



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 05:02 am GMT

PDB ID : 2JKV
Title : Structure of human Phosphogluconate Dehydrogenase in complex with NADPH at 2.53Å
Authors : Pilka, E.S.; Kavanagh, K.L.; von Delft, F.; Muniz, J.R.C.; Murray, J.; Piccaud, S.; Guo, K.; Edwards, A.; Arrowsmith, C.H.; Weigelt, J.; Bountra, C.; Oppermann, U.
Deposited on : 2008-09-01
Resolution : 2.53 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

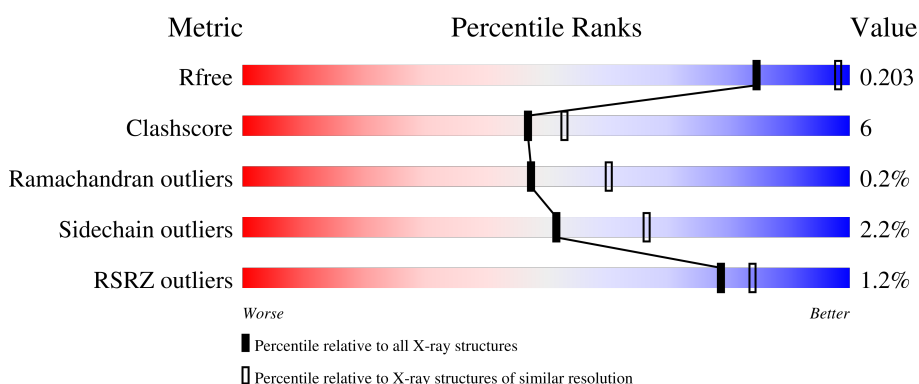
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 $\leq 5\%$. 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	505	2% 81% 13% • 5%
1	B	505	2% 83% 12% • 5%
1	C	505	2% 81% 14% 5%
1	D	505	2% 80% 15% 5%
1	E	505	82% 13% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	505	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment representing 80%, a yellow segment representing 13%, and a red segment representing 7%. A small red square is positioned at the beginning of the bar, and a small black dot is at the end of the red segment. The percentage values are printed below the bar.</p>

2 Entry composition [i](#)

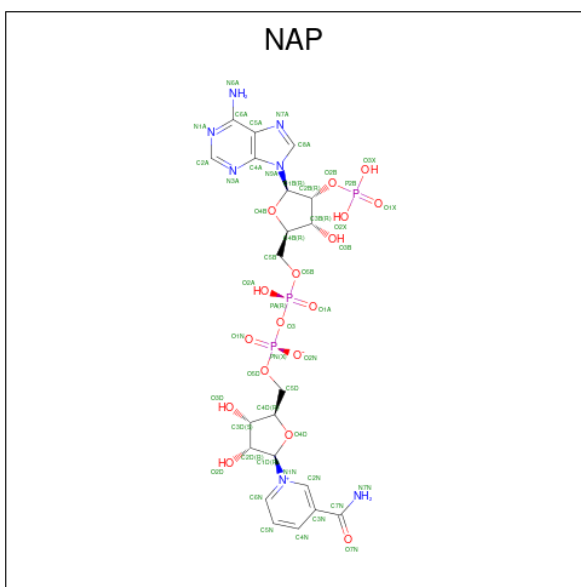
There are 5 unique types of molecules in this entry. The entry contains 23837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	Total 3708	C 2361	N 634	O 691	S 22	0	1	0
1	B	482	Total 3701	C 2358	N 634	O 687	S 22	0	1	0
1	C	482	Total 3689	C 2351	N 629	O 687	S 22	0	0	0
1	D	482	Total 3690	C 2351	N 632	O 685	S 22	0	0	0
1	E	482	Total 3693	C 2354	N 633	O 684	S 22	0	0	0
1	F	471	Total 3640	C 2322	N 626	O 670	S 22	0	0	0

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

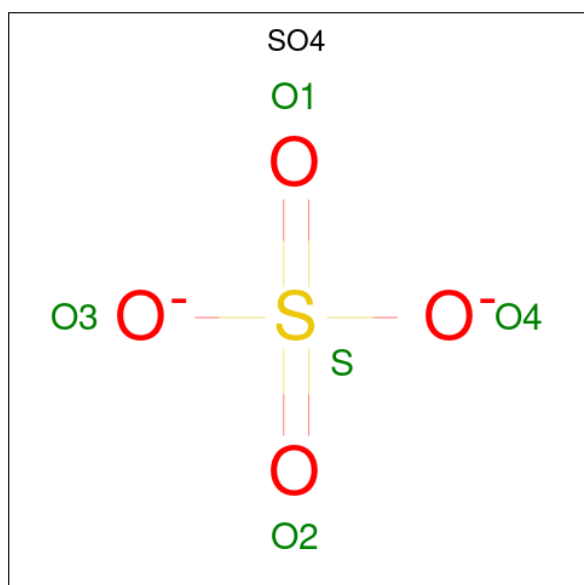


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	3	Total	Cl	0	0
			3	3		
3	D	1	Total	Cl	0	0
			1	1		
3	E	2	Total	Cl	0	0
			2	2		
3	F	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

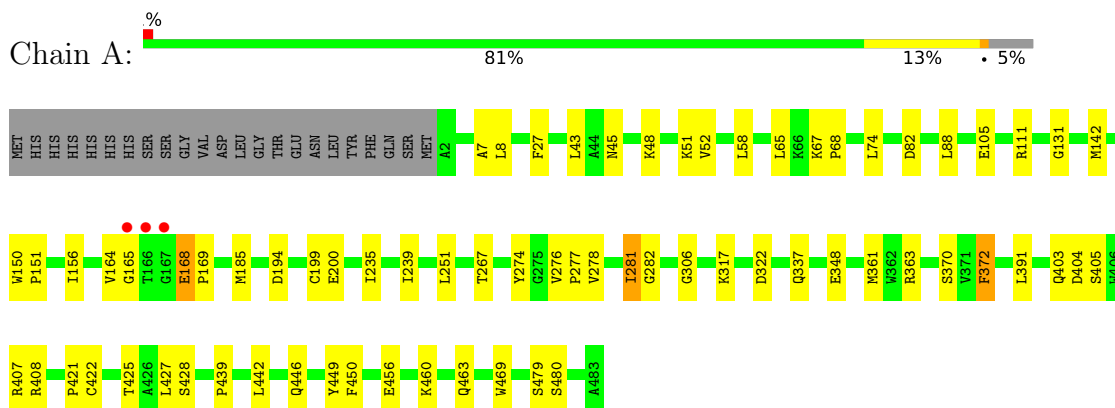
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	263	Total O 263 263	0	0
5	B	269	Total O 269 269	0	0
5	C	195	Total O 195 195	0	0
5	D	191	Total O 191 191	0	0
5	E	238	Total O 238 238	0	0
5	F	249	Total O 249 249	0	0

