Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 12:04 pm BST

PDB ID	:	2AHR
Title	:	Crystal Structures of 1-Pyrroline-5-Carboxylate Reductase from Human Pathogen Streptococcus pyogenes
Authors	:	Nocek, B.; Lezondra, L.; Holzle, D.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-07-28
Resolution	:	2.15 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:

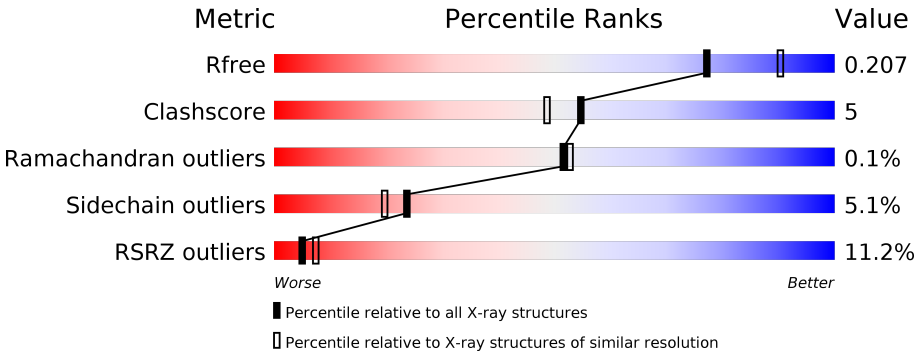
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	259	8% 83% 15%
1	B	259	11% 92% 8%
1	C	259	21% 80% 16%
1	D	259	3% 83% 15%
1	E	259	11% 88% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10547 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 putative pyrroline carboxylate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	Se	0	0	0
			1921	1224	319	370	1	7			
1	B	257	Total	C	N	O	S	Se	0	0	0
			1921	1224	319	370	1	7			
1	C	256	Total	C	N	O	S	Se	0	0	0
			1916	1221	318	369	1	7			
1	D	258	Total	C	N	O	S	Se	0	0	0
			1926	1227	320	371	1	7			
1	E	259	Total	C	N	O	S	Se	0	0	0
			1935	1231	322	374	1	7			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
A	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
A	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
A	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
B	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
B	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
B	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
C	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
C	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
C	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
D	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
D	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
D	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	-2	SER	-	CLONING ARTIFACT	UNP Q9A1S9
E	-1	ASN	-	CLONING ARTIFACT	UNP Q9A1S9
E	0	ALA	-	CLONING ARTIFACT	UNP Q9A1S9
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	11	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	49	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	86	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	109	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	112	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9
E	231	MSE	MET	MODIFIED RESIDUE	UNP Q9A1S9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

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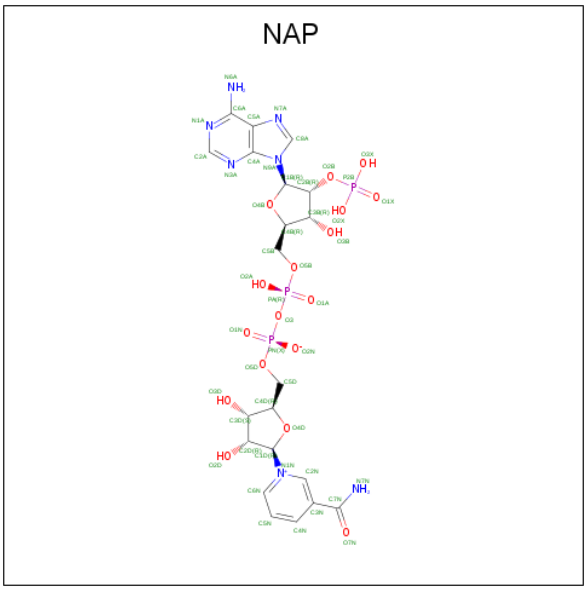
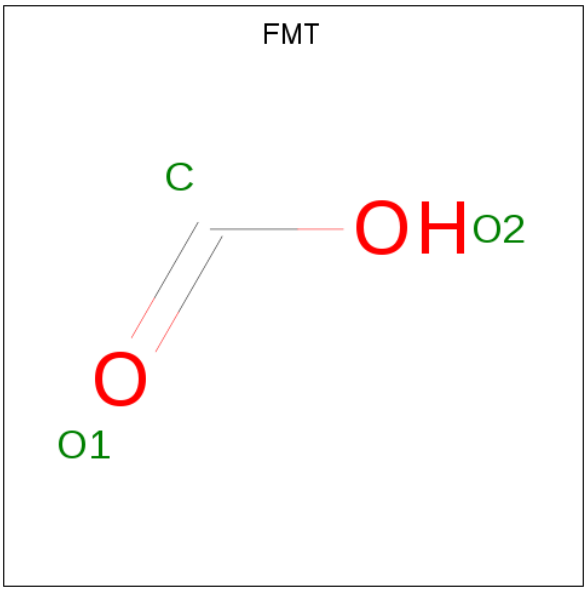
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Na 1 1	0	0

- Molecule 3 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
3	A	1	Total C N O P 48 21 7 17 3	0	0
3	B	1	Total C N O P 48 21 7 17 3	0	0
3	C	1	Total C N O P 48 21 7 17 3	0	0
3	D	1	Total C N O P 48 21 7 17 3	0	0
3	E	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

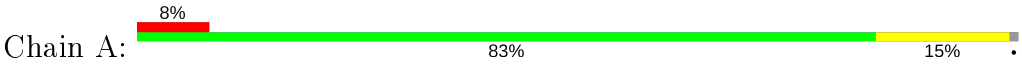
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	123	Total O 123 123	0	0
5	C	99	Total O 99 99	0	0
5	D	150	Total O 150 150	0	0
5	E	157	Total O 157 157	0	0

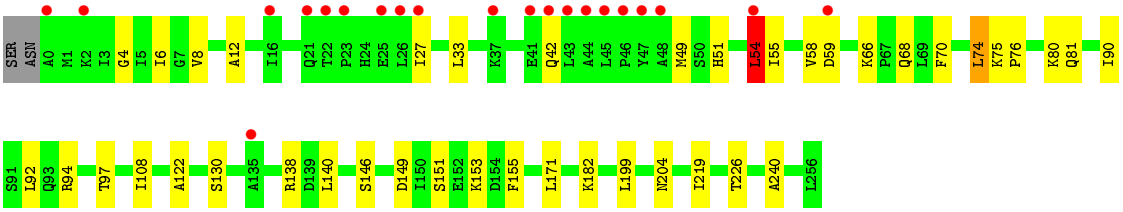
3 Residue-property plots (i)

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: putative pyrroline carboxylate reductase

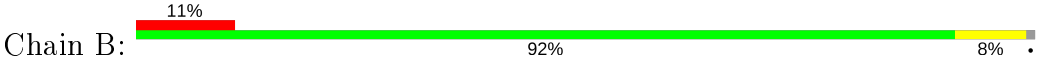
Chain A:

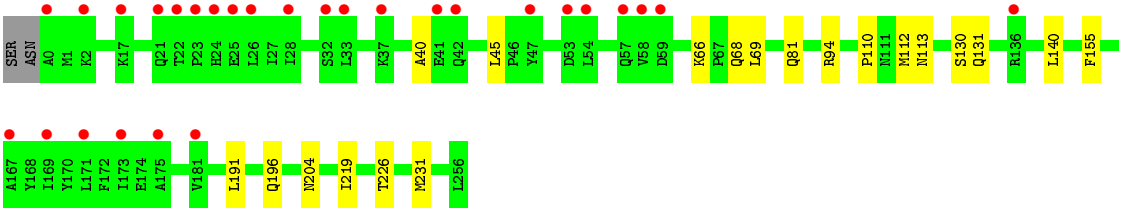




- Molecule 1: putative pyrroline carboxylate reductase

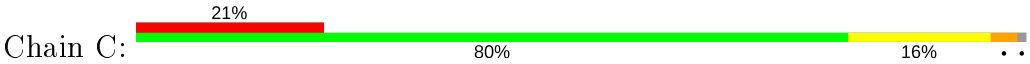
Chain B:

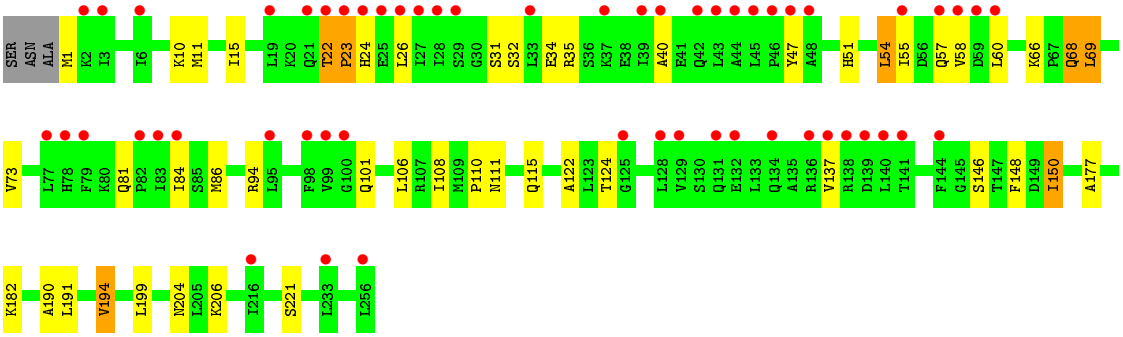




- Molecule 1: putative pyrroline carboxylate reductase

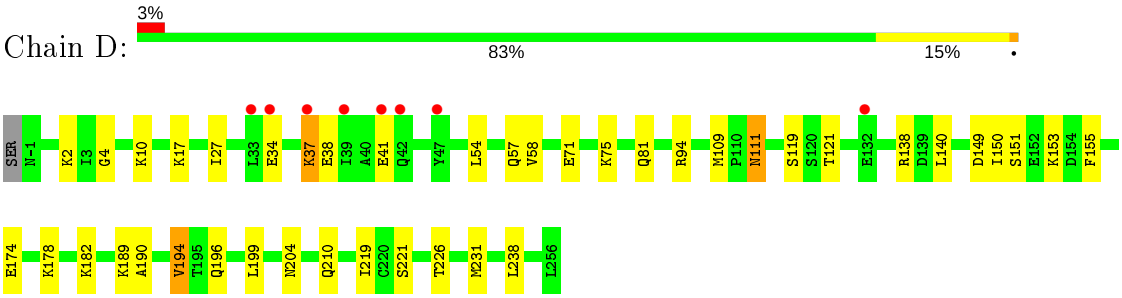
Chain C:





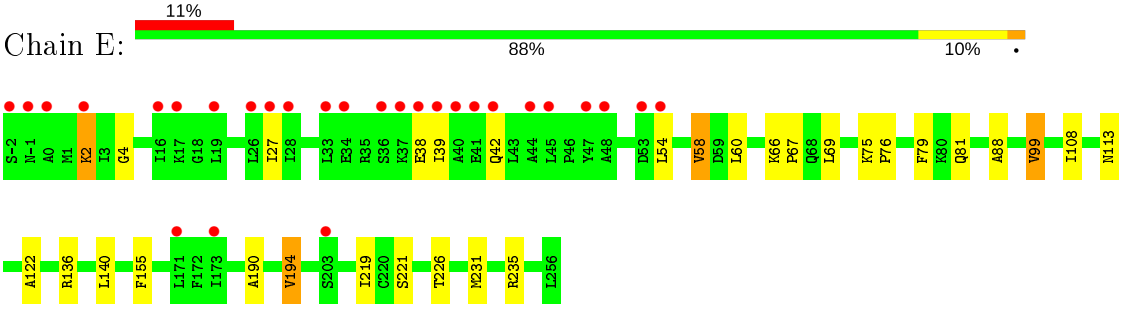
- Molecule 1: putative pyrroline carboxylate reductase

Chain D:



- Molecule 1: putative pyrroline carboxylate reductase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.63Å 109.65Å 84.03Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 45.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.15) 99.0 (45.84-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.210 0.178 , 0.207	Depositor DCC
R_{free} test set	4155 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10547	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: NA, FMT, 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	0.62	0/1940	0.63	1/2612 (0.0%)
1	B	0.60	0/1940	0.60	1/2612 (0.0%)
1	C	0.60	0/1936	0.63	2/2608 (0.1%)
1	D	0.64	0/1945	0.60	0/2619
1	E	0.62	0/1954	0.63	1/2631 (0.0%)
All	All	0.62	0/9715	0.62	5/13082 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	LEU	CA-CB-CG	6.34	129.88	115.30
1	C	69	LEU	CA-CB-CG	5.71	128.42	115.30
1	E	54	LEU	CA-CB-CG	5.53	128.03	115.30
1	C	54	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	191	LEU	CA-CB-CG	5.03	126.87	115.30

