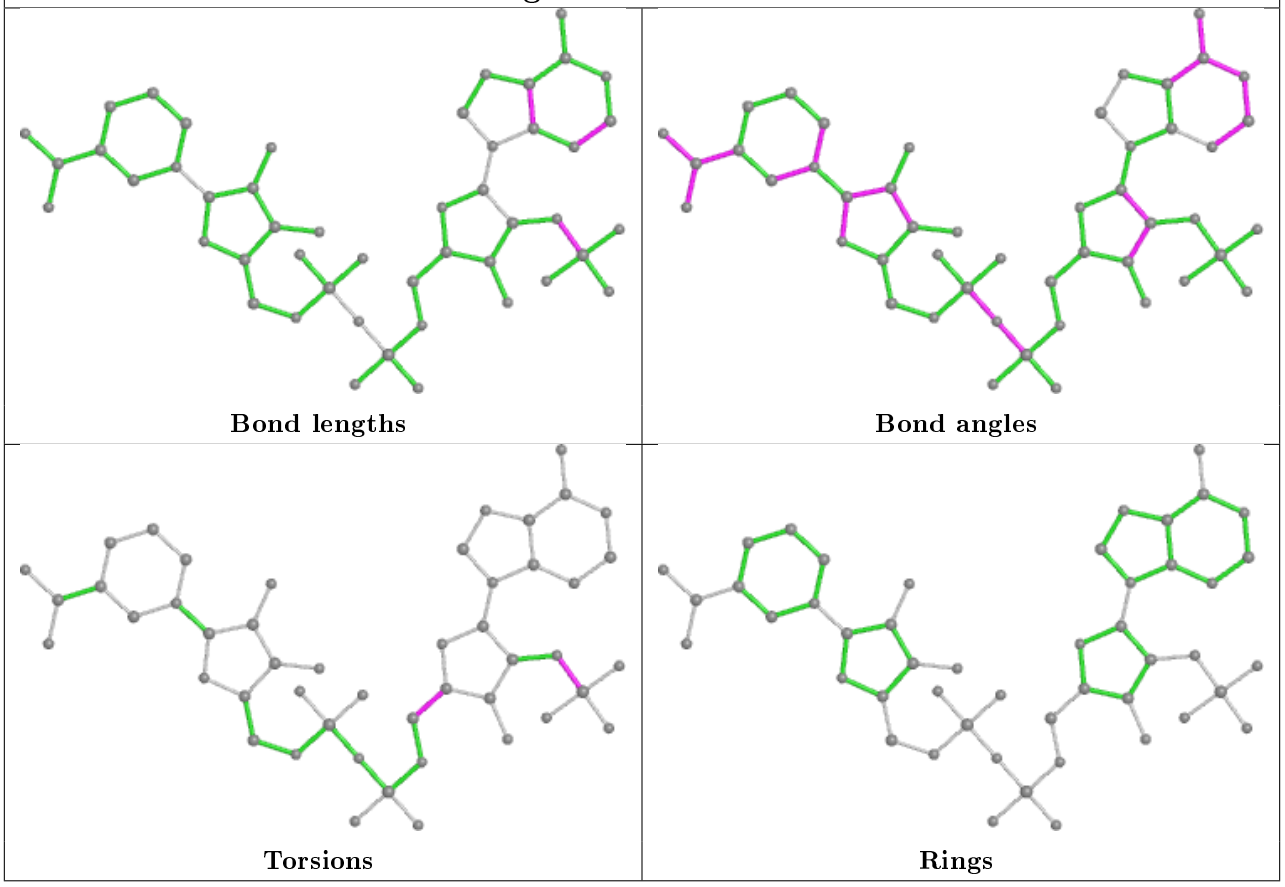


Torsions



Rings

Ligand NAP C 301



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	285/298 (95%)	-0.46	0 100 100	18, 28, 50, 90	0
1	B	284/298 (95%)	-0.43	0 100 100	24, 38, 63, 90	0
1	C	279/298 (93%)	-0.46	0 100 100	27, 37, 58, 77	0
1	D	279/298 (93%)	-0.24	4 (1%) 75 73	26, 42, 64, 84	0
1	E	283/298 (94%)	-0.21	6 (2%) 63 61	24, 44, 75, 91	0
1	F	262/298 (87%)	0.67	47 (17%) 1 1	21, 50, 107, 121	0
1	G	263/298 (88%)	0.48	35 (13%) 3 3	26, 54, 91, 105	0
1	H	281/298 (94%)	-0.39	1 (0%) 92 91	18, 33, 59, 86	0
All	All	2216/2384 (92%)	-0.14	93 (4%) 36 34	18, 39, 81, 121	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	46	LEU	6.4
1	F	55	ALA	6.4
1	F	51	ALA	6.2
1	G	77	VAL	5.2
1	G	116	ALA	5.1
1	F	77	VAL	5.0
1	G	60	ALA	4.9
1	F	83	ALA	4.7
1	F	110	LEU	4.5
1	G	113	ALA	4.5
1	G	86	PRO	4.3
1	F	69	PHE	4.2
1	F	84	GLY	4.2
1	F	60	ALA	4.1
1	F	15	LEU	4.0
1	F	36	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	113	ALA	3.9
1	G	90	GLY	3.8
1	F	39	THR	3.8
1	F	81	LEU	3.7
1	F	50	GLY	3.7
1	G	79	GLN	3.7
1	E	40	ALA	3.6
1	F	26	PHE	3.6
1	F	31	HIS	3.6
1	G	46	LEU	3.6