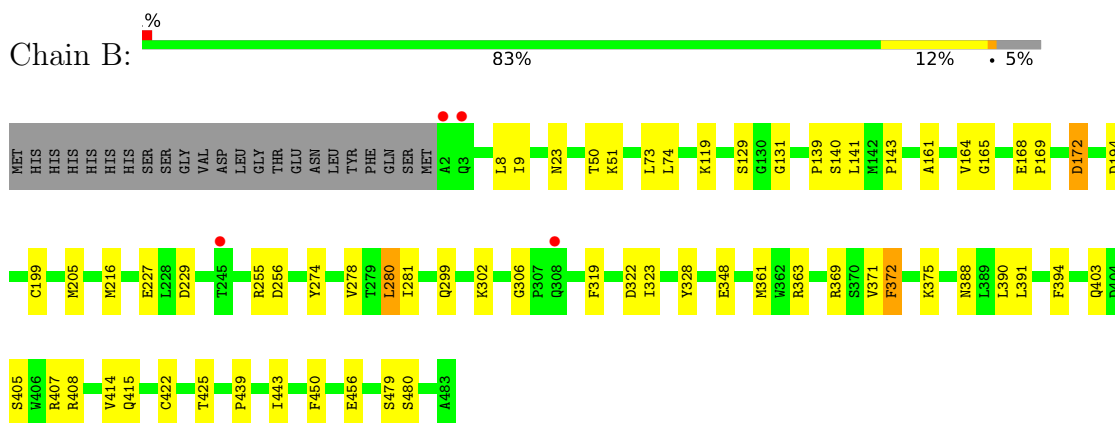
3 Residue-property plots [i](#)

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

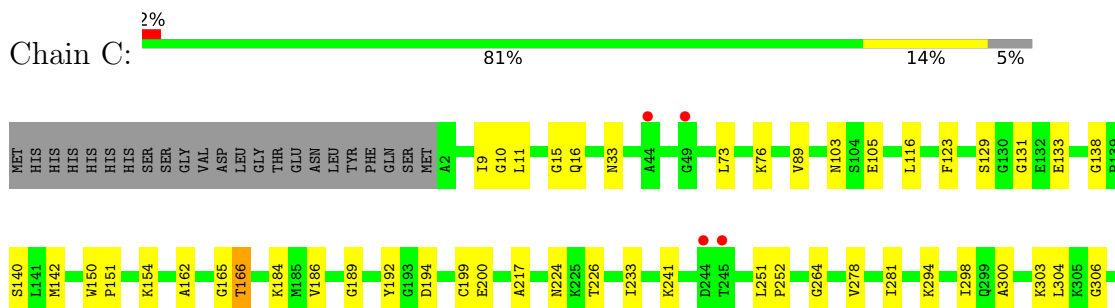
• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

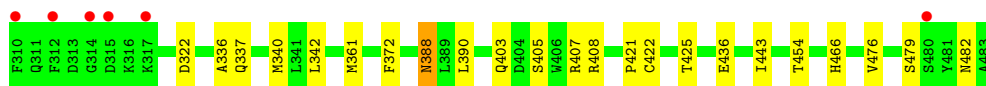


• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

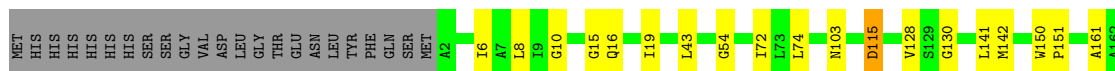
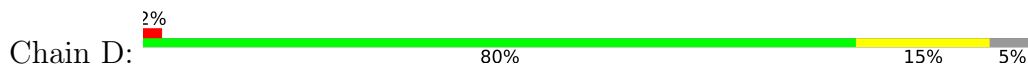


• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

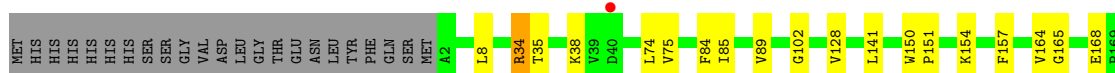
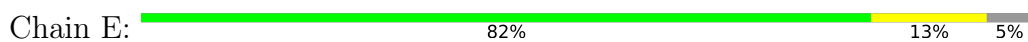




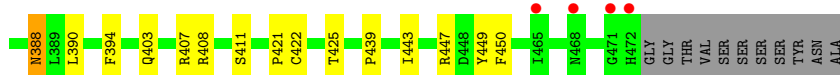
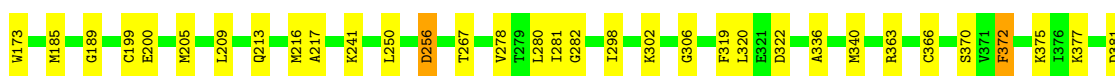
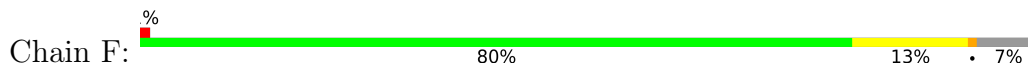
- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.64Å 204.71Å 170.32Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	36.90 – 2.53 36.90 – 2.53	Depositor EDS
% Data completeness (in resolution range)	92.2 (36.90-2.53) 97.8 (36.90-2.53)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.156 , 0.207 0.155 , 0.203	Depositor DCC
R_{free} test set	2120 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23837	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, SO4, CL