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	1921	0	2014	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1921	0	2014	9	0
1	C	1916	0	2009	32	0
1	D	1926	0	2016	27	0
1	E	1935	0	2025	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	2	0
3	E	48	0	25	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
5	A	139	0	0	1	0
5	B	123	0	0	2	0
5	C	99	0	0	1	0
5	D	150	0	0	5	0
5	E	157	0	0	4	0
All	All	10547	0	10208	104	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 (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ARG:HH22	1:D:149:ASP:HB2	1.38	0.86
1:E:88:ALA:HB3	5:E:1606:HOH:O	1.78	0.82
1:C:68:GLN:HE21	1:C:68:GLN:H	1.27	0.82
1:C:148:PHE:HB3	1:C:150:ILE:CD1	2.12	0.79
1:D:138:ARG:NH2	1:D:149:ASP:HB2	2.02	0.75
1:A:55:ILE:HG23	1:A:81:GLN:HE22	1.55	0.71
1:E:2:LYS:NZ	1:E:2:LYS:HB3	2.07	0.69
1:C:22:THR:N	1:C:23:PRO:HD2	2.09	0.68
1:C:32:SER:HB2	1:C:35:ARG:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:NZ	5:C:1538:HOH:O	2.26	0.67
1:D:178:LYS:NZ	5:D:1638:HOH:O	2.27	0.67
1:A:66:LYS:HB3	1:A:68:GLN:HE21	1.62	0.65
1:D:4:GLY:HA3	1:D:54:LEU:HD11	1.77	0.65
1:B:204:ASN:HD21	1:C:115:GLN:HE21	1.45	0.64
1:D:111:ASN:C	1:D:111:ASN:HD22	2.00	0.64
1:D:219:ILE:HG22	1:D:226:THR:HG21	1.82	0.61
1:C:22:THR:HG22	1:C:24:HIS:HD2	1.65	0.61
1:C:190:ALA:O	1:C:194:VAL:HG13	2.03	0.59
1:D:182:LYS:HD2	1:E:231:MSE:HG3	1.86	0.57
1:C:101:GLN:HG3	1:C:101:GLN:O	2.06	0.55
1:B:219:ILE:HG22	1:B:226:THR:HG21	1.88	0.55
1:E:67:PRO:HG3	5:E:1606:HOH:O	2.08	0.54
1:A:171:LEU:HD23	1:D:238:LEU:HD23	1.90	0.54
1:E:58:VAL:HG13	1:E:60:LEU:H	1.73	0.53
3:D:1503:NAP:O1A	5:D:1648:HOH:O	2.17	0.53
1:C:40:ALA:HB2	1:C:47:TYR:HB3	1.90	0.53
1:C:60:LEU:HD21	1:C:84:ILE:HD12	1.90	0.52
1:C:23:PRO:HA	1:C:24:HIS:HB2	1.92	0.51
1:D:94:ARG:HD3	5:D:1533:HOH:O	2.10	0.51
1:A:182:LYS:HD2	1:B:231:MSE:HG3	1.91	0.51
1:C:55:ILE:HG23	1:C:81:GLN:HE22	1.76	0.51
1:E:113:ASN:ND2	5:E:1576:HOH:O	2.43	0.51
1:A:94:ARG:O	1:A:97:THR:HB	2.10	0.51
1:C:22:THR:N	1:C:23:PRO:CD	2.72	0.51
1:D:138:ARG:HH22	1:D:149:ASP:CB	2.19	0.51
1:B:196:GLN:HE22	1:C:146:SER:HB2	1.75	0.51
1:E:136:ARG:NH2	5:E:1621:HOH:O	2.38	0.50
1:C:1:MSE:HB3	1:C:24:HIS:CE1	2.47	0.49
1:D:151:SER:OG	1:D:153:LYS:HG2	2.12	0.49
1:B:66:LYS:HE3	1:B:68:GLN:HB2	1.94	0.49
1:A:138:ARG:NH1	1:A:149:ASP:OD2	2.46	0.49
1:A:70:PHE:O	1:A:74:LEU:HB2	2.13	0.49
1:D:111:ASN:HD21	1:D:119:SER:HA	1.78	0.49
1:B:66:LYS:HE2	1:B:69:LEU:HD13	1.95	0.48
1:A:66:LYS:HB3	1:A:68:GLN:NE2	2.29	0.47
1:E:4:GLY:HA2	1:E:27:ILE:O	2.14	0.47
1:E:190:ALA:O	1:E:194:VAL:HG13	2.14	0.47
1:D:174:GLU:OE2	1:D:178:LYS:HE3	2.14	0.47
1:E:79:PHE:CD1	1:E:99:VAL:HG22	2.49	0.47
1:A:199:LEU:HD12	1:D:199:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:O	1:A:81:GLN:NE2	2.49	0.46
1:C:68:GLN:H	1:C:68:GLN:NE2	2.06	0.46
1:A:58:VAL:O	1:A:81:GLN:HG2	2.15	0.46
1:A:59:ASP:O	1:A:81:GLN:HB3	2.17	0.45
1:C:182:LYS:HD2	1:D:231:MSE:HG3	1.98	0.45
1:C:22:THR:CG2	1:C:24:HIS:HD2	2.27	0.45
1:D:37:LYS:HD2	1:D:38:GLU:N	2.32	0.45
1:A:6:ILE:HG23	1:A:51:HIS:CE1	2.53	0.44
1:D:4:GLY:CA	1:D:54:LEU:HD11	2.47	0.44
1:C:148:PHE:HB3	1:C:150:ILE:HD12	1.96	0.44
1:A:138:ARG:HH12	1:A:149:ASP:CG	2.21	0.44
3:D:1503:NAP:H1B	5:D:1517:HOH:O	2.18	0.44
1:C:51:HIS:O	1:C:54:LEU:HB3	2.18	0.43
1:A:75:LYS:N	1:A:76:PRO:HD2	2.34	0.43
1:C:15:ILE:HD12	1:C:86:MSE:CE	2.48	0.43
1:E:38:GLU:O	1:E:42:GLN:HG2	2.18	0.43
1:A:33:LEU:HD21	1:A:49:MSE:HA	2.01	0.43
1:C:106:LEU:HD13	1:C:137:VAL:HG21	2.00	0.43
1:E:219:ILE:HG22	1:E:226:THR:HG21	2.01	0.43
1:A:240:ALA:CB	1:E:235:ARG:HA	2.49	0.43
1:D:190:ALA:O	1:D:194:VAL:HG13	2.19	0.43
1:B:110:PRO:O	3:B:1501:NAP:H5N	2.19	0.42
1:E:108:ILE:HA	1:E:122:ALA:O	2.19	0.42
1:D:111:ASN:C	1:D:111:ASN:ND2	2.71	0.42
1:C:66:LYS:HB3	1:C:68:GLN:NE2	2.34	0.42
1:A:138:ARG:NH1	1:A:149:ASP:CG	2.73	0.42
1:A:108:ILE:HA	1:A:122:ALA:O	2.20	0.42
1:D:189:LYS:HA	1:D:189:LYS:HD3	1.88	0.41
1:D:27:ILE:HG23	1:D:54:LEU:CD1	2.50	0.41
1:A:51:HIS:O	1:A:54:LEU:HB3	2.19	0.41
1:B:40:ALA:HB1	1:B:45:LEU:O	2.21	0.41
1:C:15:ILE:HD12	1:C:86:MSE:HE1	2.01	0.41
1:E:66:LYS:HB2	1:E:67:PRO:HD2	2.02	0.41
1:C:110:PRO:O	3:C:1502:NAP:H5N	2.20	0.41
1:A:219:ILE:HG22	1:A:226:THR:HG21	2.02	0.41
1:D:109:MSE:O	1:D:121:THR:HA	2.21	0.41
1:D:210:GLN:NE2	5:D:1644:HOH:O	2.50	0.41
1:A:151:SER:OG	1:A:153:LYS:HG2	2.20	0.41
1:A:8:VAL:HA	1:A:12:ALA:HB3	2.03	0.41
1:C:108:ILE:HA	1:C:122:ALA:O	2.21	0.41
1:B:113:ASN:ND2	5:B:1556:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:MSE:HE1	1:C:111:ASN:O	2.21	0.41
1:A:4:GLY:HA2	1:A:27:ILE:O	2.20	0.41
5:B:1603:HOH:O	1:C:10:LYS:HG3	2.20	0.41
1:C:23:PRO:HA	1:C:24:HIS:C	2.40	0.41
1:A:42:GLN:NE2	5:A:1576:HOH:O	2.38	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.97	0.41
1:D:2:LYS:NZ	1:D:57:GLN:HE21	2.19	0.40
1:C:22:THR:HG22	1:C:24:HIS:CD2	2.50	0.40
1:D:71:GLU:HG3	1:D:75:LYS:HD2	2.02	0.40
1:E:75:LYS:N	1:E:76:PRO:HD2	2.37	0.40
1:C:177:ALA:CB	1:C:191:LEU:HD13	2.51	0.40
1:A:146:SER:HB2	1:D:196:GLN:HE22	1.85	0.40
1:D:34:GLU:O	1:D:38:GLU:HG3	2.21	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	255/259 (98%)	250 (98%)	5 (2%)	0	100	100
1	B	255/259 (98%)	252 (99%)	3 (1%)	0	100	100
1	C	254/259 (98%)	244 (96%)	9 (4%)	1 (0%)	34	29
1	D	256/259 (99%)	253 (99%)	3 (1%)	0	100	100
1	E	257/259 (99%)	254 (99%)	3 (1%)	0	100	100
All	All	1277/1295 (99%)	1253 (98%)	23 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	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	212/207 (102%)	204 (96%)	8 (4%)	33 31
1	B	212/207 (102%)	205 (97%)	7 (3%)	38 37
1	C	212/207 (102%)	196 (92%)	16 (8%)	13 8
1	D	212/207 (102%)	199 (94%)	13 (6%)	18 14
1	E	214/207 (103%)	204 (95%)	10 (5%)	26 23
All	All	1062/1035 (103%)	1008 (95%)	54 (5%)	24 20

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	74	LEU
1	A	80	LYS
1	A	90	ILE
1	A	130	SER
1	A	140	LEU
1	A	155	PHE
1	A	204	ASN
1	B	81	GLN
1	B	94	ARG
1	B	112	MSE
1	B	130	SER
1	B	131	GLN
1	B	140	LEU
1	B	155	PHE
1	C	22	THR
1	C	26	LEU
1	C	31	SER
1	C	34	GLU
1	C	57	GLN
1	C	58	VAL
1	C	68	GLN
1	C	69	LEU

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Mol	Chain	Res	Type
1	C	73	VAL
1	C	94	ARG
1	C	124	THR
1	C	150	ILE
1	C	194	VAL
1	C	199	LEU
1	C	204	ASN
1	C	221	SER
1	D	10	LYS
1	D	17	LYS
1	D	37	LYS
1	D	41	GLU
1	D	58	VAL
1	D	81	GLN
1	D	111	ASN
1	D	140	LEU
1	D	150	ILE
1	D	155	PHE
1	D	194	VAL
1	D	204	ASN
1	D	221	SER
1	E	2	LYS
1	E	39	ILE
1	E	58	VAL
1	E	69	LEU
1	E	81	GLN
1	E	99	VAL
1	E	140	LEU
1	E	155	PHE
1	E	194	VAL
1	E	221	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	101	GLN
1	A	196	GLN
1	A	204	ASN
1	B	113	ASN
1	B	115	GLN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	196	GLN
1	C	21	GLN
1	C	68	GLN
1	C	113	ASN
1	C	115	GLN
1	C	196	GLN
1	C	204	ASN
1	D	21	GLN
1	D	57	GLN
1	D	111	ASN
1	D	115	GLN
1	D	196	GLN
1	D	204	ASN
1	E	113	ASN
1	E	196	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\#\|Z\|>2$
4	FMT	A	1508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	E	1504	-	45,52,52	1.75	4 (8%)	56,80,80	1.29	5 (8%)
4	FMT	C	1510	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	B	1501	-	45,52,52	1.74	4 (8%)	56,80,80	1.27	4 (7%)
4	FMT	E	1512	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	A	1500	-	45,52,52	1.67	4 (8%)	56,80,80	1.27	7 (12%)
3	NAP	D	1503	-	45,52,52	1.78	4 (8%)	56,80,80	1.23	3 (5%)
4	FMT	B	1509	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	1511	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAP	C	1502	-	45,52,52	1.76	4 (8%)	56,80,80	1.16	3 (5%)

