Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2023 – 12:10 AM JST

PDB ID	:	7W5K
Title	:	The C296A mutant of L-sorbosone dehydrogenase (SNDH) from Gluconobacter Oxydans WSH-004
Authors	:	Li, D.; Hou, X.D.; Rao, Y.J.; Zhou, J.W.; Chen, J.
Deposited on	:	2021-11-30
Resolution	:	2.22 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

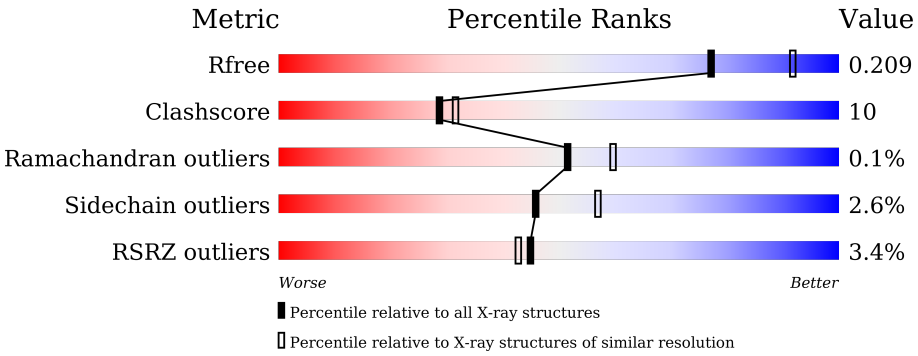
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	504	2% 74% 23% •
1	B	504	2% 73% 23% • •
1	C	504	5% 73% 22% • 5%
1	D	504	4% 74% 21% • 5%

2 Entry composition

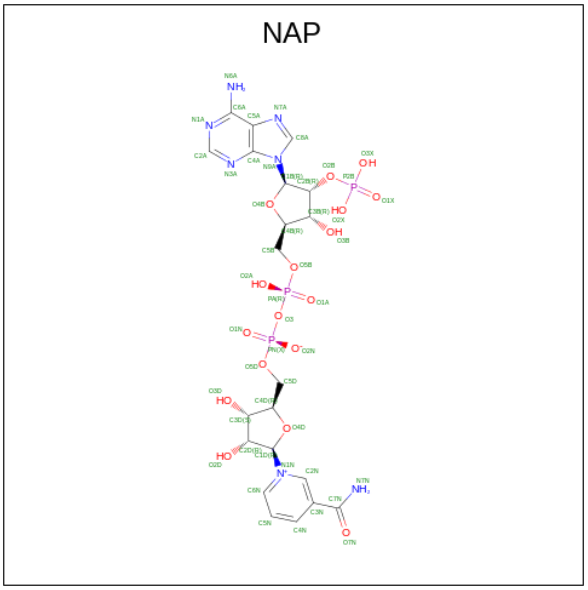
There are 3 unique types of molecules in this entry. The entry contains 15657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-sorbosone dehydrogenase, NAD(P) dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3709	2354	643	695	17			
1	B	490	Total	C	N	O	S	0	0	0
			3699	2346	642	694	17			
1	C	481	Total	C	N	O	S	0	0	0
			3632	2307	627	681	17			
1	D	481	Total	C	N	O	S	0	0	0
			3629	2304	625	683	17			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	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		

- Molecule 3 is water.

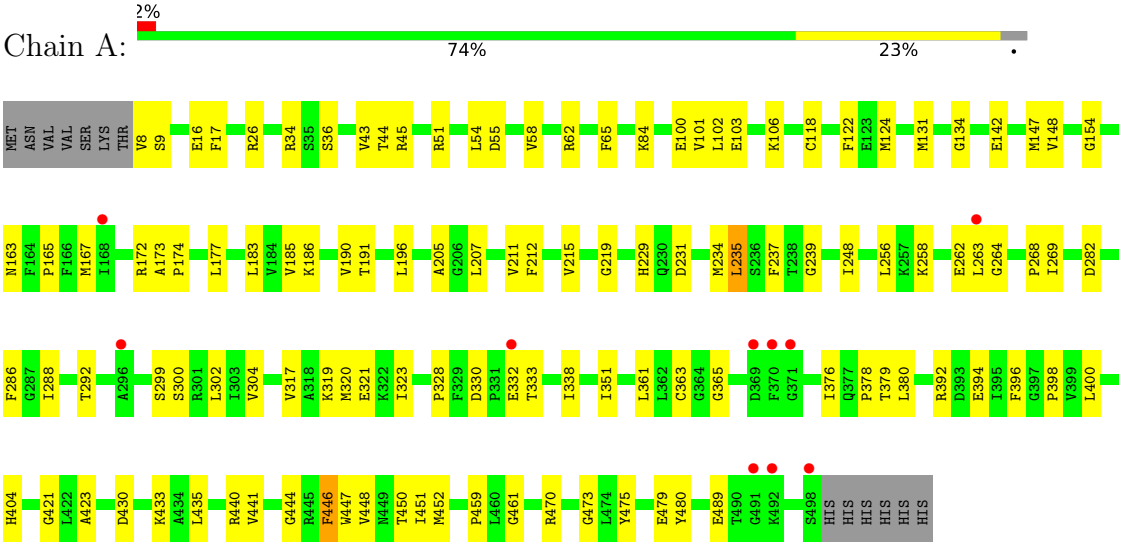
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	229	Total	O	0	0
			229	229		
3	B	237	Total	O	0	0
			237	237		
3	C	136	Total	O	0	0
			136	136		
3	D	194	Total	O	0	0
			194	194		

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.

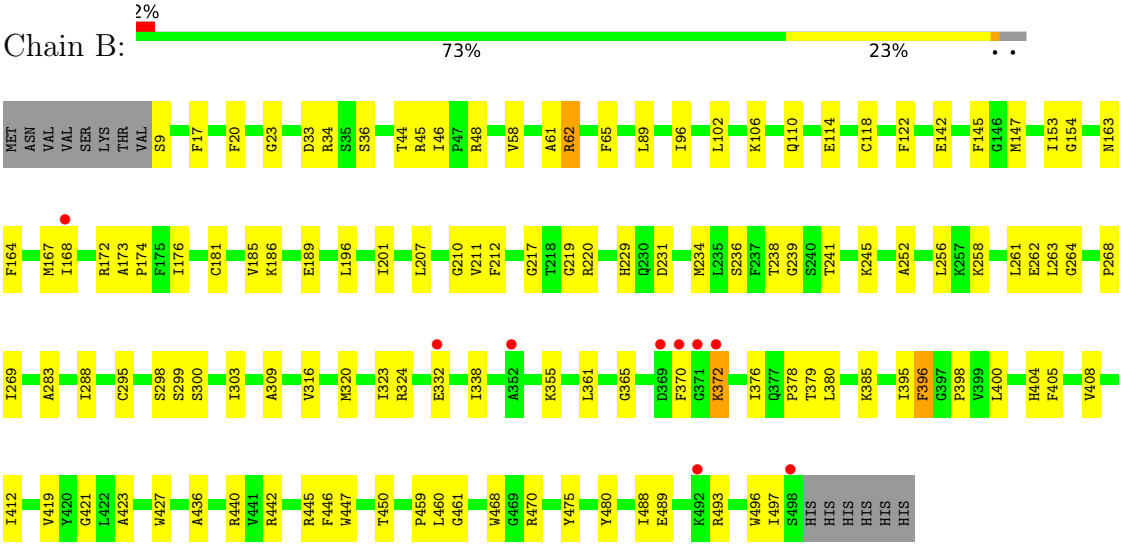
• Molecule 1: L-sorbosone dehydrogenase, NAD(P) dependent

Chain A:



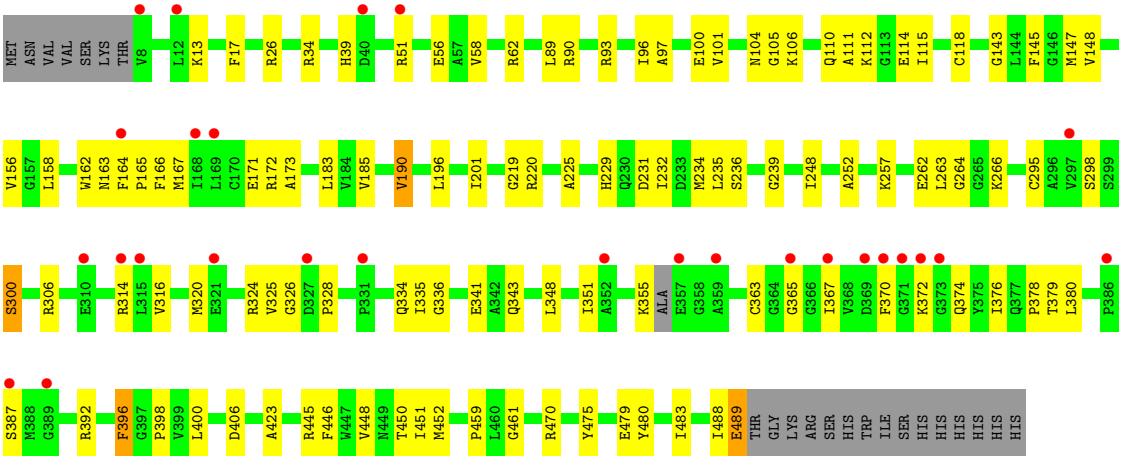
• Molecule 1: L-sorbosone dehydrogenase, NAD(P) dependent