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	0.43	0/3784	0.53	0/5105
1	B	0.43	0/3777	0.56	1/5096 (0.0%)
1	C	0.43	0/3765	0.53	0/5083
1	D	0.42	0/3766	0.52	0/5083
1	E	0.43	0/3769	0.57	0/5087
1	F	0.41	0/3715	0.56	1/5010 (0.0%)
All	All	0.42	0/22576	0.55	2/30464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ASP	N-CA-CB	-7.87	96.44	110.60
1	F	256	ASP	N-CA-CB	-6.79	98.38	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3708	0	3652	57	0
1	B	3701	0	3646	47	0
1	C	3689	0	3623	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3690	0	3628	55	0
1	E	3693	0	3639	49	0
1	F	3640	0	3614	50	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	1	0
4	F	10	0	0	0	0
5	A	263	0	0	4	0
5	B	269	0	0	3	0
5	C	195	0	0	2	0
5	D	191	0	0	1	0
5	E	238	0	0	1	0
5	F	249	0	0	3	0
All	All	23837	0	21927	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (275) 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:C:388:ASN:HD22	1:C:390:LEU:H	1.10	0.94
1:D:403:GLN:HE21	1:D:407:ARG:HH21	1.12	0.92
1:A:403:GLN:HE21	1:A:407:ARG:HH21	1.13	0.92
1:B:403:GLN:HE21	1:B:407:ARG:HH21	0.98	0.90
1:B:403:GLN:NE2	1:B:407:ARG:HH21	1.69	0.89
1:E:388:ASN:HD22	1:E:390:LEU:H	1.21	0.86
1:B:388:ASN:HD22	1:B:390:LEU:H	1.18	0.86
1:D:388:ASN:HD22	1:D:390:LEU:H	1.25	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLN:HE21	1:C:407:ARG:HH21	1.26	0.82
1:B:23:ASN:HD21	1:B:51:LYS:H	1.26	0.82
1:F:388:ASN:HD22	1:F:390:LEU:H	1.28	0.78
1:B:403:GLN:HE21	1:B:407:ARG:NH2	1.79	0.76
1:C:388:ASN:ND2	1:C:390:LEU:H	1.84	0.76
1:D:322:ASP:HA	1:D:405:SER:HB3	1.67	0.74
1:C:105:GLU:HB3	5:C:2055:HOH:O	1.87	0.73
1:E:360:LEU:HB2	1:E:377:LYS:HD2	1.71	0.73
1:B:388:ASN:ND2	1:B:390:LEU:H	1.86	0.72
1:C:200:GLU:OE2	1:C:421:PRO:HD2	1.90	0.71
1:F:403:GLN:HE21	1:F:407:ARG:HH21	1.37	0.70
1:F:164:VAL:HG21	1:F:363:ARG:CZ	2.21	0.70
1:A:403:GLN:NE2	1:A:407:ARG:HH21	1.87	0.70
1:F:213:GLN:NE2	5:F:2140:HOH:O	2.23	0.70
1:D:388:ASN:ND2	1:D:390:LEU:H	1.90	0.69
1:E:205:MET:HE2	1:E:216:MET:HG2	1.76	0.68
1:F:200:GLU:OE2	1:F:421:PRO:HD2	1.93	0.68
1:A:442:LEU:O	1:A:446:GLN:HG3	1.92	0.68
1:E:306:GLY:HA2	1:F:403:GLN:HE22	1.58	0.68
1:E:199:CYS:HB3	1:F:439:PRO:HB2	1.75	0.67
1:C:150:TRP:HB3	1:C:151:PRO:HD3	1.78	0.65
1:A:403:GLN:HE21	1:A:407:ARG:NH2	1.91	0.65
1:E:370:SER:OG	1:E:372:PHE:HB3	1.97	0.65
1:E:322:ASP:OD2	1:E:408:ARG:HD2	1.97	0.65
1:E:403:GLN:HE21	1:E:407:ARG:HH21	1.44	0.64
1:F:164:VAL:HG21	1:F:363:ARG:NH2	2.11	0.64
1:E:439:PRO:HB2	1:F:199:CYS:HB3	1.79	0.64
1:C:306:GLY:HA2	1:D:403:GLN:HE22	1.63	0.64
1:D:141:LEU:O	1:D:361:MET:HE3	1.97	0.64
1:C:403:GLN:NE2	1:C:407:ARG:HH21	1.94	0.63
1:C:403:GLN:HE21	1:C:407:ARG:NH2	1.97	0.63
1:B:205:MET:HE2	1:B:216:MET:HG2	1.80	0.62
1:C:482:ASN:HB3	5:C:2190:HOH:O	1.99	0.62
1:E:469:TRP:CH2	1:F:250:LEU:HD23	2.34	0.62
1:F:213:GLN:HG3	5:F:2249:HOH:O	1.99	0.62
1:B:274:TYR:CE1	1:B:348:GLU:HG2	2.35	0.61
1:A:58:LEU:HD22	1:A:88:LEU:HD21	1.83	0.61
1:C:166:THR:HG22	1:F:411:SER:HB3	1.81	0.61
1:C:322:ASP:HA	1:C:405:SER:HB3	1.82	0.61
1:C:403:GLN:HE22	1:D:306:GLY:HA2	1.64	0.61
1:D:305:LYS:HB3	1:D:308:GLN:HE22	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ILE:HG13	1:D:199:CYS:SG	2.42	0.60
1:C:422:CYS:HA	1:C:425:THR:HG22	1.84	0.60
1:E:85:ILE:O	1:E:89:VAL:HG23	2.01	0.60
1:A:199:CYS:HB3	1:B:439:PRO:HB2	1.82	0.60
1:E:422:CYS:HA	1:E:425:THR:HG22	1.84	0.60
1:E:128:VAL:O	1:E:184:LYS:HE3	2.01	0.60
1:A:322:ASP:HA	1:A:405:SER:HB3	1.83	0.59
1:F:205:MET:HE1	1:F:216:MET:HA	1.83	0.59
1:E:403:GLN:HE22	1:F:306:GLY:C	2.06	0.59
1:C:199:CYS:SG	1:D:443:ILE:HG13	2.42	0.59
1:B:422:CYS:HA	1:B:425:THR:HG22	1.85	0.59
1:B:278:VAL:HG12	1:B:281:ILE:HG22	1.86	0.58
1:E:360:LEU:HD12	1:E:360:LEU:O	2.02	0.58
1:A:322:ASP:OD2	1:A:408:ARG:HD2	2.04	0.58
1:B:322:ASP:HA	1:B:405:SER:HB3	1.86	0.58
1:F:3:GLN:HB2	5:F:2002:HOH:O	2.03	0.57
1:A:306:GLY:HA2	1:B:403:GLN:HE22	1.68	0.57
1:A:281:ILE:HG23	1:A:282:GLY:N	2.21	0.56
1:F:336:ALA:O	1:F:340:MET:HG3	2.04	0.56
1:A:82:ASP:OD1	1:A:111:ARG:NH2	2.38	0.56
1:C:278:VAL:HG12	1:C:281:ILE:HG22	1.87	0.56
1:A:200:GLU:OE2	1:A:421:PRO:HD2	2.05	0.56
1:D:8:LEU:HD11	1:D:74:LEU:HD12	1.88	0.56
1:F:278:VAL:O	1:F:281:ILE:HG22	2.07	0.55
1:C:9:ILE:HD12	1:C:73:LEU:HD21	1.87	0.55
1:C:131:GLY:HA3	1:D:450:PHE:O	2.05	0.55
1:D:128:VAL:HG22	1:D:141:LEU:CD2	2.36	0.55
1:D:142:MET:HA	1:D:361:MET:HE1	1.89	0.55
1:E:205:MET:HE1	1:E:216:MET:HA	1.89	0.55
1:B:129:SER:HB3	1:B:140:SER:HB3	1.89	0.55
1:C:189:GLY:HA2	1:C:281:ILE:HD13	1.88	0.55
1:E:150:TRP:CZ2	1:E:154:LYS:HG3	2.42	0.55
1:C:116:LEU:HD12	1:C:123:PHE:HB2	1.88	0.55
1:A:105[B]:GLU:HG3	5:A:2062:HOH:O	2.07	0.54
1:A:422:CYS:HA	1:A:425:THR:HG22	1.87	0.54
1:C:278:VAL:HG13	1:C:337:GLN:HB3	1.89	0.54
1:F:422:CYS:HA	1:F:425:THR:HG22	1.90	0.54
1:A:450:PHE:O	1:B:131:GLY:HA3	2.07	0.54
1:D:422:CYS:HA	1:D:425:THR:HG22	1.89	0.54
1:E:403:GLN:NE2	1:E:407:ARG:HH21	2.03	0.54
1:E:141:LEU:HD13	1:E:157:PHE:CD2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:HIS:NE2	1:E:366:CYS:HB2	2.23	0.53
1:A:460:LYS:HE2	1:A:463:GLN:OE1	2.07	0.53
1:D:388:ASN:HD22	1:D:390:LEU:N	2.02	0.53
1:C:336:ALA:O	1:C:340:MET:HG3	2.08	0.53
1:A:27:PHE:CE1	1:A:156:ILE:HG12	2.44	0.53
1:B:388:ASN:HD22	1:B:390:LEU:N	1.98	0.53
1:B:139:PRO:HD2	1:B:161:ALA:HA	1.90	0.53
1:F:375:LYS:HG3	1:F:394:PHE:CZ	2.43	0.53
1:D:360:LEU:HB2	1:D:377:LYS:HE2	1.91	0.52
1:A:142:MET:HG2	1:A:361:MET:HE2	1.91	0.52
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.92	0.52
1:A:8:LEU:HD11	1:A:74:LEU:HD12	1.91	0.52
1:E:322:ASP:HA	1:E:405:SER:HB3	1.90	0.52
1:E:251:LEU:HB3	1:E:252:PRO:HD3	1.92	0.52
1:D:442:LEU:O	1:D:446:GLN:HG3	2.10	0.52
1:A:142:MET:HA	1:A:361:MET:HE1	1.92	0.51
1:F:205:MET:HE2	1:F:216:MET:HG2	1.92	0.51
1:D:230:SER:CB	1:D:370:SER:HB3	2.40	0.51
1:D:293:LEU:O	1:D:297:ARG:HG3	2.11	0.51
1:A:403:GLN:HE22	1:B:306:GLY:C	2.13	0.51
1:B:391:LEU:HD11	5:B:2233:HOH:O	2.10	0.51
1:D:205:MET:HE1	1:D:216:MET:HA	1.93	0.51
1:A:456:GLU:HG3	1:B:255:ARG:HB3	1.92	0.50
1:A:281:ILE:CG2	1:A:282:GLY:N	2.75	0.50
1:B:322:ASP:OD2	1:B:408:ARG:HD2	2.11	0.50
1:B:363:ARG:O	1:B:369:ARG:HG3	2.12	0.50
1:A:164:VAL:HG21	1:A:363:ARG:CZ	2.41	0.50
1:A:164:VAL:HG21	1:A:363:ARG:NH2	2.27	0.50
1:E:388:ASN:ND2	1:E:390:LEU:H	1.98	0.50
1:B:229:ASP:HB3	1:B:371:VAL:HB	1.94	0.50
1:D:150:TRP:HB3	1:D:151:PRO:HD3	1.93	0.50
1:B:348:GLU:HG3	5:B:2189:HOH:O	2.12	0.49
1:F:403:GLN:NE2	1:F:407:ARG:HH21	2.07	0.49
1:D:170:CYS:HB3	1:D:361:MET:O	2.12	0.49
1:E:306:GLY:CA	1:F:403:GLN:HE22	2.23	0.49
1:E:35:THR:HB	1:E:38:LYS:HE3	1.95	0.49
1:D:375:LYS:HG3	1:D:394:PHE:CZ	2.48	0.49
1:E:265:LYS:O	1:E:269:ILE:HG13	2.12	0.49
1:D:395:PHE:O	1:D:399:VAL:HG23	2.13	0.49
1:E:360:LEU:HD22	1:E:377:LYS:HE3	1.93	0.49
1:B:143:PRO:HD2	1:B:172:ASP:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HD22	1:D:19:ILE:HD11	1.94	0.49
1:F:150:TRP:HB3	1:F:151:PRO:HD3	1.95	0.48
1:D:305:LYS:HB3	1:D:308:GLN:NE2	2.27	0.48
1:E:8:LEU:C	1:E:8:LEU:HD23	2.34	0.48
1:A:421:PRO:O	1:A:425:THR:HG22	2.12	0.48
1:B:164:VAL:HG21	1:B:363:ARG:CZ	2.43	0.48