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	NAP	D	1503	-	-	4/31/67/67	0/5/5/5
3	NAP	E	1504	-	-	4/31/67/67	0/5/5/5
3	NAP	A	1500	-	-	5/31/67/67	0/5/5/5
3	NAP	C	1502	-	-	9/31/67/67	0/5/5/5
3	NAP	B	1501	-	-	8/31/67/67	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1502	NAP	O7N-C7N	9.21	1.41	1.24
3	E	1504	NAP	O7N-C7N	9.01	1.41	1.24
3	D	1503	NAP	O7N-C7N	8.98	1.41	1.24
3	B	1501	NAP	O7N-C7N	8.86	1.41	1.24
3	A	1500	NAP	O7N-C7N	8.09	1.39	1.24
3	D	1503	NAP	C2A-N3A	4.40	1.39	1.32
3	A	1500	NAP	C2A-N3A	4.37	1.39	1.32
3	C	1502	NAP	C2A-N3A	4.25	1.38	1.32
3	B	1501	NAP	C2A-N3A	4.15	1.38	1.32
3	E	1504	NAP	C2A-N3A	3.94	1.38	1.32
3	D	1503	NAP	C2N-N1N	3.20	1.38	1.35
3	E	1504	NAP	C2N-N1N	2.94	1.38	1.35
3	B	1501	NAP	C2A-N1A	2.89	1.39	1.33
3	A	1500	NAP	C2N-N1N	2.80	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1502	NAP	C2A-N1A	2.74	1.39	1.33
3	A	1500	NAP	C2A-N1A	2.72	1.39	1.33
3	B	1501	NAP	C2N-N1N	2.67	1.38	1.35
3	E	1504	NAP	C2A-N1A	2.66	1.38	1.33
3	D	1503	NAP	C2A-N1A	2.57	1.38	1.33
3	C	1502	NAP	C2N-N1N	2.56	1.38	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1504	NAP	N3A-C2A-N1A	-5.59	119.94	128.68
3	B	1501	NAP	N3A-C2A-N1A	-5.47	120.13	128.68
3	D	1503	NAP	N3A-C2A-N1A	-5.46	120.14	128.68
3	A	1500	NAP	N3A-C2A-N1A	-5.34	120.33	128.68
3	C	1502	NAP	N3A-C2A-N1A	-5.12	120.67	128.68
3	A	1500	NAP	C3N-C7N-N7N	3.66	122.14	117.75
3	B	1501	NAP	C3N-C7N-N7N	3.45	121.89	117.75
3	B	1501	NAP	PN-O3-PA	-2.95	122.72	132.83
3	D	1503	NAP	C3N-C7N-N7N	2.73	121.02	117.75
3	A	1500	NAP	O7N-C7N-C3N	-2.69	116.42	119.63
3	B	1501	NAP	O7N-C7N-C3N	-2.60	116.53	119.63
3	E	1504	NAP	C3N-C7N-N7N	2.56	120.83	117.75
3	E	1504	NAP	PN-O3-PA	-2.55	124.06	132.83
3	E	1504	NAP	C6N-N1N-C2N	-2.53	119.67	121.97
3	D	1503	NAP	PN-O3-PA	-2.50	124.25	132.83
3	C	1502	NAP	PN-O3-PA	-2.45	124.40	132.83
3	E	1504	NAP	O7N-C7N-C3N	-2.35	116.82	119.63
3	A	1500	NAP	O3D-C3D-C4D	-2.18	104.75	111.05
3	A	1500	NAP	PN-O3-PA	-2.16	125.40	132.83
3	C	1502	NAP	C3N-C7N-N7N	2.12	120.29	117.75
3	A	1500	NAP	C1B-N9A-C4A	-2.07	123.00	126.64
3	A	1500	NAP	C2D-C3D-C4D	2.02	106.57	102.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1504	NAP	O4D-C1D-N1N-C2N
3	A	1500	NAP	C2B-O2B-P2B-O3X
3	A	1500	NAP	O4D-C1D-N1N-C2N
3	D	1503	NAP	C2B-O2B-P2B-O3X
3	D	1503	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	C	1502	NAP	C2B-O2B-P2B-O1X
3	C	1502	NAP	O4D-C1D-N1N-C2N
3	C	1502	NAP	O4D-C1D-N1N-C6N
3	B	1501	NAP	O4D-C1D-N1N-C2N
3	E	1504	NAP	C1B-C2B-O2B-P2B
3	B	1501	NAP	O4B-C4B-C5B-O5B
3	E	1504	NAP	C3B-C2B-O2B-P2B
3	A	1500	NAP	C3B-C2B-O2B-P2B
3	D	1503	NAP	C2B-O2B-P2B-O1X
3	C	1502	NAP	C2B-O2B-P2B-O3X
3	A	1500	NAP	C1B-C2B-O2B-P2B
3	C	1502	NAP	PN-O3-PA-O1A
3	A	1500	NAP	O4B-C4B-C5B-O5B
3	B	1501	NAP	PA-O3-PN-O2N
3	E	1504	NAP	O4B-C4B-C5B-O5B
3	C	1502	NAP	O4B-C4B-C5B-O5B
3	B	1501	NAP	C3B-C4B-C5B-O5B
3	C	1502	NAP	C5D-O5D-PN-O3
3	C	1502	NAP	C2D-C1D-N1N-C6N
3	B	1501	NAP	C5B-O5B-PA-O3
3	B	1501	NAP	C2B-O2B-P2B-O3X
3	C	1502	NAP	PN-O3-PA-O2A
3	B	1501	NAP	PA-O3-PN-O1N
3	B	1501	NAP	C5B-O5B-PA-O2A
3	D	1503	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

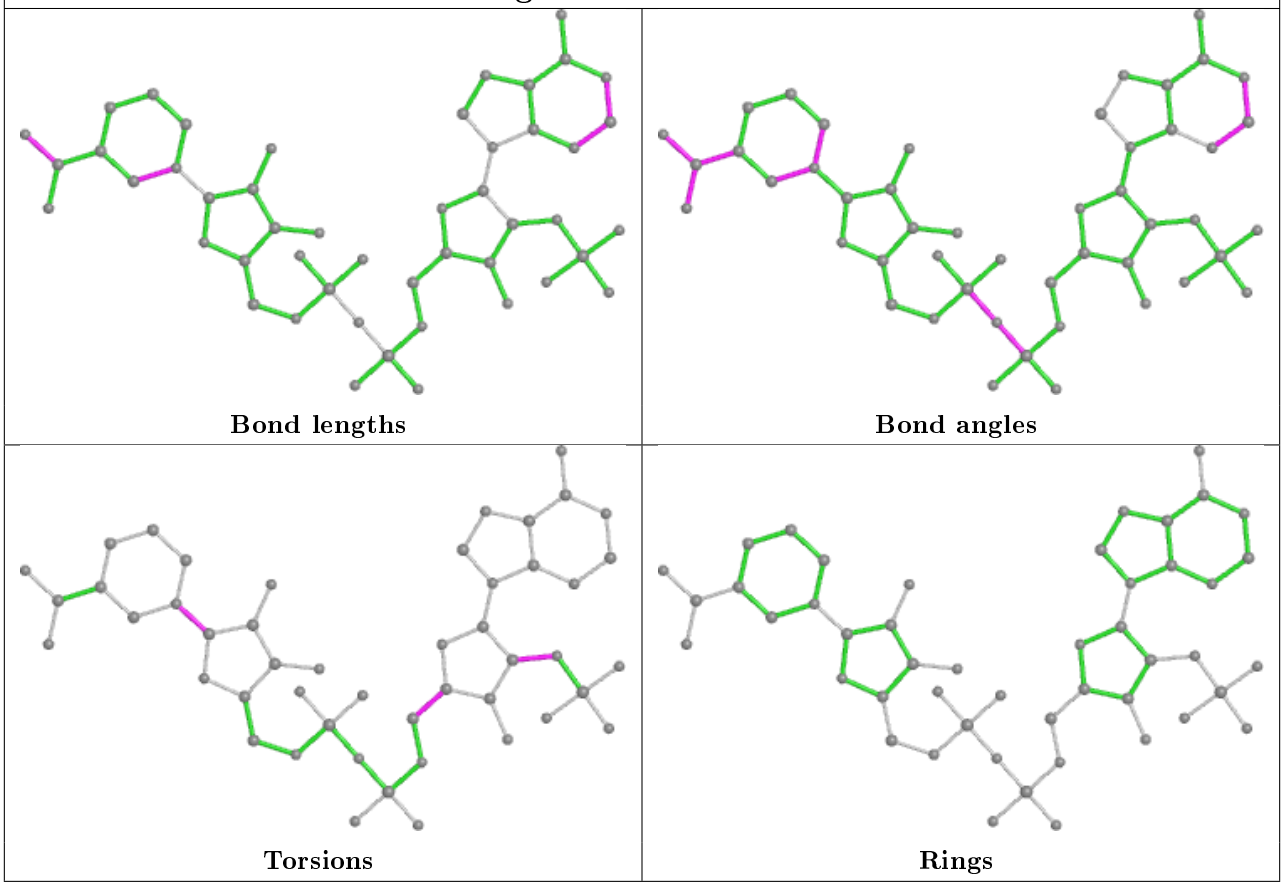
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	NAP	1	0
3	D	1503	NAP	2	0
3	C	1502	NAP	1	0