Chain B:



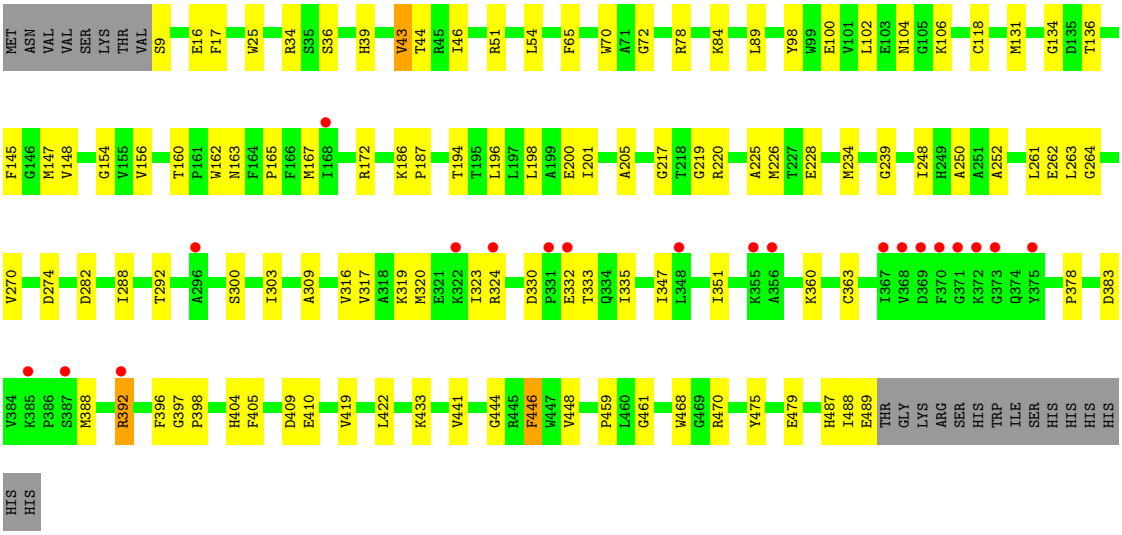
• Molecule 1: L-sorbosone dehydrogenase, NAD(P) dependent

Chain C:



• Molecule 1: L-sorbosone dehydrogenase, NAD(P) dependent

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.31Å 117.93Å 108.18Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	33.58 – 2.22 33.58 – 2.22	Depositor EDS
% Data completeness (in resolution range)	92.7 (33.58-2.22) 92.7 (33.58-2.22)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.165 , 0.204 0.171 , 0.209	Depositor DCC
R_{free} test set	4712 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15657	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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	0.50	0/3784	0.66	0/5124
1	B	0.49	0/3774	0.66	0/5112
1	C	0.45	0/3703	0.66	0/5013
1	D	0.44	0/3701	0.65	0/5011
All	All	0.47	0/14962	0.66	0/20260

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3709	0	3694	79	0
1	B	3699	0	3668	75	0
1	C	3632	0	3624	71	0
1	D	3629	0	3613	76	0
2	A	48	0	25	5	0
2	B	48	0	25	5	0
2	C	48	0	25	4	0
2	D	48	0	25	5	0
3	A	229	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	237	0	0	4	0
3	C	136	0	0	3	0
3	D	194	0	0	4	0
All	All	15657	0	14699	287	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 10.