1:F:147:LYS:HE2	1:F:173:TRP:CD1	2.48	0.48
1:F:185:MET:HG2	1:F:267:THR:OG1	2.14	0.48
1:E:260:GLN:HE22	1:E:285:VAL:HG13	1.78	0.48
1:E:75:VAL:HG11	1:E:84:PHE:CE2	2.49	0.48
1:A:251:LEU:HD12	1:A:251:LEU:O	2.13	0.48
1:D:319:PHE:O	1:D:323:ILE:HG13	2.13	0.48
1:A:131:GLY:HA3	1:B:450:PHE:O	2.15	0.47
1:A:278:VAL:O	1:A:281:ILE:HG22	2.13	0.47
1:D:420:MET:HB3	1:D:423:PHE:HB2	1.96	0.47
1:E:367:ILE:HD12	1:F:450:PHE:CD1	2.49	0.47
1:A:449:TYR:CD2	1:A:469:TRP:HB3	2.50	0.47
1:C:9:ILE:HD12	1:C:73:LEU:CD2	2.44	0.47
1:C:11:LEU:HD12	1:C:33:ASN:HB2	1.97	0.47
1:C:294:LYS:O	1:C:298:ILE:HG13	2.15	0.47
1:F:372:PHE:CD1	1:F:372:PHE:C	2.89	0.46
1:E:189:GLY:O	1:E:281:ILE:HG12	2.15	0.46
1:A:274:TYR:CE1	1:A:348:GLU:HG2	2.51	0.46
1:A:439:PRO:HB2	1:B:199:CYS:HB3	1.97	0.46
1:B:280:LEU:HD23	1:B:422:CYS:SG	2.56	0.46
1:D:142:MET:HA	1:D:361:MET:CE	2.46	0.46
1:A:168:GLU:HA	1:A:169:PRO:HD3	1.76	0.45
1:F:443:ILE:O	1:F:447:ARG:HG3	2.17	0.45
1:C:217:ALA:HB1	1:C:241:LYS:HG3	1.97	0.45
1:A:199:CYS:SG	1:B:443:ILE:HG13	2.56	0.45
1:B:375:LYS:HG3	1:B:394:PHE:CZ	2.51	0.45
1:E:34:ARG:HE	1:E:34:ARG:HB3	1.40	0.45
1:E:150:TRP:HB3	1:E:151:PRO:HD3	1.99	0.45
1:A:45:ASN:O	1:A:48:LYS:HB2	2.16	0.45
1:F:27:PHE:CE1	1:F:156:ILE:HG12	2.52	0.45
1:D:205:MET:HE2	1:D:216:MET:HG2	1.99	0.45
1:F:209:LEU:HD21	1:F:319:PHE:CD2	2.52	0.45
1:C:150:TRP:CZ2	1:C:154:LYS:HG3	2.52	0.45
1:F:141:LEU:C	1:F:143:PRO:HD3	2.38	0.45
1:D:329:ALA:O	1:D:332:ILE:HB	2.17	0.45
1:B:168:GLU:HA	1:B:169:PRO:HD3	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:OD1	1:C:184:LYS:HE3	2.17	0.44
1:C:186:VAL:HG21	1:C:342:LEU:CD2	2.47	0.44
1:C:251:LEU:HB3	1:C:252:PRO:HD3	1.98	0.44
1:C:403:GLN:HE22	1:D:306:GLY:CA	2.28	0.44
1:D:115:ASP:HB2	5:D:2077:HOH:O	2.15	0.44
1:D:403:GLN:HE21	1:D:407:ARG:NH2	1.95	0.44
1:E:251:LEU:N	1:E:252:PRO:CD	2.80	0.44
1:E:343:ARG:HA	1:E:355:TYR:OH	2.16	0.44
1:C:138:GLY:O	1:C:162:ALA:HB2	2.18	0.44
1:C:300:ALA:HB1	1:C:304:LEU:HD12	1.99	0.44
1:D:128:VAL:HG22	1:D:141:LEU:HD23	2.00	0.44
1:A:67:LYS:HA	1:A:68:PRO:C	2.38	0.44
1:A:403:GLN:HE22	1:B:306:GLY:HA2	1.83	0.44
1:F:10:GLY:O	1:F:15:GLY:HA3	2.18	0.44
1:C:16:GLN:NE2	1:D:476:VAL:HG21	2.32	0.44
1:F:377:LYS:HE3	1:F:381:ASP:OD2	2.18	0.44
1:A:278:VAL:HG13	1:A:337:GLN:HB3	2.00	0.44
1:C:388:ASN:HD22	1:C:390:LEU:N	1.93	0.44
1:D:43:LEU:HD11	1:D:54:GLY:HA3	1.99	0.44
1:D:130:GLY:CA	1:D:365:GLY:O	2.66	0.44
1:B:141:LEU:O	1:B:361:MET:CE	2.66	0.44
1:F:129:SER:HB3	1:F:140:SER:HB3	2.00	0.44
1:D:6:ILE:HD11	1:D:72:ILE:HG13	2.00	0.43
1:D:326:ALA:HB2	1:D:406:TRP:HA	2.01	0.43
1:E:403:GLN:HE22	1:F:306:GLY:CA	2.32	0.43
1:F:99:ILE:HG21	1:F:157:PHE:HZ	1.83	0.43
1:A:105[B]:GLU:CD	5:A:2062:HOH:O	2.56	0.43
1:A:43:LEU:HD21	1:A:52:VAL:HG12	2.00	0.43
1:A:460:LYS:O	1:A:460:LYS:HG3	2.17	0.43
1:B:372:PHE:CD1	1:B:372:PHE:C	2.92	0.43
1:A:168:GLU:H	1:A:168:GLU:HG3	1.55	0.43
1:B:9:ILE:HD12	1:B:73:LEU:CD2	2.48	0.43
1:E:373:LEU:HD23	1:E:376:ILE:HD12	2.01	0.43
1:B:8:LEU:HD11	1:B:74:LEU:HD12	2.00	0.43
1:F:209:LEU:HD21	1:F:319:PHE:HD2	1.83	0.43
1:E:205:MET:CE	1:E:216:MET:HA	2.49	0.43
1:D:274:TYR:CD1	1:D:348:GLU:HG3	2.54	0.42
1:B:119:LYS:HE3	5:B:2085:HOH:O	2.19	0.42
1:C:142:MET:HG2	1:C:361:MET:HE2	2.01	0.42
1:C:224:ASN:HB2	1:C:233:ILE:HG22	2.00	0.42
1:D:278:VAL:CG1	1:D:281:ILE:HD12	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:HG13	1:E:170:CYS:SG	2.59	0.42
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.81	0.42
1:F:74:LEU:HD23	1:F:74:LEU:HA	1.87	0.42
1:A:51:LYS:HE2	1:A:51:LYS:HB2	1.81	0.42
1:A:372:PHE:CD1	1:A:372:PHE:C	2.93	0.42
1:D:103:ASN:OD1	1:D:184:LYS:HE3	2.18	0.42
1:C:476:VAL:HG21	1:D:16:GLN:NE2	2.34	0.42
1:E:403:GLN:HE22	1:F:306:GLY:HA2	1.84	0.42
1:A:150:TRP:N	1:A:151:PRO:CD	2.81	0.42
1:A:317:LYS:HB2	1:A:317:LYS:NZ	2.35	0.42
1:F:388:ASN:ND2	1:F:390:LEU:H	2.06	0.42
1:D:150:TRP:N	1:D:151:PRO:CD	2.83	0.42
2:C:500:NAP:H2N	2:C:500:NAP:H2D	1.88	0.42
1:D:10:GLY:O	1:D:15:GLY:HA3	2.20	0.42
1:F:372:PHE:C	1:F:372:PHE:HD1	2.23	0.42
1:A:185:MET:HG2	1:A:267:THR:OG1	2.20	0.42
1:C:129:SER:HB3	1:C:140:SER:HB3	2.02	0.42
1:D:375:LYS:HG3	1:D:394:PHE:CE2	2.55	0.42
1:A:391:LEU:HD11	5:A:2219:HOH:O	2.20	0.41
1:C:322:ASP:OD2	1:C:408:ARG:HD2	2.20	0.41
1:E:102:GLY:HA3	5:E:2051:HOH:O	2.20	0.41
1:D:403:GLN:HG2	1:D:407:ARG:HE	1.85	0.41
1:F:281:ILE:HG23	1:F:282:GLY:N	2.36	0.41
1:B:375:LYS:HD3	1:B:375:LYS:HA	1.77	0.41
1:F:322:ASP:OD2	1:F:408:ARG:HD2	2.20	0.41
1:A:403:GLN:O	1:A:407:ARG:HG3	2.21	0.41
1:A:427:LEU:HD21	1:B:414:VAL:HG13	2.03	0.41
1:B:23:ASN:ND2	1:B:50:THR:HB	2.35	0.41
1:D:205:MET:CE	1:D:216:MET:HA	2.50	0.41
1:F:189:GLY:HA2	1:F:281:ILE:HD13	2.02	0.41
1:A:142:MET:CG	1:A:361:MET:HE2	2.50	0.41
1:B:227:GLU:HB3	1:B:328:TYR:CZ	2.55	0.41
1:C:454:THR:HG22	1:C:466:HIS:HB2	2.02	0.41
1:E:420:MET:HB3	1:E:423:PHE:HB2	2.02	0.41
1:C:76:LYS:HE3	1:D:481:TYR:CD1	2.56	0.41
1:C:142:MET:HA	1:C:361:MET:HE1	2.02	0.41
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.94	0.41
1:A:7:ALA:HB2	1:A:65:LEU:HD21	2.02	0.41
1:A:403:GLN:HE22	1:B:306:GLY:CA	2.34	0.41
1:A:428:SER:HA	5:A:2217:HOH:O	2.21	0.41
1:C:192:TYR:CE2	1:C:264:GLY:HA3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:TRP:CE2	1:E:324:ARG:HB2	2.56	0.41
1:F:205:MET:HE3	1:F:320:LEU:HD11	2.03	0.41
1:F:217:ALA:HB1	1:F:241:LYS:HG3	2.03	0.41
1:D:164:VAL:HG13	1:D:170:CYS:SG	2.61	0.40
1:D:331:LYS:O	1:D:335:TYR:HD1	2.04	0.40
1:E:187:HIS:CD2	1:E:368:ILE:HG12	2.56	0.40
1:E:436:GLU:HG3	1:F:298:ILE:HG12	2.03	0.40
1:F:141:LEU:O	1:F:143:PRO:HD3	2.21	0.40
1:D:161:ALA:O	1:D:163:LYS:HE3	2.21	0.40
1:D:187:HIS:NE2	1:D:366:CYS:HB2	2.36	0.40
1:A:235:ILE:O	1:A:239:ILE:HG13	2.22	0.40
1:A:276:VAL:HA	1:A:277:PRO:HD3	1.86	0.40
2:A:500:NAP:H2N	2:A:500:NAP:H2D	1.84	0.40
1:C:10:GLY:O	1:C:15:GLY:HA3	2.21	0.40
1:B:299:GLN:O	1:B:302:LYS:HB2	2.21	0.40
1:B:319:PHE:O	1:B:323:ILE:HG13	2.21	0.40
1:B:205:MET:HE1	1:B:216:MET:HA	2.04	0.40
1:E:249:HIS:N	4:E:1484:SO4:O3	2.47	0.40
1:E:335:TYR:HE2	1:E:373:LEU:HD21	1.85	0.40
1:F:140:SER:HB2	1:F:366:CYS:HB2	2.03	0.40
1:F:141:LEU:HB2	1:F:171:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	481/505 (95%)	463 (96%)	17 (4%)	1 (0%)	47 60
1	B	481/505 (95%)	461 (96%)	19 (4%)	1 (0%)	47 60
1	C	480/505 (95%)	466 (97%)	13 (3%)	1 (0%)	47 60
1	D	480/505 (95%)	462 (96%)	16 (3%)	2 (0%)	34 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	480/505 (95%)	459 (96%)	20 (4%)	1 (0%)	47 60
1	F	469/505 (93%)	453 (97%)	15 (3%)	1 (0%)	47 60
All	All	2871/3030 (95%)	2764 (96%)	100 (4%)	7 (0%)	47 60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLY
1	B	165	GLY
1	C	165	GLY
1	D	165	GLY
1	D	386	LEU
1	E	165	GLY
1	F	165	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	380/410 (93%)	372 (98%)	8 (2%)	53 68
1	B	378/410 (92%)	370 (98%)	8 (2%)	53 68
1	C	376/410 (92%)	366 (97%)	10 (3%)	44 59
1	D	376/410 (92%)	370 (98%)	6 (2%)	62 77
1	E	377/410 (92%)	369 (98%)	8 (2%)	53 68
1	F	375/410 (92%)	365 (97%)	10 (3%)	44 59
All	All	2262/2460 (92%)	2212 (98%)	50 (2%)	52 66