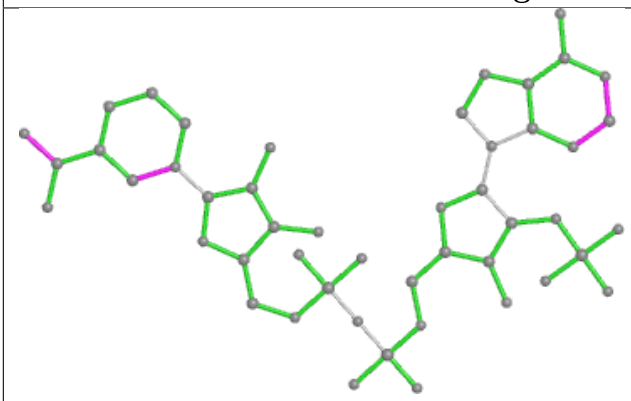
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

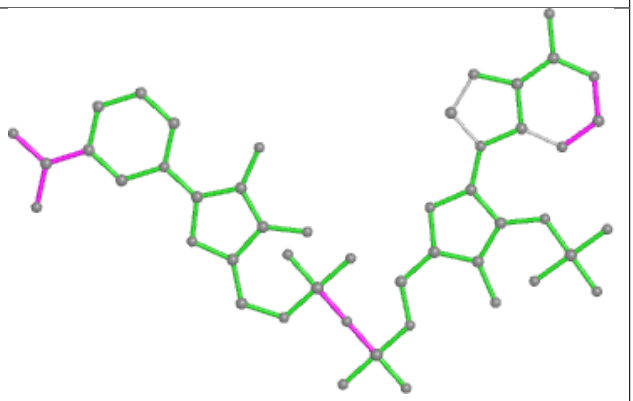
Ligand NAP E 1504



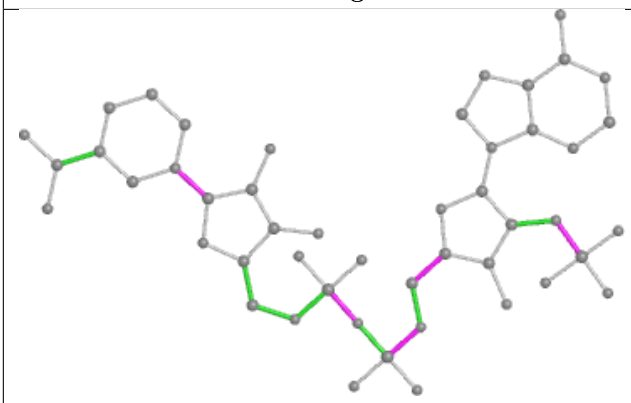
Ligand NAP B 1501



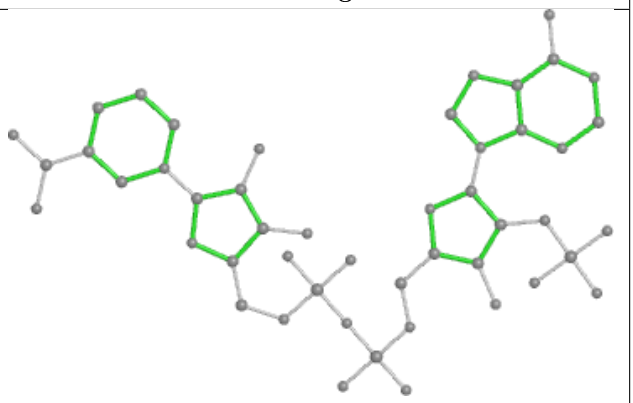
Bond lengths



Bond angles

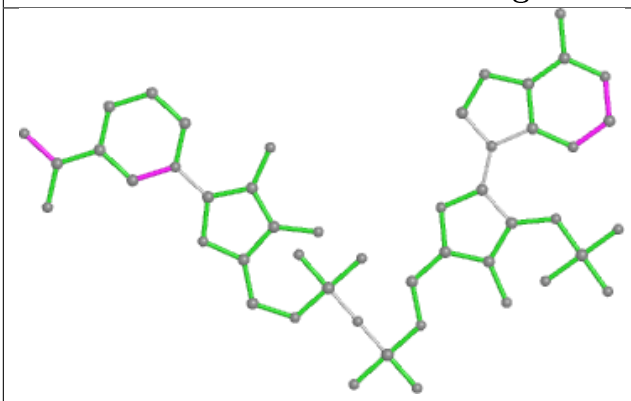


Torsions

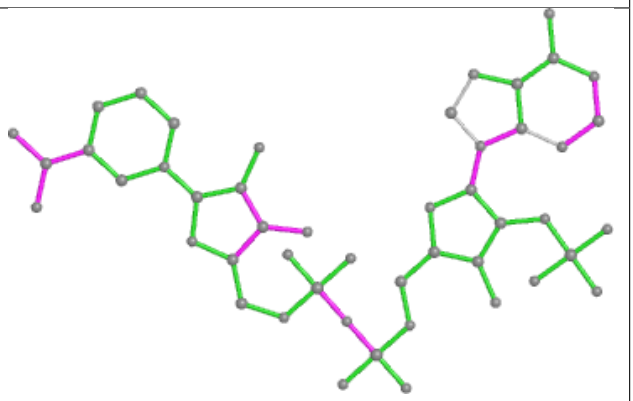


Rings

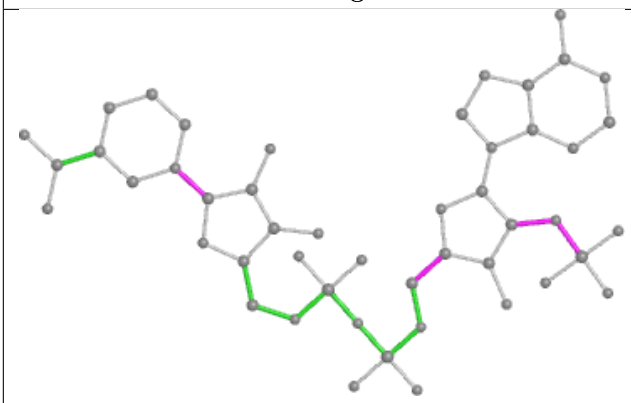
Ligand NAP A 1500



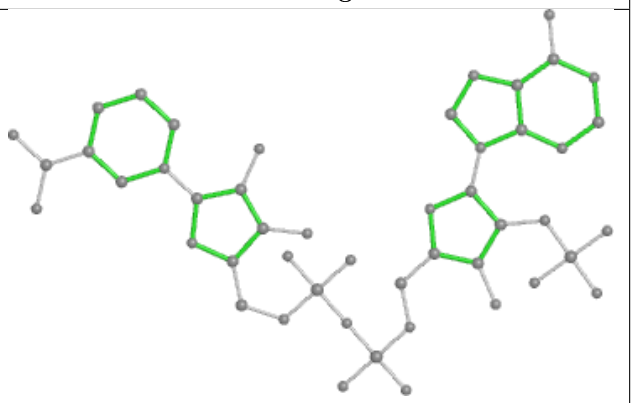
Bond lengths



Bond angles

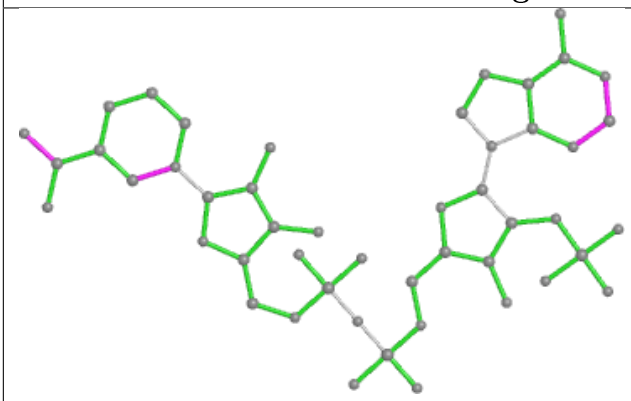


Torsions

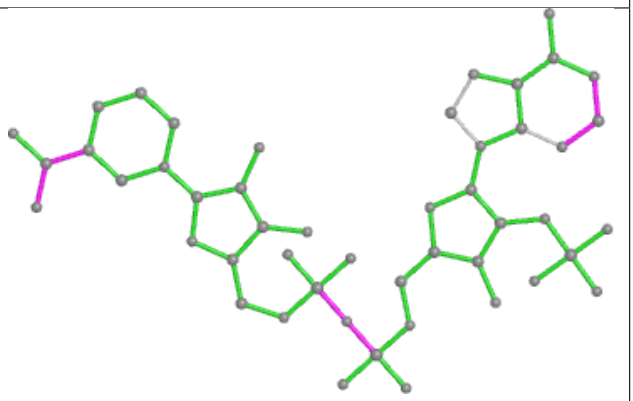


Rings

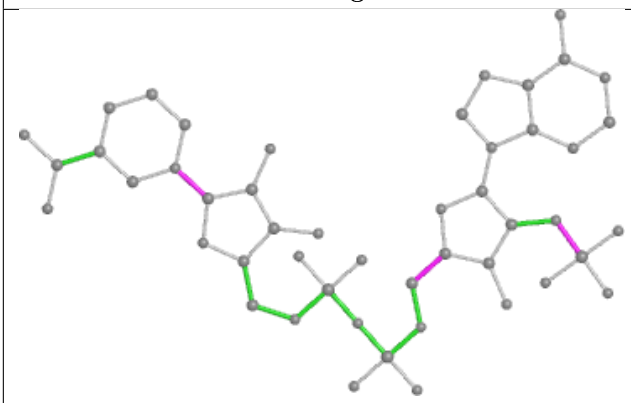
Ligand NAP D 1503



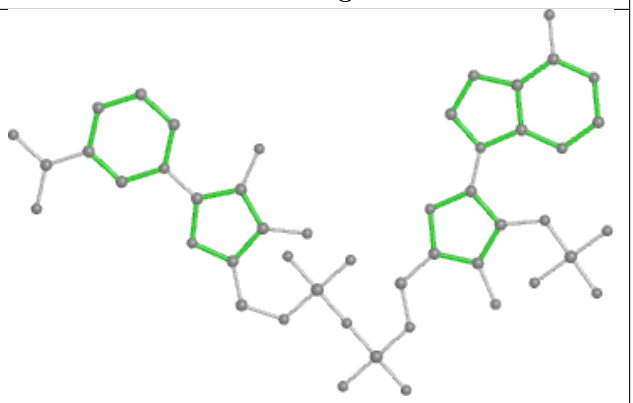
Bond lengths



Bond angles

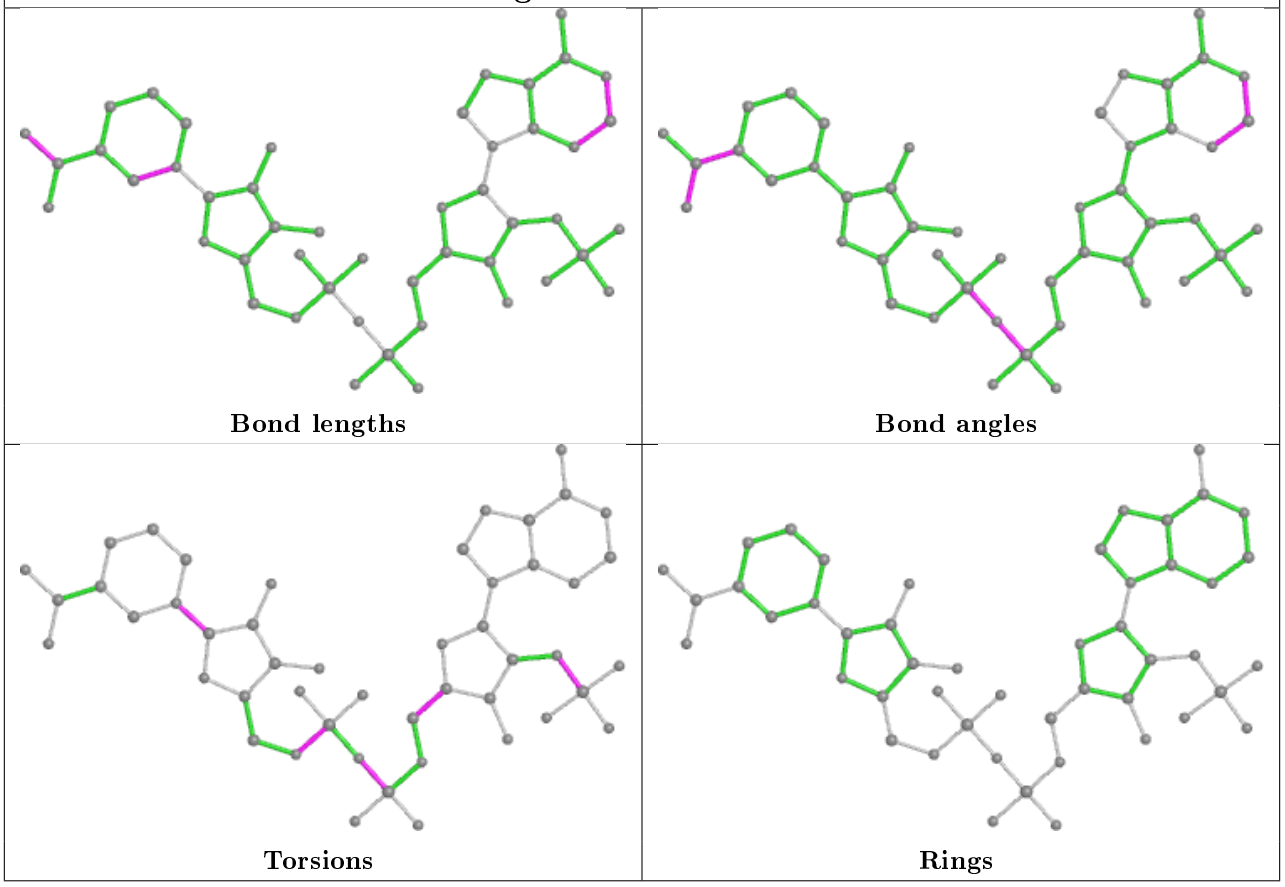


Torsions



Rings

Ligand NAP C 1502



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	250/259 (96%)	0.57	21 (8%) 11 15	29, 41, 58, 67	1 (0%)
1	B	250/259 (96%)	0.69	28 (11%) 5 7	30, 43, 63, 70	1 (0%)
1	C	249/259 (96%)	1.15	55 (22%) 0 0	30, 50, 84, 89	0
1	D	251/259 (96%)	0.39	8 (3%) 47 56	28, 41, 57, 67	2 (0%)
1	E	252/259 (97%)	0.73	28 (11%) 5 7	28, 40, 65, 71	2 (0%)
All	All	1252/1295 (96%)	0.71	140 (11%) 5 7	28, 42, 70, 89	6 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	LEU	6.3
1	C	45	LEU	6.1
1	E	27	ILE	5.8
1	C	22	THR	5.5
1	C	60	LEU	5.4
1	E	39	ILE	5.0
1	A	48	ALA	4.7
1	E	37	LYS	4.5
1	B	0	ALA	4.5
1	C	26	LEU	4.3
1	E	45	LEU	4.3
1	A	22	THR	4.3
1	C	136	ARG	4.2
1	C	58	VAL	4.2
1	B	22	THR	4.2
1	C	132	GLU	4.1
1	C	46	PRO	4.1
1	C	6	ILE	4.0
1	A	47	TYR	3.9
1	C	129	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	3.9
1	B	28	ILE	3.7
1	C	43	LEU	3.7
1	E	48	ALA	3.7
1	E	47	TYR	3.7
1	C	19	LEU	3.7
1	E	33	LEU	3.7
1	A	23	PRO	3.7
1	C	48	ALA	3.7
1	D	37	LYS	3.7
1	C	24	HIS	3.6