All (287) 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:489:GLU:HG3	3:B:711:HOH:O	1.81	0.81
1:C:325:VAL:HG22	1:C:335:ILE:HD11	1.69	0.75
1:A:451:ILE:HG13	1:A:452:MET:HG3	1.70	0.73
1:B:89:LEU:HD12	1:B:201:ILE:HD13	1.73	0.71
1:C:341:GLU:HA	1:C:374:GLN:HE22	1.56	0.70
1:D:292:THR:HG23	1:D:335:ILE:HD12	1.74	0.69
1:A:26:ARG:HD2	3:A:715:HOH:O	1.93	0.69
1:B:241:THR:HG22	1:B:245:LYS:HE2	1.74	0.68
1:B:62:ARG:HD2	1:B:231:ASP:OD2	1.93	0.68
1:C:39:HIS:HA	1:C:372:LYS:HD2	1.76	0.68
1:A:282:ASP:HA	1:A:319:LYS:HD2	1.77	0.67
1:B:153:ILE:HD13	1:B:234:MET:HB2	1.77	0.66
1:B:355:LYS:HE3	1:B:361:LEU:HD22	1.76	0.66
1:C:363:CYS:SG	1:C:380:LEU:HB3	2.36	0.66
1:C:96:ILE:HD11	1:C:201:ILE:HD11	1.78	0.65
1:D:89:LEU:HD23	1:D:201:ILE:HD13	1.78	0.65
1:D:43:VAL:HG22	1:D:102:LEU:HD13	1.78	0.64
1:B:396:PHE:CE1	2:B:601:NAP:H2D	2.33	0.64
1:A:396:PHE:CE1	2:A:601:NAP:H2D	2.32	0.63
1:B:33:ASP:OD1	1:B:45:ARG:HD2	1.99	0.63
1:D:396:PHE:CE1	2:D:601:NAP:H2D	2.33	0.63
1:B:320:MET:HB3	1:B:378:PRO:HB2	1.81	0.62
1:D:320:MET:HB3	1:D:378:PRO:HB2	1.82	0.62
1:D:282:ASP:HA	1:D:319:LYS:HD2	1.81	0.62
1:B:48:ARG:NE	1:B:189:GLU:OE2	2.22	0.61
1:D:186:LYS:HE2	1:D:217:GLY:O	2.00	0.61
1:C:396:PHE:CE1	2:C:601:NAP:H2D	2.36	0.60
1:B:361:LEU:HD21	1:B:365:GLY:HA3	1.83	0.60
1:D:320:MET:HA	1:D:323:ILE:HD12	1.82	0.60
1:A:124:MET:HE2	1:A:473:GLY:HA2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.66	0.60
1:A:470:ARG:O	1:A:479:GLU:HG3	2.00	0.60
1:A:84:LYS:HD3	1:A:205:ALA:HA	1.82	0.59
1:D:145:PHE:CE2	1:D:147:MET:HG3	2.37	0.59
1:B:46:ILE:HG13	3:B:751:HOH:O	2.02	0.59
1:D:470:ARG:O	1:D:479:GLU:HG3	2.01	0.59
1:A:62:ARG:NH2	3:A:709:HOH:O	2.35	0.59
1:C:111:ALA:O	1:C:115:ILE:HG12	2.02	0.59
1:D:84:LYS:HG2	1:D:205:ALA:HA	1.85	0.58
1:A:239:GLY:O	1:A:263:LEU:HA	2.04	0.58
1:C:380:LEU:HD13	1:C:400:LEU:HD23	1.86	0.58
1:A:62:ARG:HD2	1:A:231:ASP:OD2	2.04	0.57
1:B:186:LYS:HE2	1:B:217:GLY:O	2.03	0.57
1:A:319:LYS:HD3	1:B:497:ILE:HB	1.86	0.57
3:C:786:HOH:O	1:D:487:HIS:HD2	1.88	0.57
1:C:341:GLU:HA	1:C:374:GLN:NE2	2.20	0.56
1:B:288:ILE:HD13	1:B:300:SER:HA	1.89	0.55
1:A:320:MET:HA	1:A:323:ILE:HD12	1.88	0.55
1:A:447:TRP:HB3	1:A:450:THR:HG23	1.88	0.55
1:C:97:ALA:O	1:C:101:VAL:HG23	2.06	0.55
1:B:219:GLY:HA3	2:B:601:NAP:C8A	2.37	0.55
1:C:488:ILE:HG12	1:D:448:VAL:HB	1.89	0.55
1:D:274:ASP:OD2	1:D:433:LYS:NZ	2.28	0.55
1:C:450:THR:HB	1:D:489:GLU:HB2	1.89	0.55
1:C:367:ILE:HG22	1:C:376:ILE:HG12	1.89	0.54
1:B:145:PHE:CE2	1:B:147:MET:HG2	2.42	0.54
1:C:470:ARG:O	1:C:479:GLU:HG3	2.08	0.54
1:C:264:GLY:HA2	2:C:601:NAP:O2D	2.08	0.54
1:B:408:VAL:O	1:B:412:ILE:HG23	2.08	0.54
1:C:51:ARG:HD2	1:C:225:ALA:HB2	1.90	0.54
1:D:316:VAL:O	1:D:320:MET:HG3	2.08	0.54
1:A:65:PHE:CZ	1:A:154:GLY:HA2	2.43	0.54
1:B:436:ALA:O	1:B:440:ARG:HG3	2.07	0.54
1:A:394:GLU:HG3	3:A:891:HOH:O	2.07	0.53
1:C:324:ARG:HB2	1:C:334:GLN:HG3	1.89	0.53
1:D:264:GLY:HA2	2:D:601:NAP:O2D	2.07	0.53
1:A:450:THR:HB	1:B:489:GLU:HB2	1.90	0.53
1:A:441:VAL:HB	1:A:446:PHE:CZ	2.44	0.53
1:B:338:ILE:HG13	1:B:376:ILE:HD12	1.91	0.53
1:C:62:ARG:NH2	3:C:708:HOH:O	2.38	0.53
1:B:309:ALA:HB1	1:B:404:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HG2	1:A:440:ARG:HH11	1.73	0.53
1:C:145:PHE:CE2	1:C:147:MET:HG2	2.44	0.53
1:B:380:LEU:HD13	1:B:400:LEU:HD23	1.90	0.52
1:B:106:LYS:HE2	1:B:114:GLU:OE2	2.10	0.52
1:C:89:LEU:HD23	1:C:201:ILE:HD13	1.92	0.52
1:A:264:GLY:HA2	2:A:601:NAP:O2D	2.08	0.52
1:D:118:CYS:SG	1:D:167:MET:HA	2.50	0.52
1:D:470:ARG:HB2	1:D:475:TYR:CD2	2.44	0.52
1:B:236:SER:HB2	1:B:480:TYR:OH	2.09	0.52
1:C:93:ARG:NH1	1:C:112:LYS:HB3	2.25	0.52
1:A:163:ASN:OD1	2:A:601:NAP:H5N	2.10	0.51
1:A:361:LEU:HD21	1:A:365:GLY:HA3	1.93	0.51
1:B:303:ILE:HG22	1:B:405:PHE:CD2	2.46	0.51
1:A:186:LYS:HE2	1:A:219:GLY:HA2	1.93	0.51
1:B:96:ILE:HD11	1:B:201:ILE:HD11	1.93	0.51
1:D:9:SER:O	1:D:98:TYR:OH	2.23	0.51
1:B:269:ILE:HB	1:B:299:SER:HB2	1.92	0.51
1:C:62:ARG:HD2	1:C:231:ASP:OD2	2.11	0.51
1:D:186:LYS:NZ	1:D:187:PRO:O	2.30	0.50
1:C:26:ARG:NH2	1:C:56:GLU:OE2	2.36	0.50
1:C:316:VAL:O	1:C:320:MET:HG3	2.12	0.50
1:B:440:ARG:NH1	3:B:701:HOH:O	2.21	0.50
1:C:105:GLY:O	1:C:336:GLY:HA3	2.12	0.50
1:D:145:PHE:HE2	1:D:147:MET:HG3	1.77	0.50
1:A:292:THR:HG22	1:A:398:PRO:HG3	1.93	0.50
1:C:164:PHE:CD1	1:C:167:MET:HE2	2.46	0.50
1:D:405:PHE:HB2	1:D:410:GLU:HB3	1.93	0.50
1:A:450:THR:HB	1:B:489:GLU:CB	2.42	0.50
1:D:100:GLU:OE2	1:D:165:PRO:HD2	2.12	0.49
1:D:172:ARG:NH2	1:D:262:GLU:HG3	2.26	0.49
1:D:54:LEU:HD23	1:D:225:ALA:CB	2.42	0.49
1:A:16:GLU:HA	1:A:45:ARG:HB3	1.94	0.49
1:D:461:GLY:HA3	1:D:470:ARG:HD3	1.94	0.49
1:D:239:GLY:O	1:D:263:LEU:HA	2.13	0.49
1:C:163:ASN:OD1	2:C:601:NAP:H5N	2.12	0.49
1:C:459:PRO:HB3	1:C:475:TYR:HB2	1.94	0.49
1:C:118:CYS:SG	1:C:167:MET:HA	2.52	0.49
1:C:143:GLY:O	1:C:489:GLU:HB3	2.12	0.49
1:B:459:PRO:HB3	1:B:475:TYR:HB2	1.93	0.49
1:B:370:PHE:C	1:B:372:LYS:H	2.16	0.49
1:C:461:GLY:HA3	1:C:470:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:VAL:CG1	1:C:328:PRO:HB2	2.44	0.48
1:D:51:ARG:HG2	1:D:225:ALA:HB2	1.95	0.48
1:C:219:GLY:HA3	2:C:601:NAP:C8A	2.43	0.48
1:A:448:VAL:HB	1:B:488:ILE:HG12	1.94	0.48
1:C:306:ARG:NH1	1:C:406:ASP:OD2	2.46	0.48
1:D:317:VAL:HG13	1:D:363:CYS:HB3	1.95	0.48
1:A:286:PHE:HD1	1:B:496:TRP:CD2	2.32	0.48
1:A:489:GLU:HB2	1:B:450:THR:HB	1.95	0.48
1:A:459:PRO:HB3	1:A:475:TYR:HB2	1.96	0.47
1:C:348:LEU:HD21	1:C:367:ILE:HG23	1.96	0.47
1:C:90:ARG:HG3	1:C:90:ARG:NH1	2.28	0.47
1:D:220:ARG:NH2	3:D:712:HOH:O	2.47	0.47
1:A:332:GLU:OE2	1:A:332:GLU:HA	2.14	0.47
1:A:380:LEU:HD13	1:A:400:LEU:HD23	1.95	0.47
1:C:295:CYS:HB3	1:C:298:SER:HB3	1.95	0.47
1:D:70:TRP:CH2	1:D:78:ARG:HA	2.49	0.47
1:A:34:ARG:HB3	1:A:44:THR:OG1	2.15	0.47
1:A:338:ILE:HG13	1:A:376:ILE:HD12	1.97	0.47
1:B:239:GLY:O	1:B:263:LEU:HA	2.14	0.47
1:B:316:VAL:O	1:B:320:MET:HG3	2.15	0.47
1:D:163:ASN:OD1	2:D:601:NAP:H5N	2.13	0.47
1:B:268:PRO:HD2	1:B:423:ALA:O	2.15	0.47
1:A:173:ALA:HA	1:A:183:LEU:HD11	1.97	0.47
1:D:388:MET:O	1:D:392:ARG:HG3	2.14	0.47
1:A:269:ILE:HB	1:A:299:SER:HB2	1.96	0.46
1:B:164:PHE:HB2	1:B:168:ILE:HG13	1.96	0.46
1:C:17:PHE:HB3	1:C:196:LEU:HD13	1.96	0.46
1:C:239:GLY:O	1:C:263:LEU:HA	2.15	0.46
1:C:162:TRP:HH2	1:C:343:GLN:HG2	1.79	0.46
1:C:351:ILE:HG21	1:C:365:GLY:HA2	1.97	0.46
1:C:252:ALA:HB2	1:D:248:ILE:HB	1.97	0.46
1:D:65:PHE:CZ	1:D:154:GLY:HA2	2.51	0.46
1:D:104:ASN:ND2	1:D:162:TRP:O	2.46	0.46
1:A:36:SER:HA	1:A:102:LEU:O	2.15	0.46
1:A:65:PHE:CE1	1:A:154:GLY:HA2	2.50	0.46
1:B:17:PHE:HB3	1:B:196:LEU:HD13	1.98	0.46