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	GLU
1	A	194	ASP
1	A	281	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	SER
1	A	372	PHE
1	A	404	ASP
1	A	479	SER
1	A	480	SER
1	B	172	ASP
1	B	194	ASP
1	B	280	LEU
1	B	372	PHE
1	B	415	GLN
1	B	456	GLU
1	B	479	SER
1	B	480	SER
1	C	89	VAL
1	C	133	GLU
1	C	166	THR
1	C	194	ASP
1	C	226	THR
1	C	303	LYS
1	C	372	PHE
1	C	388	ASN
1	C	436	GLU
1	C	479	SER
1	D	115	ASP
1	D	168	GLU
1	D	280	LEU
1	D	388	ASN
1	D	411	SER
1	D	480	SER
1	E	34	ARG
1	E	168	GLU
1	E	263	THR
1	E	280	LEU
1	E	388	ASN
1	E	456	GLU
1	E	479	SER
1	E	480	SER
1	F	139	PRO
1	F	168	GLU
1	F	172	ASP
1	F	256	ASP
1	F	280	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	302	LYS
1	F	370	SER
1	F	372	PHE
1	F	388	ASN
1	F	449	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	403	GLN
1	B	23	ASN
1	B	152	HIS
1	B	388	ASN
1	B	403	GLN
1	C	388	ASN
1	C	401	ASN
1	C	403	GLN
1	C	415	GLN
1	D	152	HIS
1	D	308	GLN
1	D	388	ASN
1	D	403	GLN
1	E	103	ASN
1	E	152	HIS
1	E	260	GLN
1	E	388	ASN
1	E	403	GLN
1	F	388	ASN
1	F	403	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 11 are monoatomic - leaving 17 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
2	NAP	D	500	-	45,52,52	1.72	4 (8%)	56,80,80	1.16	2 (3%)
4	SO4	C	1484	-	4,4,4	0.22	0	6,6,6	0.42	0
2	NAP	B	500	-	45,52,52	1.67	3 (6%)	56,80,80	1.20	3 (5%)
4	SO4	B	1486	-	4,4,4	0.20	0	6,6,6	0.61	0
4	SO4	D	1485	-	4,4,4	0.12	0	6,6,6	0.15	0
2	NAP	C	500	-	45,52,52	1.68	4 (8%)	56,80,80	1.18	4 (7%)
4	SO4	E	1484	-	4,4,4	0.16	0	6,6,6	0.26	0
2	NAP	E	500	-	45,52,52	1.69	4 (8%)	56,80,80	1.17	2 (3%)
4	SO4	A	1486	-	4,4,4	0.22	0	6,6,6	0.18	0
2	NAP	A	500	-	45,52,52	1.69	3 (6%)	56,80,80	1.13	2 (3%)
4	SO4	C	1485	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	D	1484	-	4,4,4	0.15	0	6,6,6	0.32	0
4	SO4	F	1475	-	4,4,4	0.11	0	6,6,6	0.29	0
4	SO4	B	1487	-	4,4,4	0.17	0	6,6,6	0.22	0
4	SO4	E	1485	-	4,4,4	0.18	0	6,6,6	0.60	0
4	SO4	F	1474	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	A	1485	-	4,4,4	0.12	0	6,6,6	0.41	0