1	C	47	TYR	3.6
1	A	45	LEU	3.5
1	C	131	GLN	3.5
1	B	37	LYS	3.5
1	C	27	ILE	3.5
1	C	128	LEU	3.5
1	C	37	LYS	3.4
1	A	27	ILE	3.4
1	B	32	SER	3.4
1	B	47	TYR	3.4
1	C	42	GLN	3.4
1	B	54	LEU	3.4
1	E	42	GLN	3.3
1	C	23	PRO	3.3
1	E	26	LEU	3.3
1	C	25	GLU	3.2
1	D	39	ILE	3.2
1	C	139	ASP	3.2
1	E	44	ALA	3.2
1	B	58	VAL	3.1
1	E	0	ALA	3.1
1	A	43	LEU	3.1
1	D	47	TYR	3.1
1	E	-2	SER	3.0
1	C	28	ILE	3.0
1	C	55	ILE	3.0
1	C	59	ASP	3.0
1	C	84	ILE	3.0
1	E	2	LYS	3.0
1	A	42	GLN	3.0
1	D	33	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	39	ILE	2.9
1	A	26	LEU	2.9
1	C	79	PHE	2.9
1	B	171	LEU	2.9
1	E	173	ILE	2.7
1	A	25	GLU	2.7
1	C	77	LEU	2.7
1	C	137	VAL	2.7
1	C	216	ILE	2.7
1	A	54	LEU	2.7
1	B	41	GLU	2.7
1	E	203	SER	2.6
1	A	59	ASP	2.6
1	A	21	GLN	2.6
1	A	135	ALA	2.6
1	B	57	GLN	2.6
1	E	16	ILE	2.6
1	D	41	GLU	2.6
1	C	44	ALA	2.6
1	C	82	PRO	2.6
1	E	41	GLU	2.6
1	C	40	ALA	2.5
1	A	37	LYS	2.5
1	C	95	LEU	2.5
1	B	23	PRO	2.5
1	E	28	ILE	2.5
1	C	98	PHE	2.5
1	B	33	LEU	2.5
1	E	38	GLU	2.5
1	C	134	GLN	2.5
1	C	29	SER	2.5
1	D	34	GLU	2.5
1	C	21	GLN	2.4
1	E	-1	ASN	2.4
1	E	53	ASP	2.4
1	B	2	LYS	2.4
1	E	40	ALA	2.4
1	B	42	GLN	2.4
1	C	100	GLY	2.4
1	E	171	LEU	2.4
1	C	138	ARG	2.4
1	A	16	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	17	LYS	2.3
1	B	53	ASP	2.3
1	D	42	GLN	2.3
1	B	175	ALA	2.3
1	A	2	LYS	2.3
1	B	181	VAL	2.3
1	B	169	ILE	2.3
1	B	25	GLU	2.3
1	C	57	GLN	2.3
1	C	141	THR	2.2
1	E	54	LEU	2.2
1	C	78	HIS	2.2
1	E	36	SER	2.2
1	D	132	GLU	2.2
1	C	140	LEU	2.2
1	B	173	ILE	2.1
1	E	19	LEU	2.1
1	B	21	GLN	2.1
1	C	83	ILE	2.1
1	B	26	LEU	2.1
1	B	24	HIS	2.1
1	B	167	ALA	2.1
1	E	34	GLU	2.1
1	A	46	PRO	2.1
1	C	3	ILE	2.1
1	B	136	ARG	2.1
1	B	17	LYS	2.1
1	A	41	GLU	2.1
1	C	99	VAL	2.0
1	C	144	PHE	2.0
1	C	233	LEU	2.0
1	C	256	LEU	2.0
1	A	44	ALA	2.0
1	C	125	GLY	2.0
1	C	2	LYS	2.0
1	B	59	ASP	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)