1	F	14	GLY	3.6
1	F	37	ASN	3.5
1	F	53	LEU	3.5
1	G	112	SER	3.5
1	F	62	ALA	3.4
1	G	92	THR	3.4
1	F	8	THR	3.3
1	G	36	TRP	3.2
1	G	24	THR	3.1
1	F	72	LEU	3.1
1	F	40	ALA	3.1
1	F	56	THR	3.1
1	G	110	LEU	3.1
1	G	80	THR	3.1
1	G	111	ALA	3.1
1	F	52	HIS	3.1
1	D	6	THR	3.0
1	G	53	LEU	3.0
1	E	47	VAL	3.0
1	E	220	THR	3.0
1	G	32	THR	2.9
1	F	160	GLY	2.9
1	F	42	LYS	2.9
1	F	111	ALA	2.8
1	E	43	ALA	2.8
1	G	56	THR	2.8
1	G	25	GLN	2.8
1	F	61	ILE	2.7
1	F	88	LEU	2.7
1	F	107	LEU	2.7
1	G	54	ALA	2.6
1	F	86	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	203	VAL	2.6
1	F	134	HIS	2.6
1	D	82	ALA	2.5
1	G	72	LEU	2.5
1	F	43	ALA	2.5
1	G	61	ILE	2.5
1	F	48	GLU	2.5
1	G	85	PRO	2.5
1	F	38	ARG	2.5
1	F	89	ALA	2.5
1	G	87	SER	2.5
1	F	33	PRO	2.4
1	G	55	ALA	2.4
1	G	37	ASN	2.4
1	G	89	ALA	2.4
1	G	81	LEU	2.3
1	G	75	ALA	2.3
1	E	236	THR	2.3
1	D	47	VAL	2.3
1	F	12	ILE	2.3
1	G	33	PRO	2.2
1	F	112	SER	2.2
1	E	150	SER	2.2
1	G	31	HIS	2.2
1	G	51	ALA	2.2
1	D	7	THR	2.2
1	G	91	LYS	2.1
1	F	68	ILE	2.1
1	F	66	LEU	2.1
1	F	47	VAL	2.1
1	G	52	HIS	2.0
1	F	45	PRO	2.0
1	F	67	LEU	2.0
1	F	34	THR	2.0
1	G	82	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