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	D	500	-	-	6/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	500	-	-	6/31/67/67	0/5/5/5
2	NAP	C	500	-	-	6/31/67/67	0/5/5/5
2	NAP	E	500	-	-	6/31/67/67	0/5/5/5
2	NAP	A	500	-	-	6/31/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	O7N-C7N	9.10	1.41	1.24
2	E	500	NAP	O7N-C7N	8.74	1.40	1.24
2	A	500	NAP	O7N-C7N	8.62	1.40	1.24
2	B	500	NAP	O7N-C7N	8.57	1.40	1.24
2	C	500	NAP	O7N-C7N	8.43	1.40	1.24
2	C	500	NAP	C2A-N3A	4.18	1.38	1.32
2	A	500	NAP	C2A-N3A	4.15	1.38	1.32
2	D	500	NAP	C2A-N3A	4.06	1.38	1.32
2	E	500	NAP	C2A-N3A	3.98	1.38	1.32
2	B	500	NAP	C2A-N3A	3.84	1.38	1.32
2	C	500	NAP	C2A-N1A	2.63	1.38	1.33
2	A	500	NAP	C2A-N1A	2.57	1.38	1.33
2	B	500	NAP	C2A-N1A	2.51	1.38	1.33
2	D	500	NAP	C2A-N1A	2.42	1.38	1.33
2	E	500	NAP	C2A-N1A	2.37	1.38	1.33
2	C	500	NAP	C2N-N1N	2.21	1.37	1.35
2	E	500	NAP	C2N-N1N	2.19	1.37	1.35
2	D	500	NAP	C2N-N1N	2.08	1.37	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAP	N3A-C2A-N1A	-5.88	119.49	128.68
2	E	500	NAP	N3A-C2A-N1A	-5.85	119.54	128.68
2	C	500	NAP	N3A-C2A-N1A	-5.49	120.10	128.68
2	A	500	NAP	N3A-C2A-N1A	-5.46	120.15	128.68
2	B	500	NAP	N3A-C2A-N1A	-5.37	120.28	128.68
2	C	500	NAP	C3N-C7N-N7N	2.79	121.09	117.75
2	B	500	NAP	C3B-C2B-C1B	-2.73	97.75	102.89
2	B	500	NAP	C3N-C7N-N7N	2.72	121.01	117.75
2	C	500	NAP	C3B-C2B-C1B	-2.64	97.93	102.89
2	D	500	NAP	C3B-C2B-C1B	-2.50	98.18	102.89
2	A	500	NAP	C3B-C2B-C1B	-2.40	98.37	102.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	NAP	C3B-C2B-C1B	-2.38	98.41	102.89
2	C	500	NAP	O2N-PN-O1N	2.01	122.19	112.24