1:A:17:PHE:HB3	1:A:196:LEU:HD13	1.97	0.46
1:B:320:MET:HA	1:B:323:ILE:HD12	1.98	0.46
1:B:34:ARG:HB3	1:B:44:THR:OG1	2.16	0.46
1:D:261:LEU:HB2	1:D:468:TRP:H	1.81	0.46
1:A:190:VAL:HG23	1:A:191:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HB2	1:A:400:LEU:HD21	1.98	0.45
1:B:110:GLN:O	1:B:114:GLU:HG3	2.16	0.45
1:D:160:THR:OG1	1:D:187:PRO:HA	2.16	0.45
1:D:309:ALA:HB1	1:D:404:HIS:CD2	2.51	0.45
1:B:122:PHE:CE1	1:B:174:PRO:HG3	2.51	0.45
1:C:110:GLN:O	1:C:114:GLU:HG3	2.16	0.45
1:A:288:ILE:HD13	1:A:300:SER:HA	1.98	0.45
1:B:207:LEU:HD11	1:B:211:VAL:HG11	1.99	0.45
1:B:361:LEU:HD11	1:B:379:THR:HG23	1.99	0.45
1:D:104:ASN:OD1	1:D:106:LYS:HE2	2.17	0.45
1:B:163:ASN:OD1	2:B:601:NAP:H5N	2.17	0.45
1:B:264:GLY:HA2	2:B:601:NAP:O2D	2.16	0.45
1:D:360:LYS:HE3	1:D:383:ASP:OD2	2.17	0.45
1:C:423:ALA:HA	1:C:445:ARG:O	2.17	0.45
1:D:347:ILE:HG12	1:D:397:GLY:HA3	1.99	0.45
1:B:185:VAL:HG21	1:B:212:PHE:CE1	2.52	0.45
1:B:153:ILE:HD12	1:B:258:LYS:HD3	1.99	0.45
1:B:320:MET:HA	1:B:323:ILE:CD1	2.46	0.45
1:D:36:SER:HA	1:D:102:LEU:O	2.17	0.45
1:B:172:ARG:NH2	1:B:262:GLU:HG3	2.32	0.44
1:C:34:ARG:HD3	1:C:190:VAL:HG22	1.99	0.44
1:C:58:VAL:HG11	1:C:229:HIS:CE1	2.52	0.44
1:C:104:ASN:ND2	1:C:162:TRP:O	2.48	0.44
1:C:248:ILE:CG2	1:D:252:ALA:HB2	2.47	0.44
1:A:219:GLY:HA3	2:A:601:NAP:N9A	2.31	0.44
1:A:461:GLY:HA3	1:A:470:ARG:HD3	1.99	0.44
1:C:320:MET:HE2	1:C:320:MET:HB3	1.65	0.44
1:C:101:VAL:HG13	1:C:328:PRO:HB2	1.99	0.44
1:D:16:GLU:O	3:D:701:HOH:O	2.21	0.44
1:D:475:TYR:O	1:D:479:GLU:HG2	2.17	0.44
1:D:459:PRO:HB2	1:D:470:ARG:HB3	1.98	0.44
1:A:441:VAL:HB	1:A:446:PHE:HZ	1.81	0.44
1:A:234:MET:HG3	1:A:258:LYS:HB2	1.99	0.44
1:C:378:PRO:HA	1:C:398:PRO:HB2	1.98	0.44
1:C:262:GLU:OE2	3:C:701:HOH:O	2.21	0.44
1:A:134:GLY:HA3	1:A:148:VAL:O	2.17	0.43
1:A:351:ILE:HG21	1:A:365:GLY:O	2.17	0.43
1:C:451:ILE:HG13	1:C:452:MET:HG3	1.99	0.43
1:C:158:LEU:HB3	1:C:185:VAL:HG22	2.00	0.43
1:A:480:TYR:HB2	3:A:772:HOH:O	2.18	0.43
1:B:36:SER:HA	1:B:102:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ALA:CB	1:B:427:TRP:CZ2	3.02	0.43
1:D:54:LEU:HD23	1:D:225:ALA:HB3	2.00	0.43
1:B:395:ILE:HB	3:B:840:HOH:O	2.19	0.43
1:D:34:ARG:HB3	1:D:44:THR:OG1	2.18	0.43
1:B:186:LYS:NZ	2:B:601:NAP:O3B	2.50	0.43
1:D:324:ARG:NH1	1:D:332:GLU:O	2.48	0.43
1:A:101:VAL:HG13	1:A:328:PRO:HB2	2.01	0.43
1:D:134:GLY:HA3	1:D:148:VAL:O	2.18	0.43
1:A:147:MET:HB2	1:D:136:THR:HG21	2.01	0.43
1:A:317:VAL:HG13	1:A:363:CYS:HB3	1.99	0.43
1:A:378:PRO:HA	1:A:398:PRO:HB2	2.01	0.43
1:A:142:GLU:OE2	1:D:72:GLY:HA3	2.19	0.43
1:A:268:PRO:HD2	1:A:423:ALA:O	2.18	0.43
1:D:46:ILE:HG13	3:D:702:HOH:O	2.19	0.43
1:A:34:ARG:NH2	1:A:103:GLU:O	2.42	0.43
1:A:106:LYS:HB3	1:A:106:LYS:HE2	1.80	0.43
1:A:330:ASP:HB3	1:A:333:THR:OG1	2.19	0.42
1:B:20:PHE:CZ	1:B:23:GLY:HA2	2.54	0.42
1:B:238:THR:HA	1:B:262:GLU:O	2.19	0.42
1:B:261:LEU:HB2	1:B:468:TRP:H	1.83	0.42
1:C:232:ILE:O	1:C:257:LYS:HE3	2.19	0.42
1:D:17:PHE:HB3	1:D:196:LEU:HD13	2.01	0.42
1:A:235:LEU:CD2	1:A:237:PHE:HB2	2.49	0.42
1:C:171:GLU:HB3	1:C:172:ARG:NH1	2.34	0.42
1:C:262:GLU:OE1	1:C:461:GLY:HA2	2.19	0.42
1:C:363:CYS:O	1:C:379:THR:HA	2.19	0.42
1:A:219:GLY:HA3	2:A:601:NAP:C8A	2.50	0.42
1:B:118:CYS:SG	1:B:167:MET:HA	2.59	0.42
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.89	0.42
1:B:153:ILE:CD1	1:B:258:LYS:HD3	2.50	0.42
1:B:295:CYS:HB3	1:B:298:SER:HB3	2.01	0.42
1:D:100:GLU:HB2	1:D:194:THR:HG21	2.01	0.42
1:D:288:ILE:HD13	1:D:300:SER:HA	2.02	0.42
1:D:441:VAL:HB	1:D:446:PHE:CE2	2.55	0.42
1:A:58:VAL:HG11	1:A:229:HIS:CE1	2.55	0.42
1:B:461:GLY:HA3	1:B:470:ARG:HD3	2.01	0.42
1:C:320:MET:CE	1:C:363:CYS:SG	3.08	0.42
1:A:430:ASP:HB3	1:A:433:LYS:HD2	2.02	0.42
1:C:89:LEU:HD21	1:C:166:PHE:HZ	1.84	0.42
1:D:54:LEU:HD11	1:D:226:MET:HG2	2.01	0.42
1:A:131:MET:HB2	1:A:131:MET:HE3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HG13	1:C:483:ILE:HG23	2.02	0.41
1:C:173:ALA:HA	1:C:183:LEU:HD11	2.02	0.41
1:C:266:LYS:HE3	1:C:300:SER:HB2	2.01	0.41
1:D:36:SER:OG	1:D:39:HIS:ND1	2.34	0.41
1:A:122:PHE:CE1	1:A:174:PRO:HG3	2.55	0.41
1:D:219:GLY:HA3	2:D:601:NAP:N9A	2.35	0.41
1:B:447:TRP:HB3	1:B:450:THR:HG23	2.02	0.41
1:D:219:GLY:HA3	2:D:601:NAP:C8A	2.50	0.41
1:B:61:ALA:HA	1:B:210:GLY:O	2.20	0.41
1:B:378:PRO:HA	1:B:398:PRO:HB2	2.02	0.41
1:D:347:ILE:O	1:D:351:ILE:HG13	2.19	0.41
1:D:378:PRO:HA	1:D:398:PRO:HB2	2.02	0.41
1:A:55:ASP:OD1	1:A:229:HIS:NE2	2.48	0.41
1:A:304:VAL:O	1:A:404:HIS:HA	2.19	0.41
1:D:270:VAL:HA	1:D:303:ILE:O	2.21	0.41
1:D:156:VAL:HA	1:D:234:MET:O	2.19	0.41
1:A:54:LEU:HA	1:A:215:VAL:HG11	2.03	0.41
1:A:172:ARG:NH2	1:A:262:GLU:HG3	2.36	0.41
1:B:173:ALA:HB3	1:B:174:PRO:HD3	2.03	0.41
1:A:444:GLY:HA3	1:A:461:GLY:O	2.20	0.41
1:B:58:VAL:HG11	1:B:229:HIS:CE1	2.56	0.41
1:C:156:VAL:HA	1:C:234:MET:O	2.20	0.41
1:C:236:SER:HB2	1:C:480:TYR:OH	2.20	0.41
1:D:43:VAL:HG13	1:D:44:THR:HG23	2.02	0.41
1:A:43:VAL:HG23	1:A:44:THR:HG23	2.01	0.41
1:A:248:ILE:HB	1:B:252:ALA:HB2	2.03	0.41
1:B:445:ARG:HD2	1:B:460:LEU:HB2	2.03	0.41
1:C:100:GLU:OE2	1:C:165:PRO:HD2	2.21	0.41
1:C:459:PRO:HB2	1:C:470:ARG:HB3	2.03	0.41
1:D:228:GLU:HG3	1:D:250:ALA:HB1	2.03	0.41
1:D:422:LEU:HD11	3:D:810:HOH:O	2.20	0.41
1:A:118:CYS:SG	1:A:167:MET:HA	2.61	0.41
1:A:361:LEU:HD11	1:A:379:THR:HG23	2.03	0.41
1:C:101:VAL:HG13	1:C:106:LYS:O	2.21	0.41
1:A:100:GLU:OE2	1:A:165:PRO:HD2	2.21	0.40
1:A:207:LEU:HD11	1:A:211:VAL:HG11	2.03	0.40
1:B:65:PHE:CE1	1:B:154:GLY:HA2	2.56	0.40
1:B:269:ILE:CG2	1:B:299:SER:HB2	2.51	0.40
1:C:326:GLY:HA2	1:C:370:PHE:CE2	2.56	0.40
1:D:330:ASP:HB3	1:D:333:THR:OG1	2.20	0.40
1:A:101:VAL:CG1	1:A:328:PRO:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:HG2	3:A:801:HOH:O	2.20	0.40
1:A:185:VAL:HG21	1:A:212:PHE:CE1	2.56	0.40
1:B:324:ARG:HD2	1:B:332:GLU:O	2.21	0.40
1:A:447:TRP:CZ2	1:A:452:MET:HA	2.56	0.40
1:D:198:LEU:HD12	1:D:198:LEU:HA	1.92	0.40
1:D:444:GLY:HA3	1:D:461:GLY:O	2.21	0.40
1:B:176:ILE:O	1:B:181:CYS:HB2	2.21	0.40
1:C:448:VAL:HB	1:D:488:ILE:HG12	2.03	0.40
1:D:54:LEU:CD2	1:D:225:ALA:HB3	2.51	0.40
1:B:258:LYS:HB3	1:B:258:LYS:HE3	1.93	0.40
1:D:25:TRP:HZ2	1:D:200:GLU:HB2	1.87	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	489/504 (97%)	474 (97%)	14 (3%)	1 (0%)	47	54
1	B	488/504 (97%)	476 (98%)	11 (2%)	1 (0%)	47	54
1	C	477/504 (95%)	464 (97%)	13 (3%)	0	100	100
1	D	479/504 (95%)	466 (97%)	13 (3%)	0	100	100
All	All	1933/2016 (96%)	1880 (97%)	51 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	GLY
1	B	421	GLY