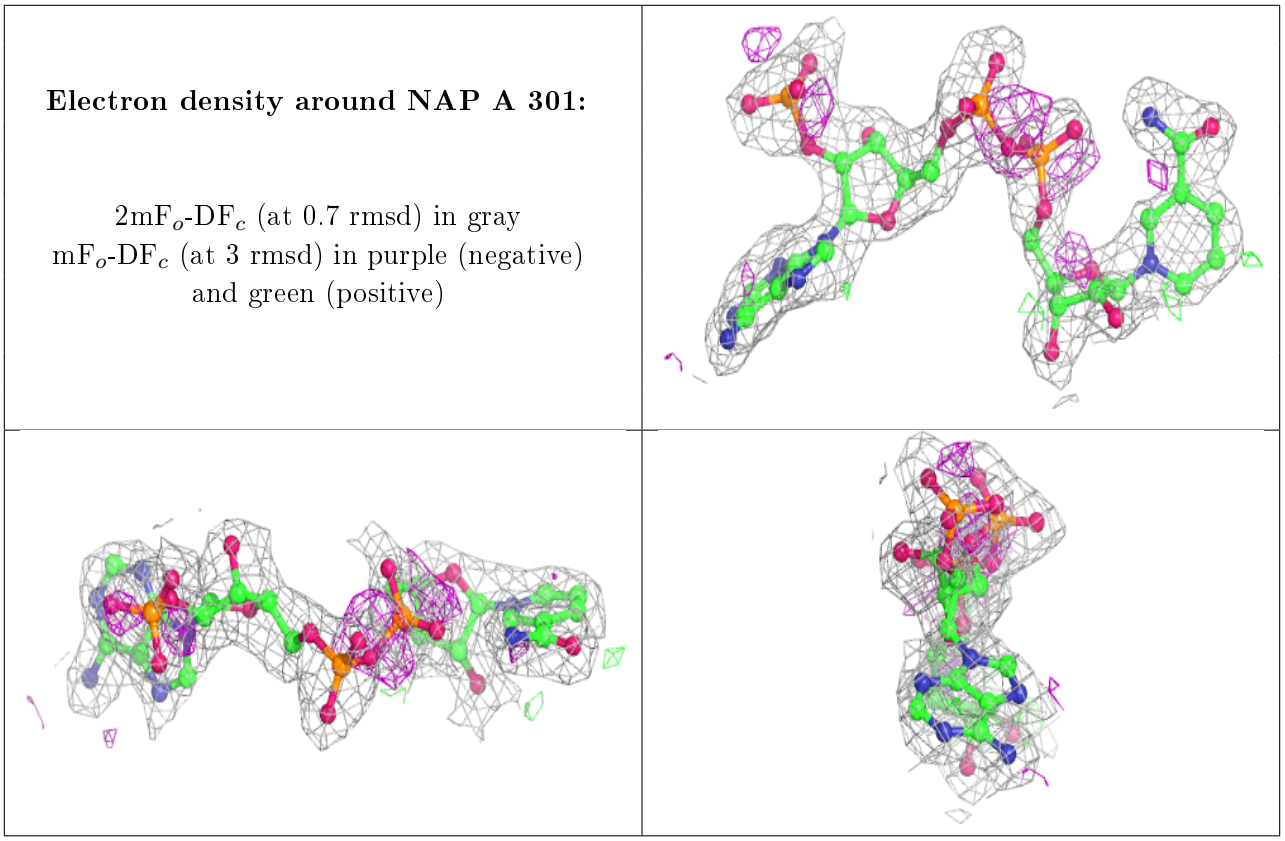
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	A	301	48/48	0.89	0.16	32,49,58,59	0
2	NAP	B	301	48/48	0.94	0.11	32,44,52,58	0
2	NAP	C	301	48/48	0.96	0.11	34,43,51,53	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.

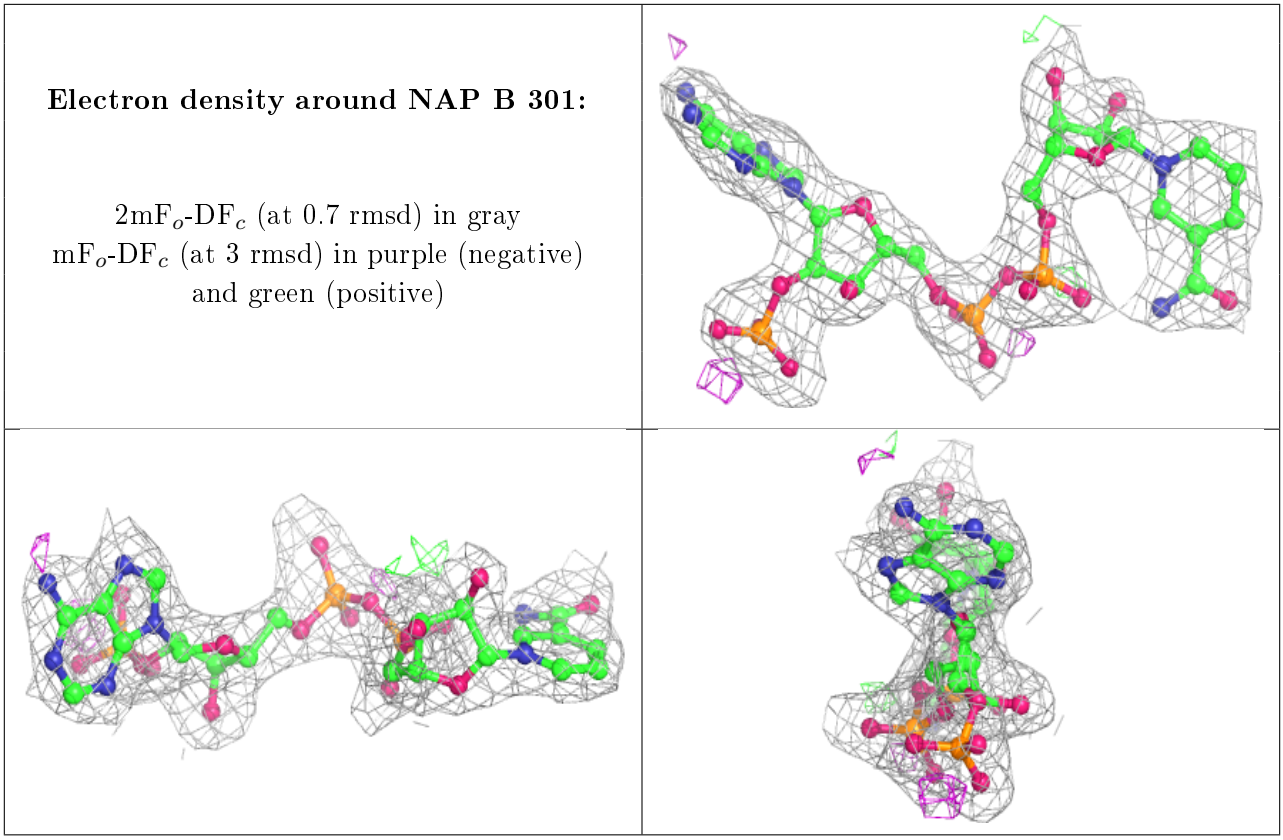
Electron density around NAP A 301:

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



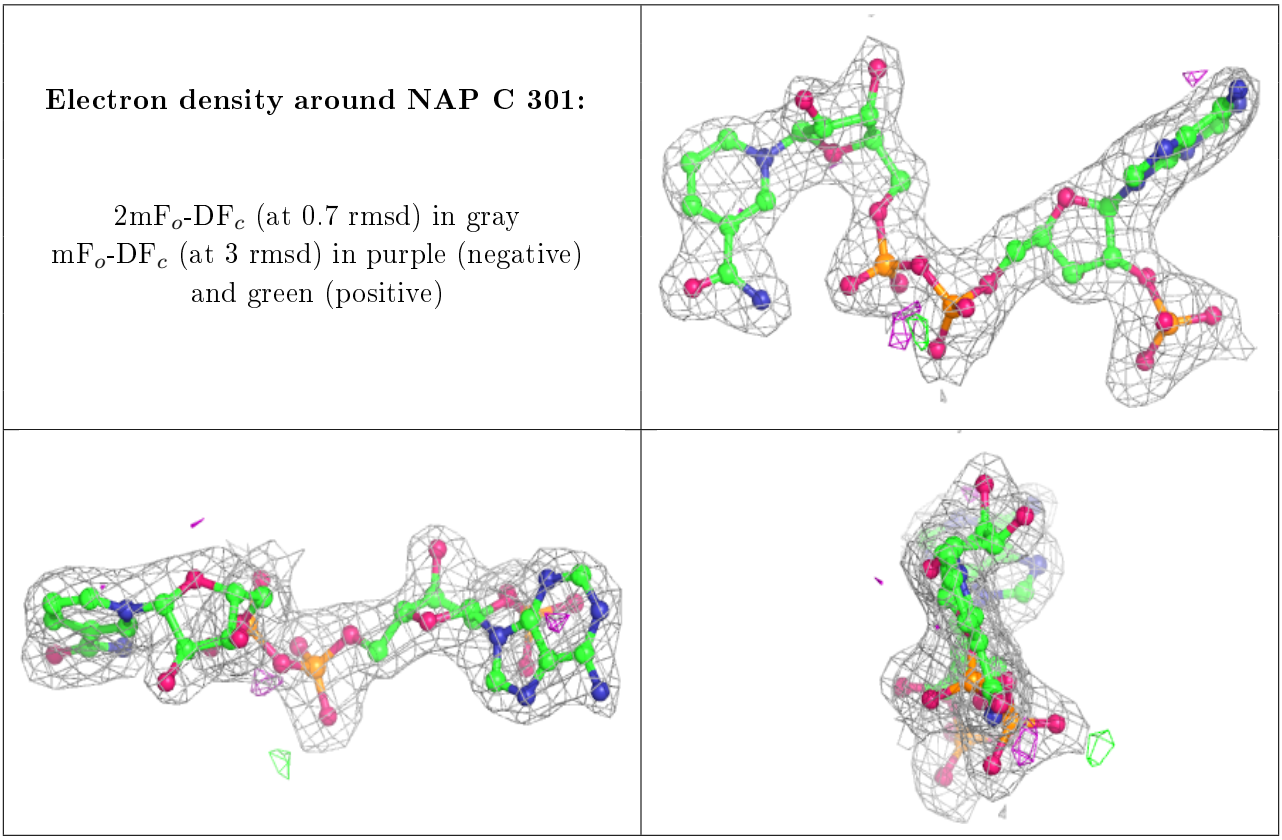
Electron density around NAP B 301:

$2mF_o$-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 C 301:

$2mF_o$-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.