There are no chirality outliers.

All (30) torsion outliers are listed below:

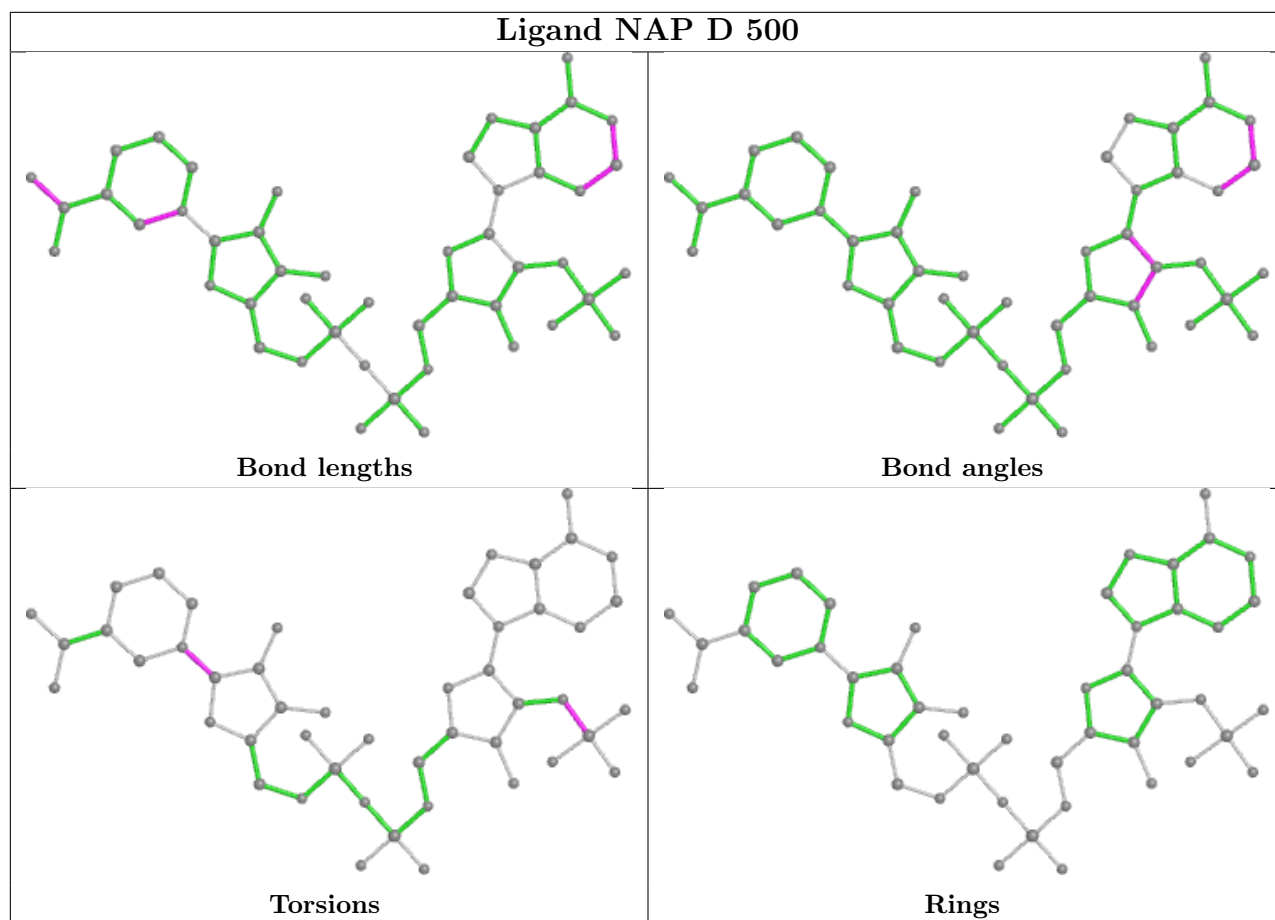
Mol	Chain	Res	Type	Atoms
2	A	500	NAP	C2B-O2B-P2B-O1X
2	A	500	NAP	O4D-C1D-N1N-C2N
2	A	500	NAP	O4D-C1D-N1N-C6N
2	A	500	NAP	C2D-C1D-N1N-C2N
2	A	500	NAP	C2D-C1D-N1N-C6N
2	B	500	NAP	C2B-O2B-P2B-O3X
2	B	500	NAP	O4D-C1D-N1N-C2N
2	B	500	NAP	O4D-C1D-N1N-C6N
2	B	500	NAP	C2D-C1D-N1N-C2N
2	B	500	NAP	C2D-C1D-N1N-C6N
2	C	500	NAP	C2B-O2B-P2B-O1X
2	C	500	NAP	O4D-C1D-N1N-C2N
2	C	500	NAP	O4D-C1D-N1N-C6N
2	C	500	NAP	C2D-C1D-N1N-C2N
2	C	500	NAP	C2D-C1D-N1N-C6N
2	D	500	NAP	C2B-O2B-P2B-O1X
2	D	500	NAP	C2B-O2B-P2B-O3X
2	D	500	NAP	O4D-C1D-N1N-C2N
2	D	500	NAP	O4D-C1D-N1N-C6N
2	D	500	NAP	C2D-C1D-N1N-C2N
2	D	500	NAP	C2D-C1D-N1N-C6N
2	E	500	NAP	C2B-O2B-P2B-O3X
2	E	500	NAP	O4D-C1D-N1N-C2N
2	E	500	NAP	O4D-C1D-N1N-C6N
2	E	500	NAP	C2D-C1D-N1N-C2N
2	E	500	NAP	C2D-C1D-N1N-C6N
2	B	500	NAP	C2B-O2B-P2B-O1X
2	E	500	NAP	C2B-O2B-P2B-O1X
2	A	500	NAP	C2B-O2B-P2B-O3X
2	C	500	NAP	C2B-O2B-P2B-O3X

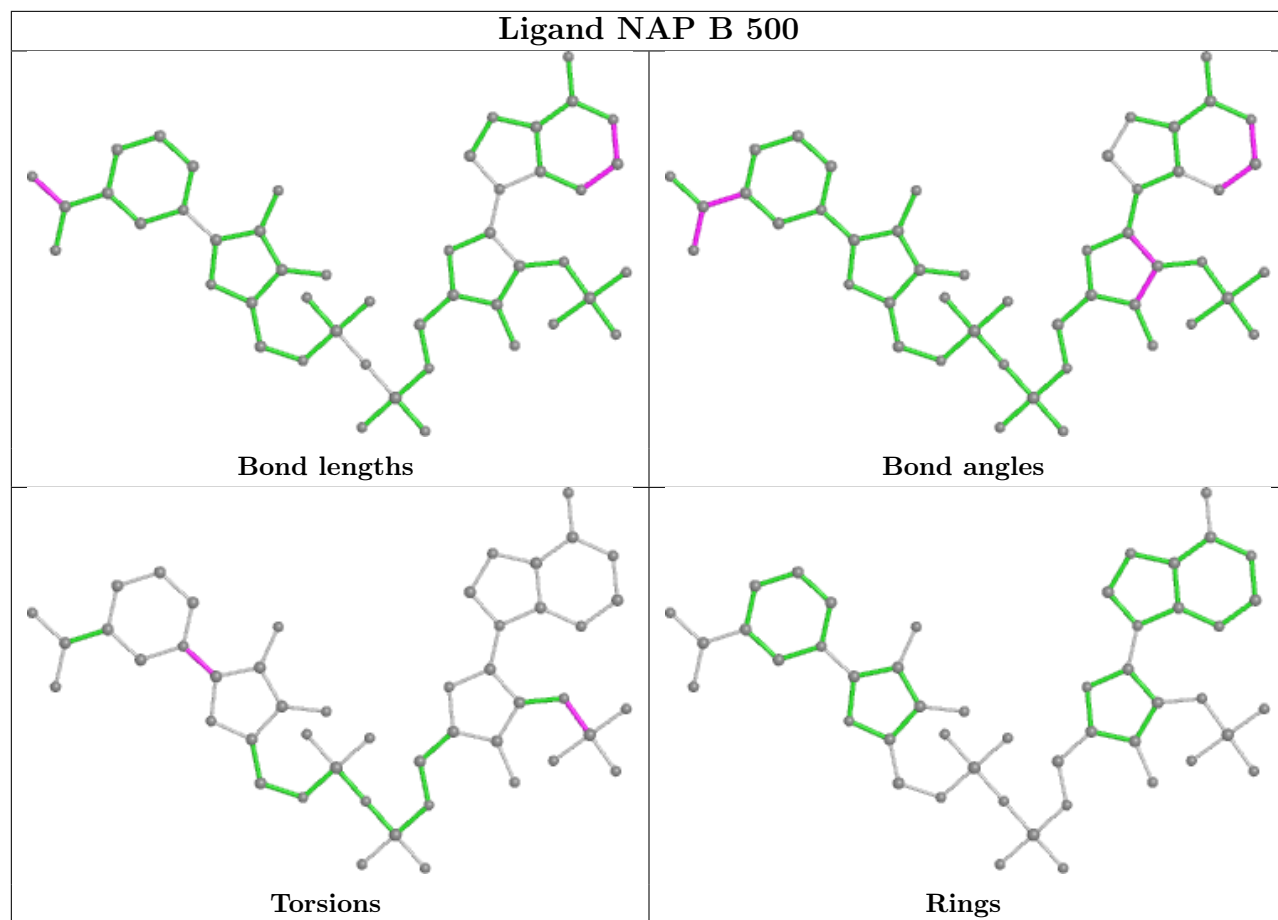
There are no ring outliers.