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	382/396 (96%)	373 (98%)	9 (2%)	49	60
1	B	378/396 (96%)	366 (97%)	12 (3%)	39	49
1	C	374/396 (94%)	362 (97%)	12 (3%)	39	49
1	D	373/396 (94%)	367 (98%)	6 (2%)	62	75
All	All	1507/1584 (95%)	1468 (97%)	39 (3%)	46	57

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	9	SER
1	A	51	ARG
1	A	177	LEU
1	A	235	LEU
1	A	256	LEU
1	A	321	GLU
1	A	392	ARG
1	A	446	PHE
1	B	9	SER
1	B	62	ARG
1	B	142	GLU
1	B	220	ARG
1	B	256	LEU
1	B	372	LYS
1	B	385	LYS
1	B	396	PHE
1	B	419	VAL
1	B	442	ARG
1	B	446	PHE
1	B	493	ARG
1	C	13	LYS
1	C	190	VAL
1	C	220	ARG

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Mol	Chain	Res	Type
1	C	235	LEU
1	C	300	SER
1	C	314	ARG
1	C	355	LYS
1	C	387	SER
1	C	392	ARG
1	C	396	PHE
1	C	446	PHE
1	C	489	GLU
1	D	43	VAL
1	D	131	MET
1	D	392	ARG
1	D	409	ASP
1	D	419	VAL
1	D	446	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	C	230	GLN
1	C	374	GLN
1	D	465	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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	A	601	-	45,52,52	0.67	1 (2%)	56,80,80	0.79	3 (5%)
2	NAP	B	601	-	45,52,52	0.69	1 (2%)	56,80,80	0.83	3 (5%)
2	NAP	D	601	-	45,52,52	0.66	0	56,80,80	0.82	3 (5%)
2	NAP	C	601	-	45,52,52	0.68	0	56,80,80	0.81	2 (3%)

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	A	601	-	-	4/31/67/67	0/5/5/5
2	NAP	B	601	-	-	5/31/67/67	0/5/5/5
2	NAP	D	601	-	-	5/31/67/67	0/5/5/5
2	NAP	C	601	-	-	4/31/67/67	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C8A-N7A	-2.03	1.31	1.34
2	A	601	NAP	C8A-N7A	-2.02	1.31	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NAP	C6N-N1N-C2N	-2.67	119.54	121.97
2	D	601	NAP	C6N-N1N-C2N	-2.65	119.56	121.97
2	A	601	NAP	C6N-N1N-C2N	-2.60	119.61	121.97
2	B	601	NAP	C6N-N1N-C2N	-2.55	119.65	121.97
2	D	601	NAP	O4D-C1D-C2D	-2.53	103.23	106.93
2	A	601	NAP	O4D-C1D-C2D	-2.44	103.36	106.93
2	B	601	NAP	O4D-C1D-C2D	-2.32	103.53	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	NAP	C5A-C6A-N6A	2.32	123.88	120.35
2	C	601	NAP	C5A-C6A-N6A	2.28	123.82	120.35
2	A	601	NAP	C5A-C6A-N6A	2.23	123.73	120.35
2	D	601	NAP	C5A-C6A-N6A	2.10	123.54	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C3D-C4D-C5D-O5D
2	B	601	NAP	C2B-O2B-P2B-O1X
2	C	601	NAP	C3D-C4D-C5D-O5D
2	A	601	NAP	O4D-C4D-C5D-O5D
2	D	601	NAP	O4D-C4D-C5D-O5D
2	D	601	NAP	C3D-C4D-C5D-O5D
2	C	601	NAP	O4D-C4D-C5D-O5D
2	B	601	NAP	C3D-C4D-C5D-O5D
2	A	601	NAP	C4D-C5D-O5D-PN
2	B	601	NAP	C4D-C5D-O5D-PN
2	A	601	NAP	PN-O3-PA-O5B
2	B	601	NAP	PN-O3-PA-O5B
2	C	601	NAP	PN-O3-PA-O5B
2	D	601	NAP	PN-O3-PA-O5B
2	B	601	NAP	O4D-C4D-C5D-O5D
2	C	601	NAP	C4D-C5D-O5D-PN
2	D	601	NAP	C4D-C5D-O5D-PN
2	D	601	NAP	C2B-O2B-P2B-O1X

There are no ring outliers.

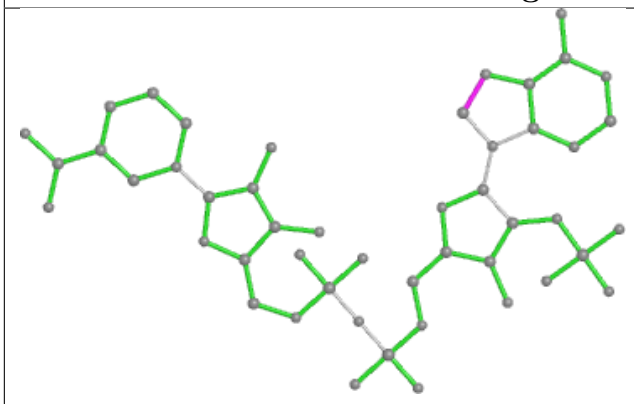
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAP	5	0
2	B	601	NAP	5	0
2	D	601	NAP	5	0
2	C	601	NAP	4	0

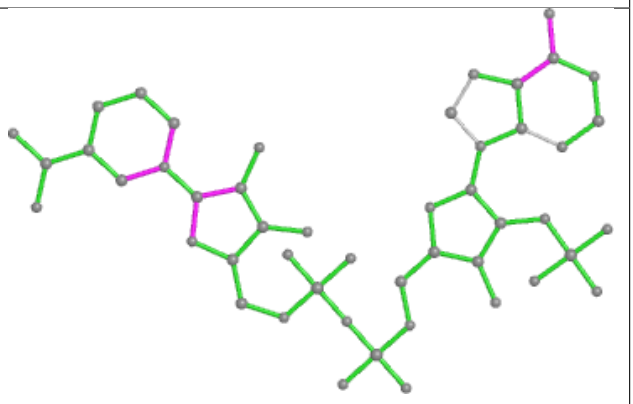
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