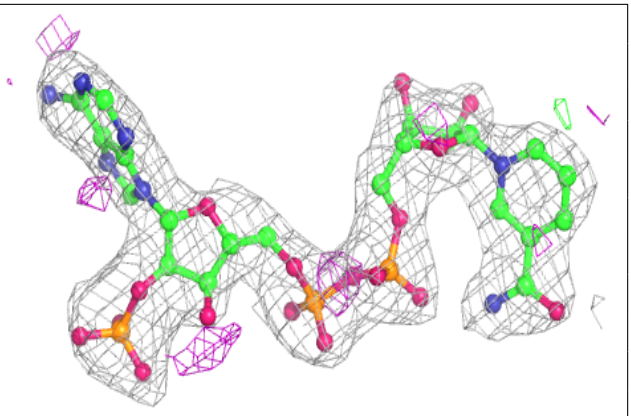
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

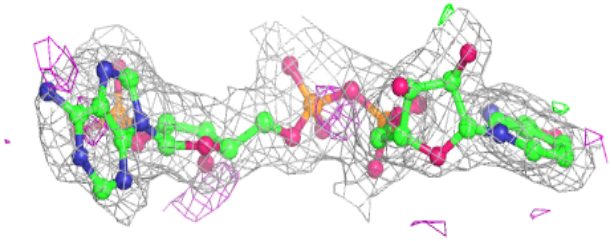
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	B	1509	3/3	0.82	0.12	59,59,60,61	0
4	FMT	C	1510	3/3	0.87	0.12	66,66,66,66	0
3	NAP	B	1501	48/48	0.88	0.15	52,75,81,83	0
2	NA	B	1258	1/1	0.90	0.05	46,46,46,46	0
4	FMT	A	1508	3/3	0.90	0.16	62,62,62,62	0
3	NAP	E	1504	48/48	0.91	0.13	47,71,80,81	0
3	NAP	C	1502	48/48	0.93	0.13	51,66,78,78	0
4	FMT	E	1512	3/3	0.93	0.10	64,64,65,65	0
3	NAP	D	1503	48/48	0.93	0.14	49,60,69,71	0
4	FMT	D	1511	3/3	0.94	0.10	64,64,64,65	0
3	NAP	A	1500	48/48	0.94	0.11	41,53,58,60	0
2	NA	D	1260	1/1	0.94	0.16	37,37,37,37	0
2	NA	C	1259	1/1	0.94	0.07	48,48,48,48	0
2	NA	A	1257	1/1	0.97	0.06	41,41,41,41	0
2	NA	E	1261	1/1	0.98	0.07	40,40,40,40	0

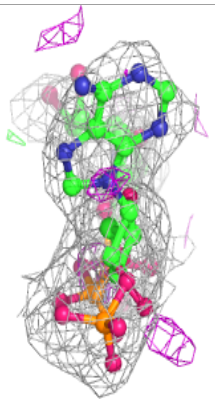
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 1501:

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

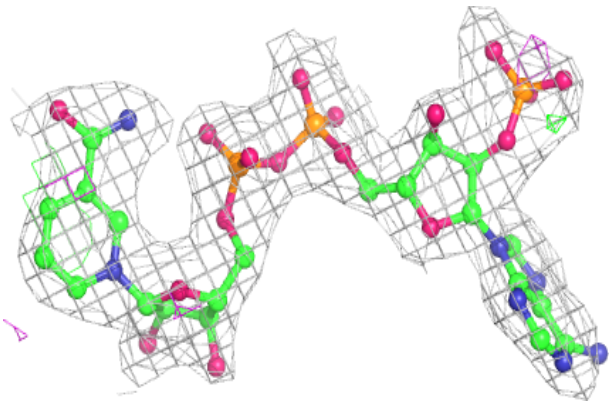


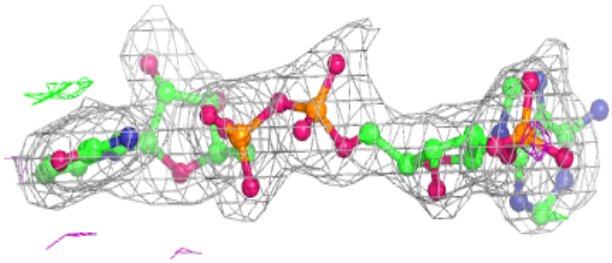


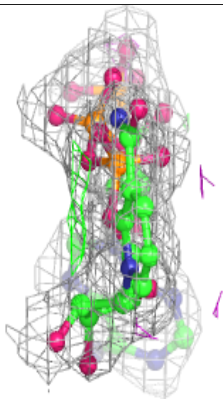


Electron density around NAP E 1504:

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

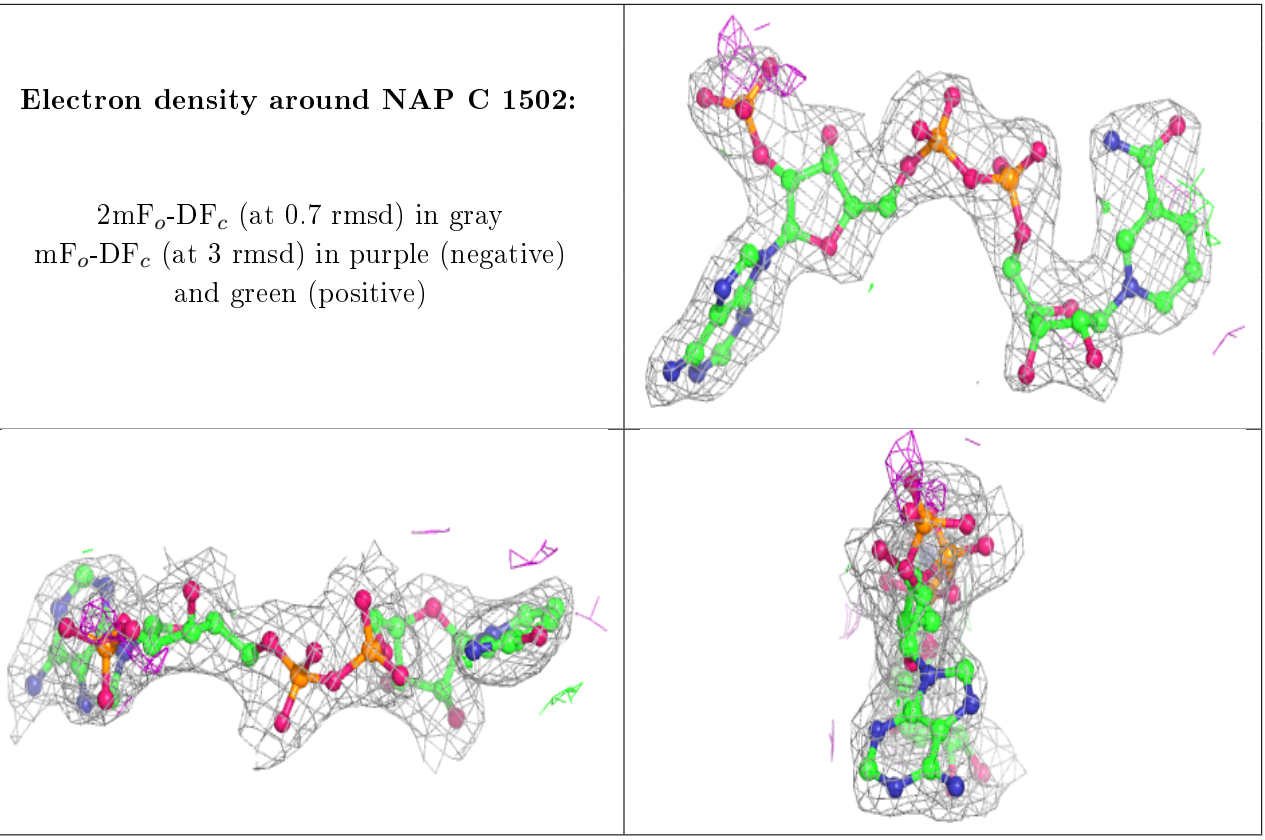






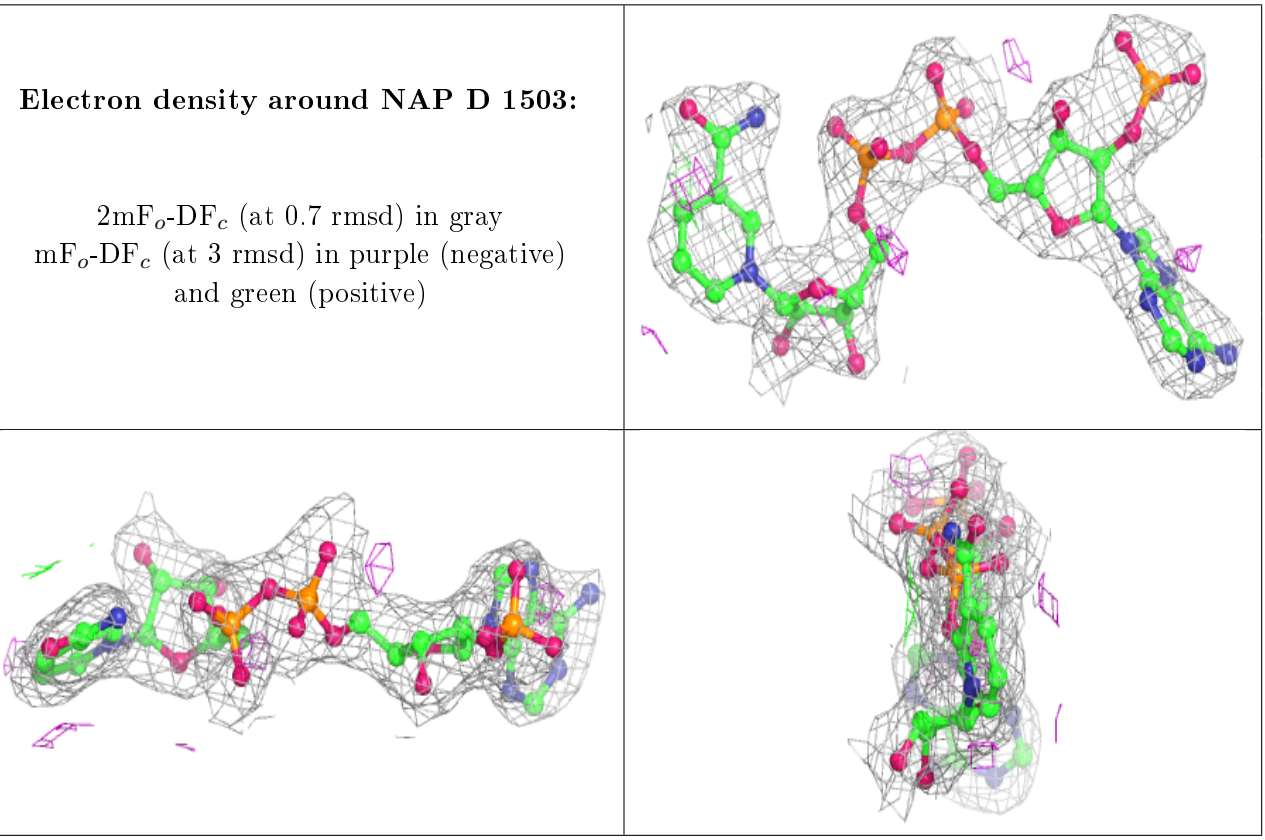
Electron density around NAP C 1502:

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



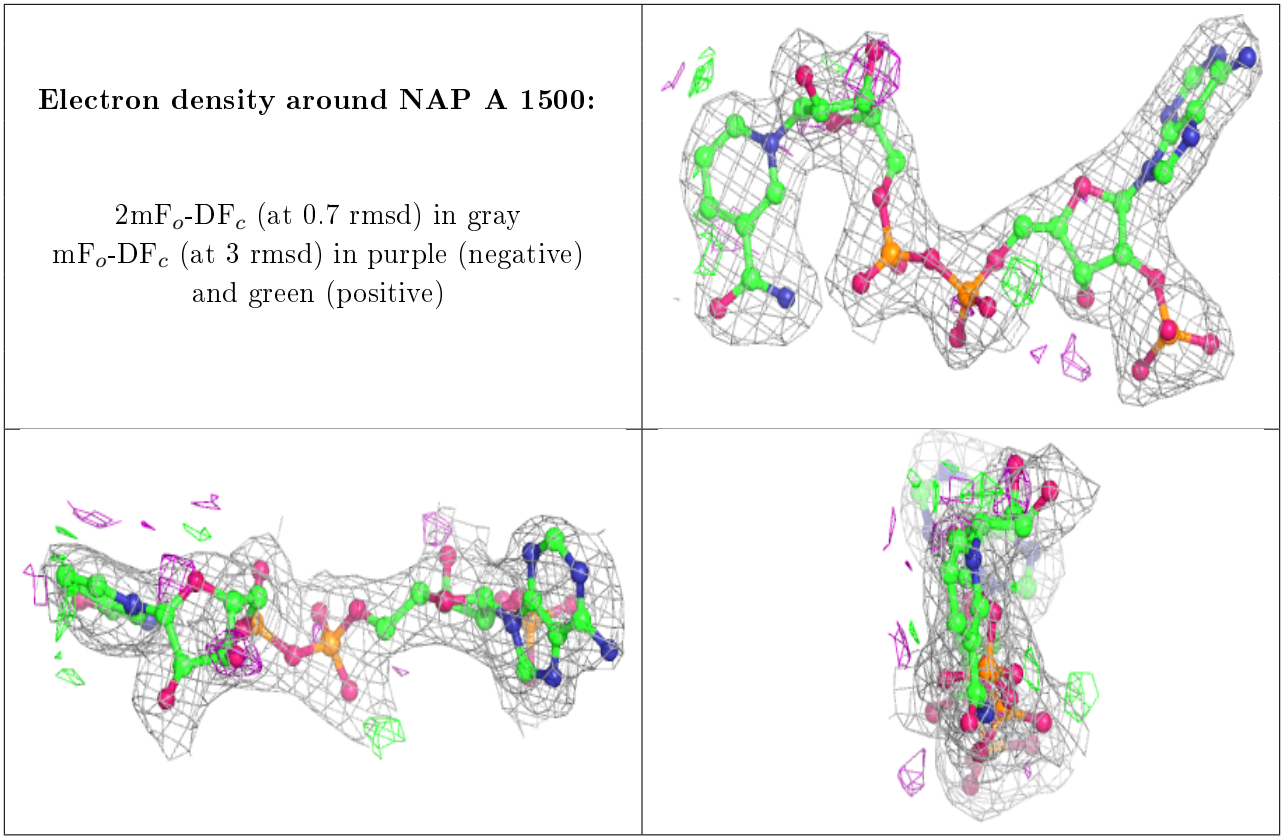
Electron density around NAP D 1503:

$2mF_o$-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 1500:

$2mF_o$-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.