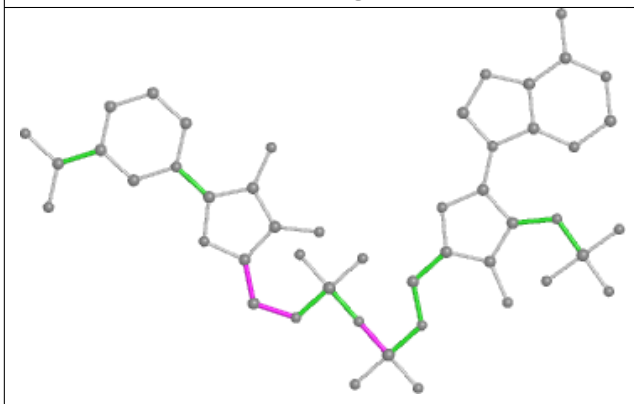
Ligand NAP A 601



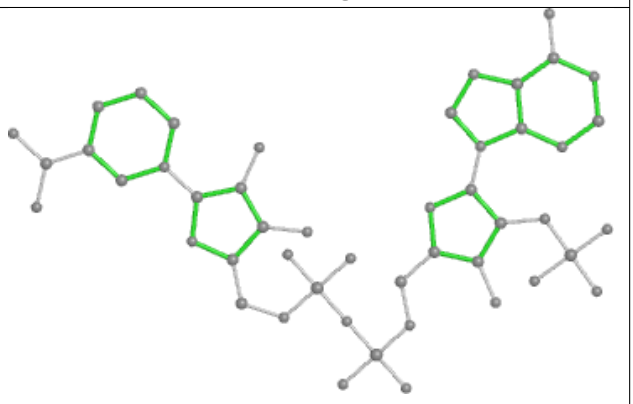
Bond lengths



Bond angles

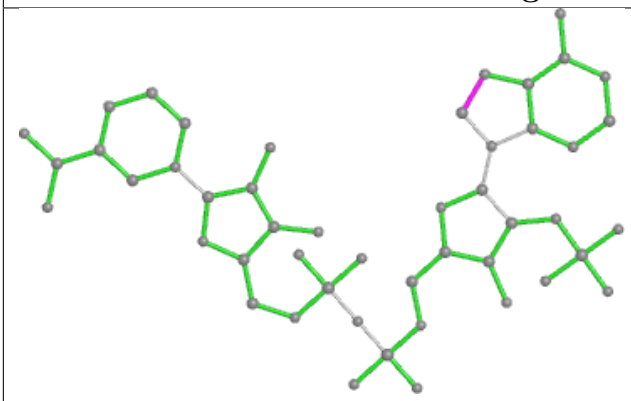


Torsions

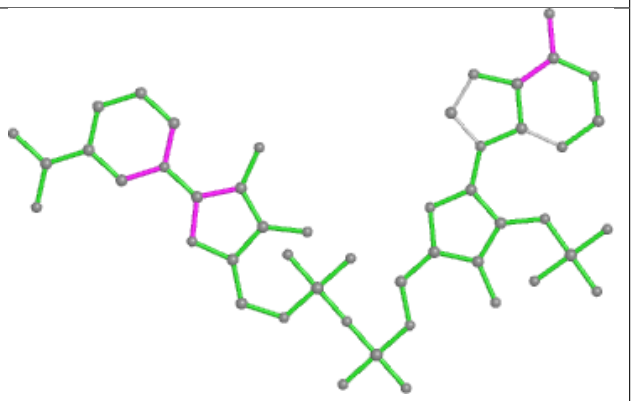


Rings

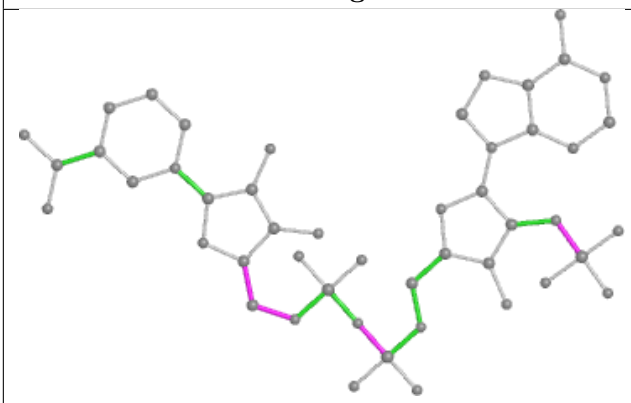
Ligand NAP B 601



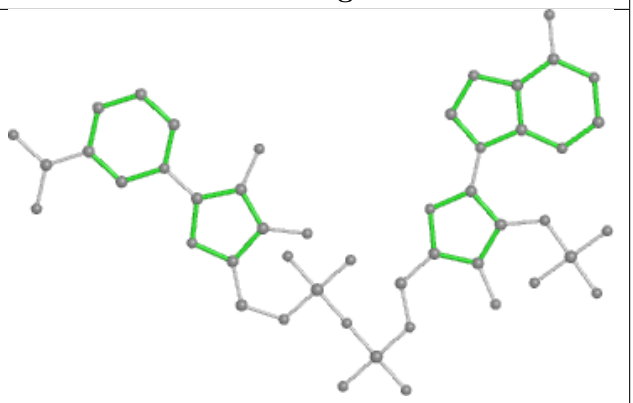
Bond lengths



Bond angles

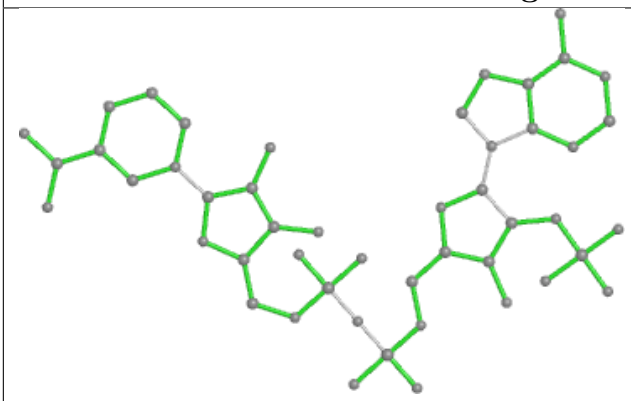


Torsions

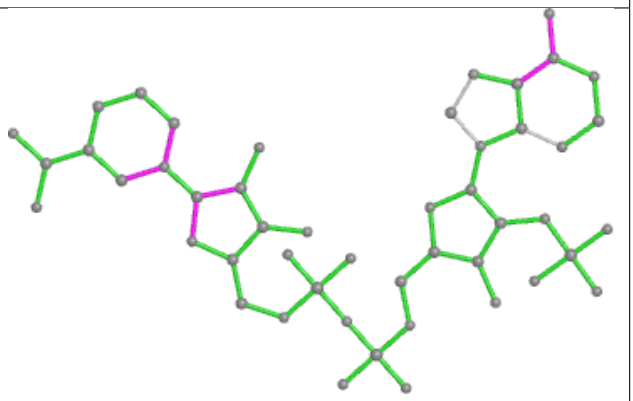


Rings

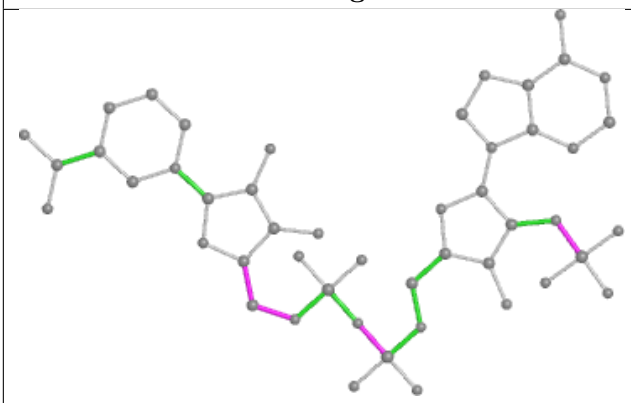
Ligand NAP D 601



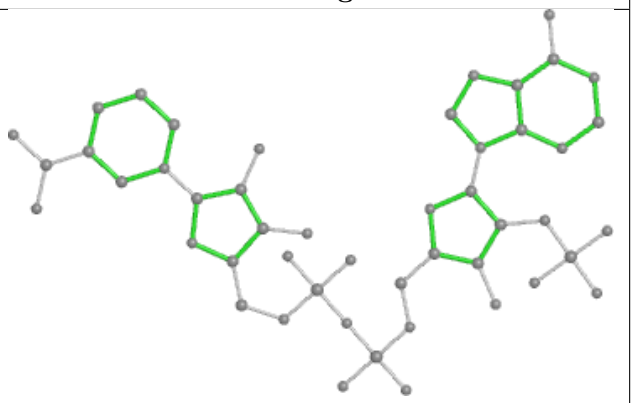
Bond lengths



Bond angles

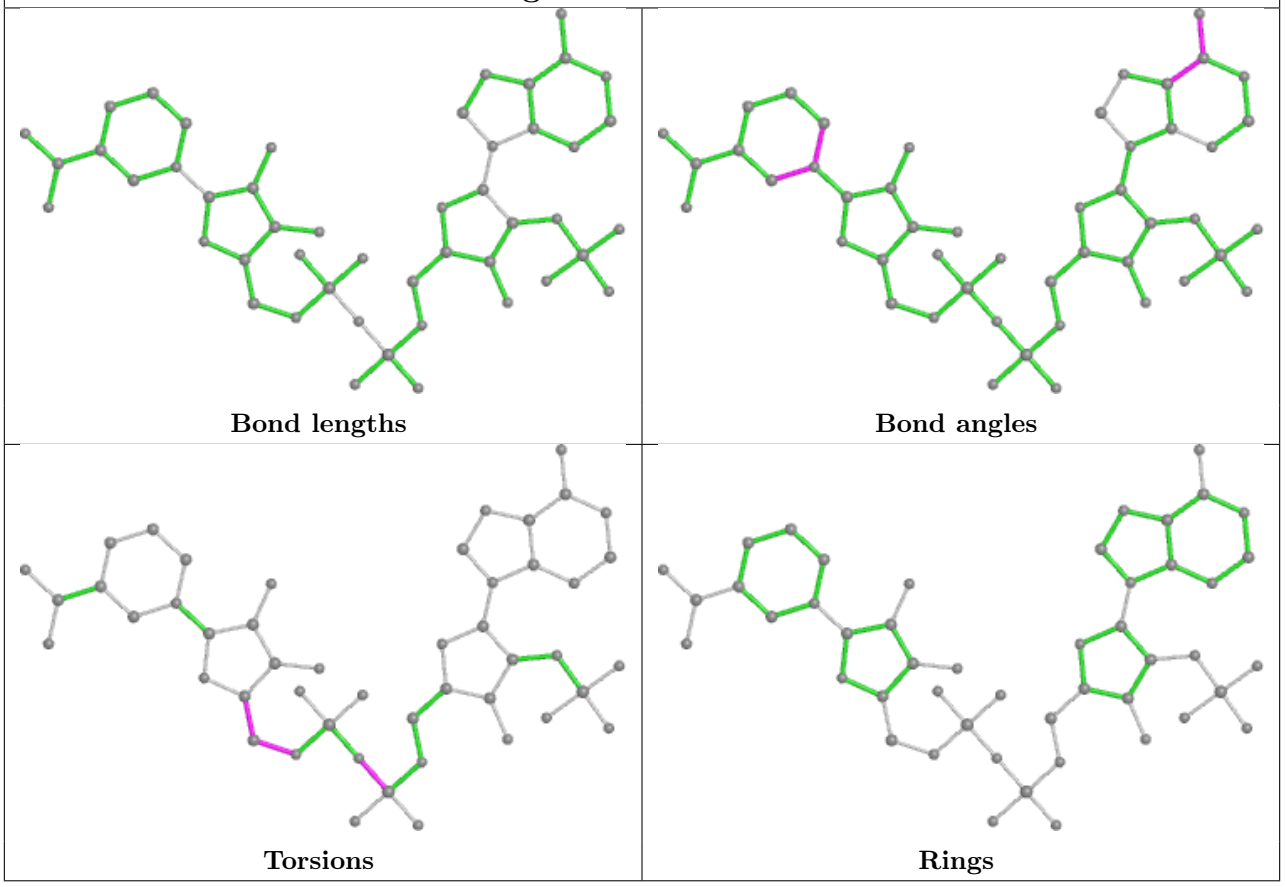


Torsions



Rings

Ligand NAP C 601



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	491/504 (97%)	-0.22	10 (2%)	65 63	21, 30, 44, 66	0
1	B	490/504 (97%)	-0.24	9 (1%)	68 66	23, 30, 43, 62	0
1	C	481/504 (95%)	0.12	27 (5%)	24 23	24, 37, 61, 77	0
1	D	481/504 (95%)	-0.08	20 (4%)	36 34	25, 35, 53, 69	0
All	All	1943/2016 (96%)	-0.11	66 (3%)	45 43	21, 33, 54, 77	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	GLY	4.6
1	C	369	ASP	4.6
1	C	367	ILE	4.2
1	D	370	PHE	4.1
1	D	371	GLY	4.1
1	C	370	PHE	4.1
1	A	491	GLY	3.8
1	C	386	PRO	3.7
1	C	371	GLY	3.6
1	D	369	ASP	3.5
1	D	331	PRO	3.5
1	C	12	LEU	3.4
1	D	324	ARG	3.3
1	C	373	GLY	3.3
1	C	169	LEU	3.2
1	C	331	PRO	3.2
1	A	498	SER	3.2
1	C	164	PHE	3.2
1	D	367	ILE	3.1
1	B	370	PHE	3.1
1	C	387	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	387	SER	2.9
1	C	8	VAL	2.9
1	C	168	ILE	2.9
1	C	51	ARG	2.9
1	B	498	SER	2.9
1	C	359	ALA	2.8
1	D	385	LYS	2.7
1	A	371	GLY	2.7
1	D	392	ARG	2.6
1	C	372	LYS	2.6
1	D	372	LYS	2.6
1	A	369	ASP	2.6
1	C	314	ARG	2.6
1	C	310	GLU	2.5
1	C	40	ASP	2.5
1	C	297	VAL	2.5
1	C	321	GLU	2.5
1	C	352	ALA	2.5
1	D	356	ALA	2.4
1	B	168	ILE	2.4
1	D	332	GLU	2.4
1	C	365	GLY	2.3
1	D	375	TYR	2.3
1	D	296	ALA	2.3
1	B	492	LYS	2.3
1	A	168	ILE	2.3
1	D	373	GLY	2.2
1	A	332	GLU	2.2
1	D	322	LYS	2.2
1	C	315	LEU	2.2
1	C	327	ASP	2.2
1	A	296	ALA	2.2
1	A	492	LYS	2.1
1	C	357	GLU	2.1
1	A	370	PHE	2.1
1	B	352	ALA	2.1
1	A	263	LEU	2.1
1	B	369	ASP	2.1
1	D	368	VAL	2.1
1	D	168	ILE	2.1
1	D	348	LEU	2.1
1	B	332	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	355	LYS	2.0
1	C	389	GLY	2.0
1	B	372	LYS	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)

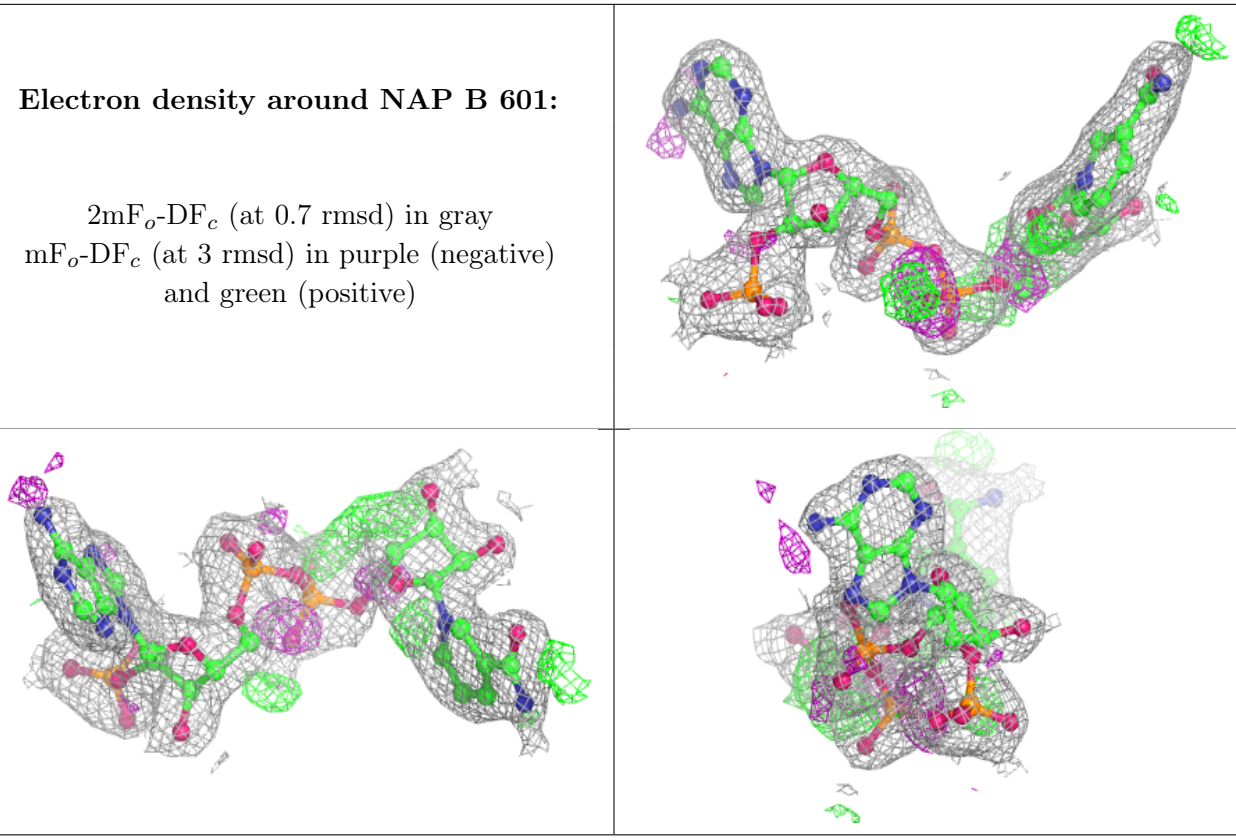
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAP	B	601	48/48	0.94	0.15	25,33,41,50	0
2	NAP	C	601	48/48	0.94	0.13	38,43,53,58	0
2	NAP	A	601	48/48	0.95	0.12	23,32,38,44	0
2	NAP	D	601	48/48	0.95	0.14	31,40,50,56	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.

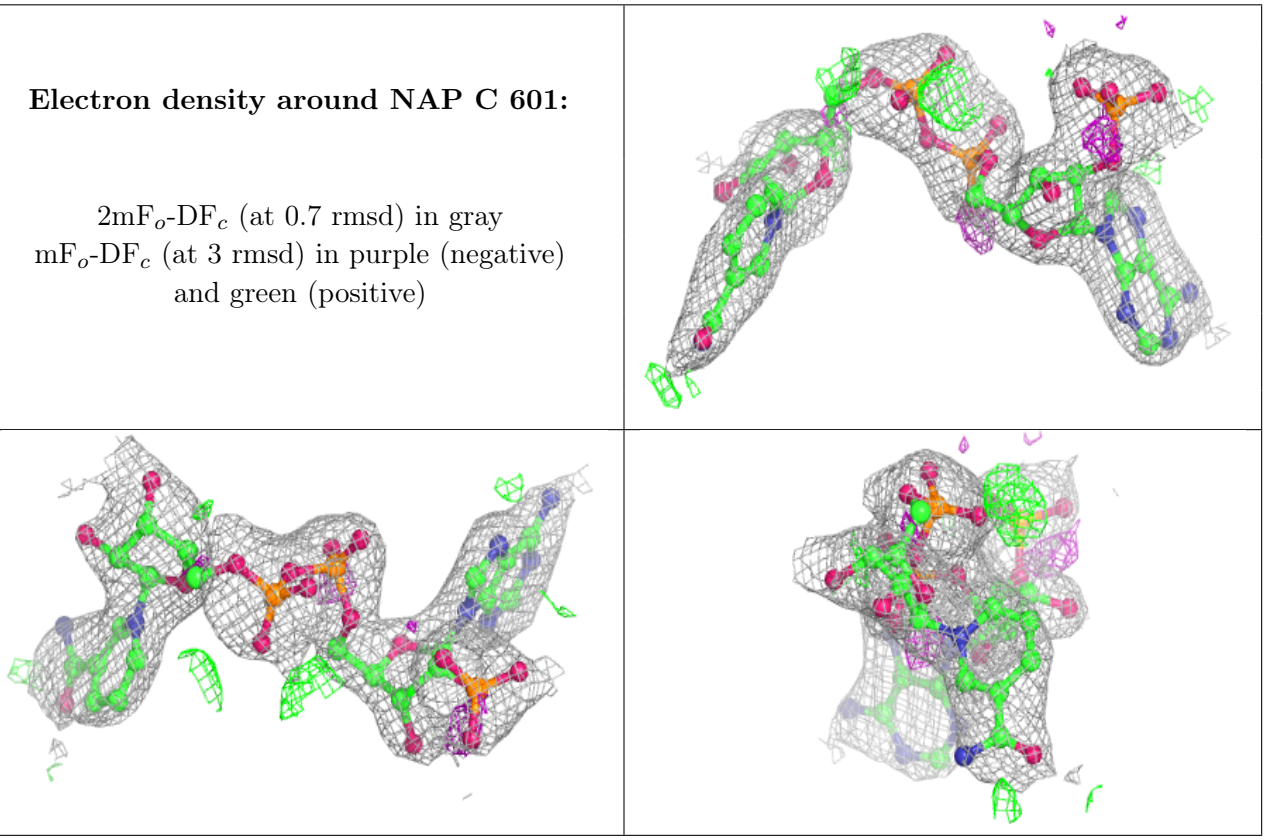
Electron density around NAP B 601:

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



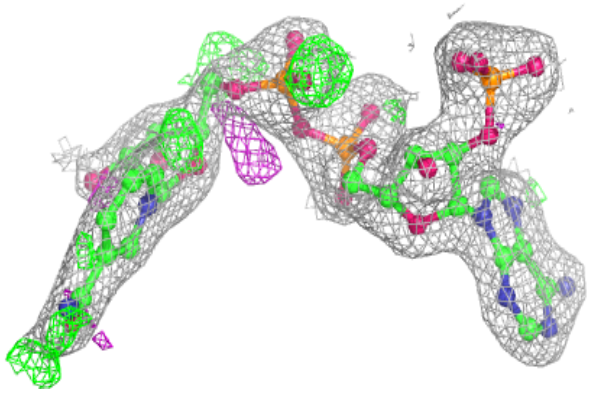
Electron density around NAP C 601:

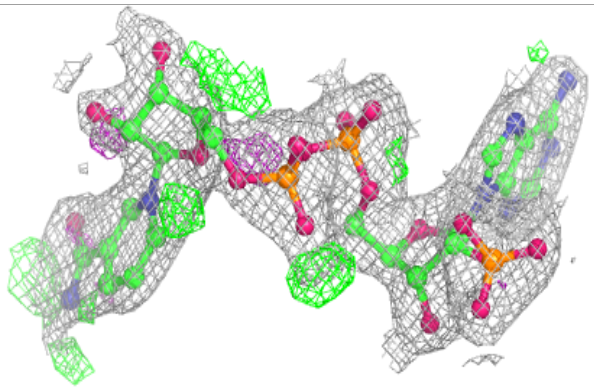
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

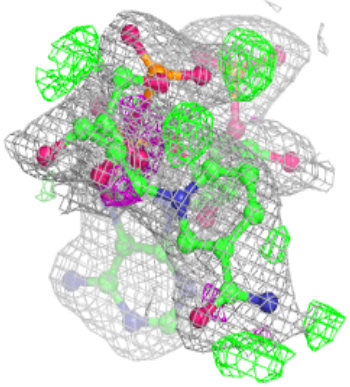


Electron density around NAP A 601:

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

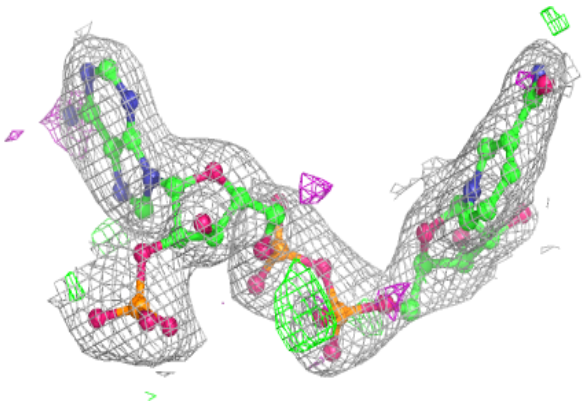


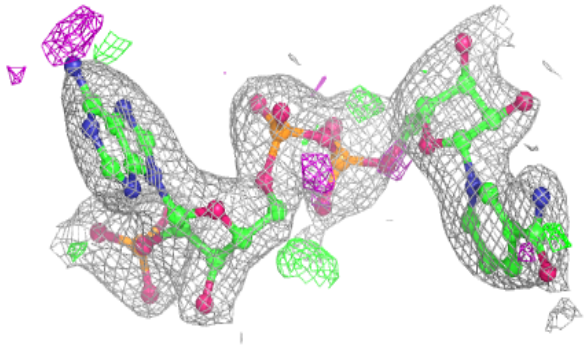


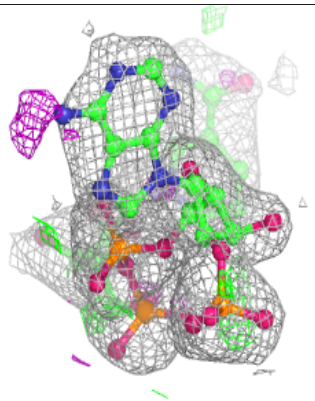


Electron density around NAP D 601:

$2mF_o$-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.