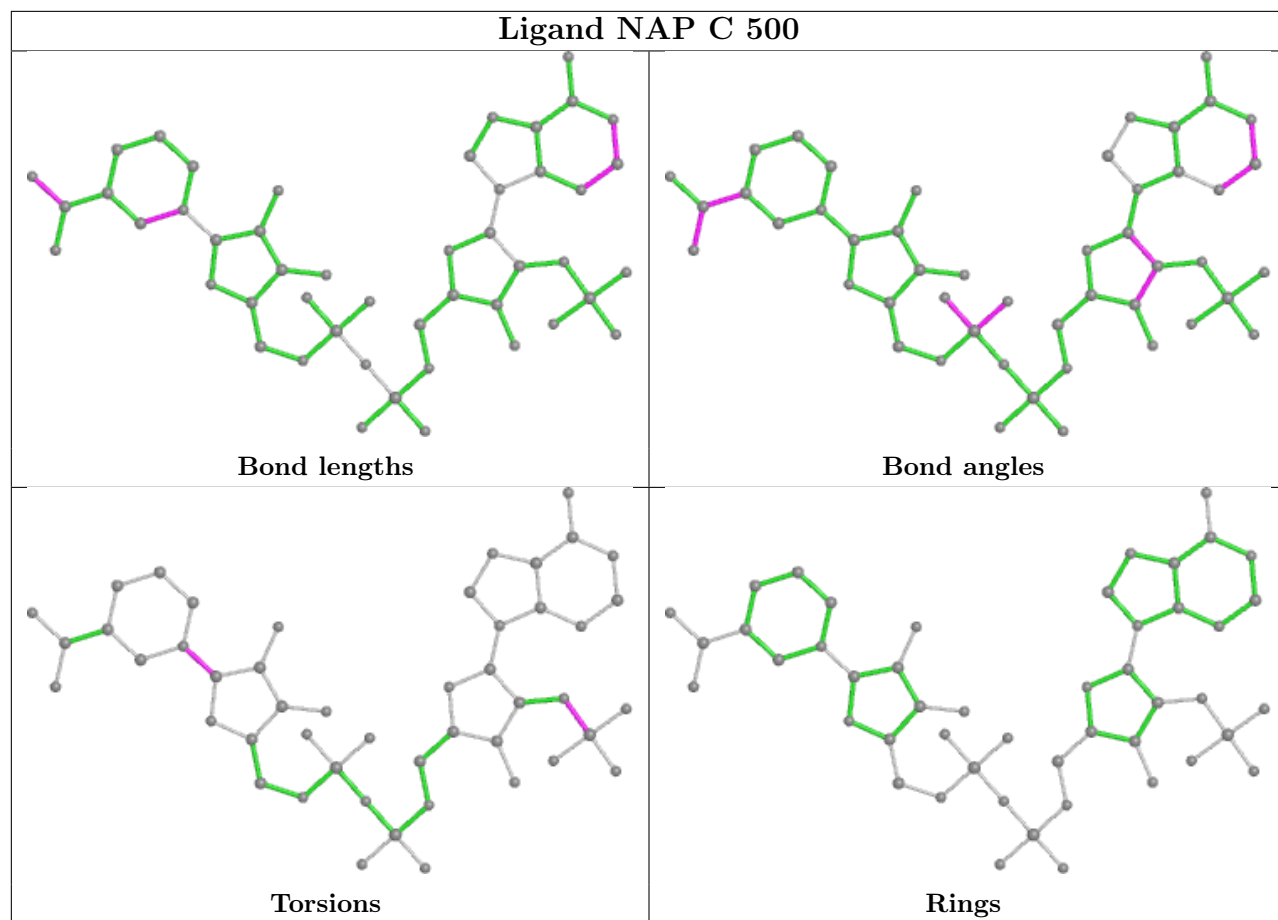
3 monomers are involved in 3 short contacts:

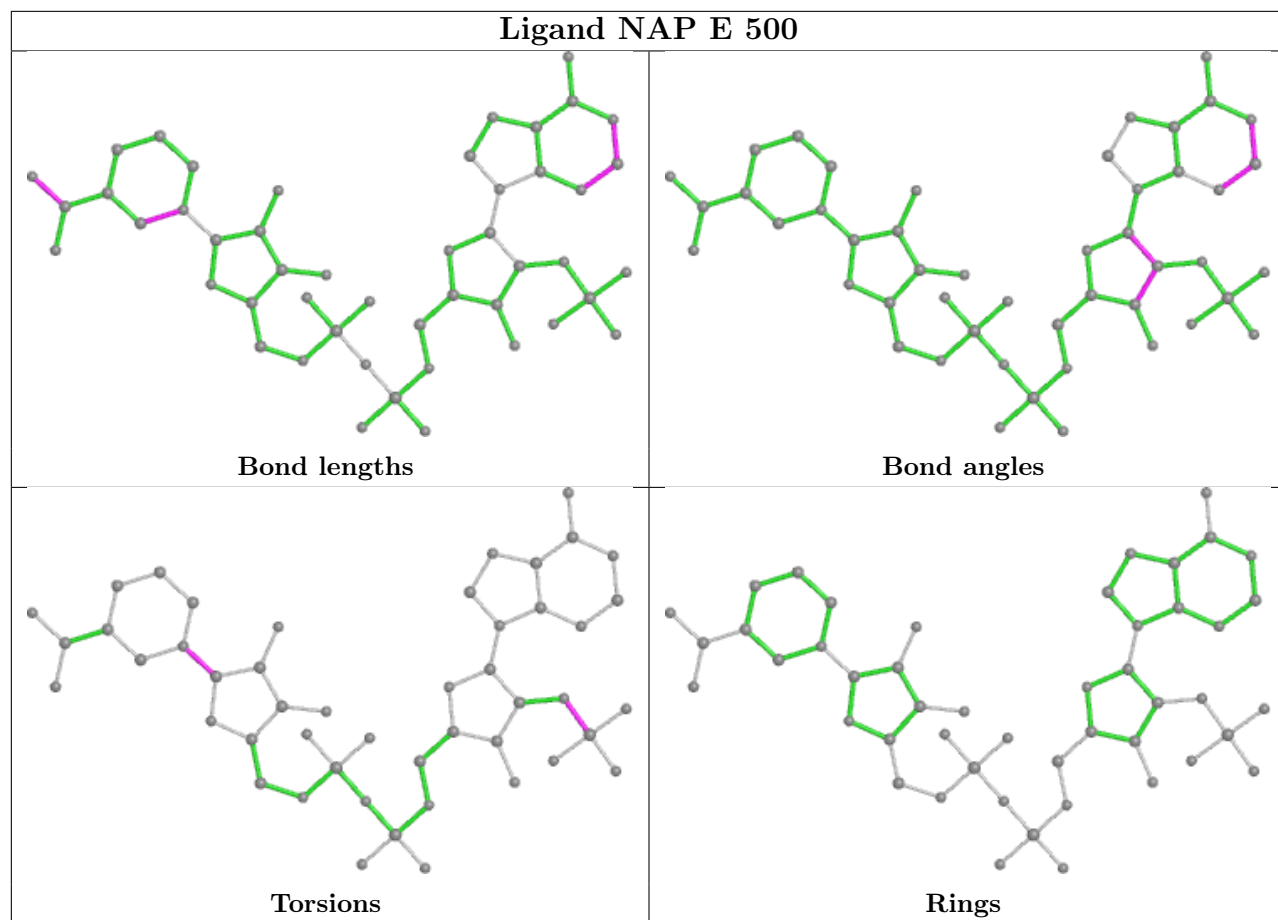
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	NAP	1	0
4	E	1484	SO4	1	0
2	A	500	NAP	1	0

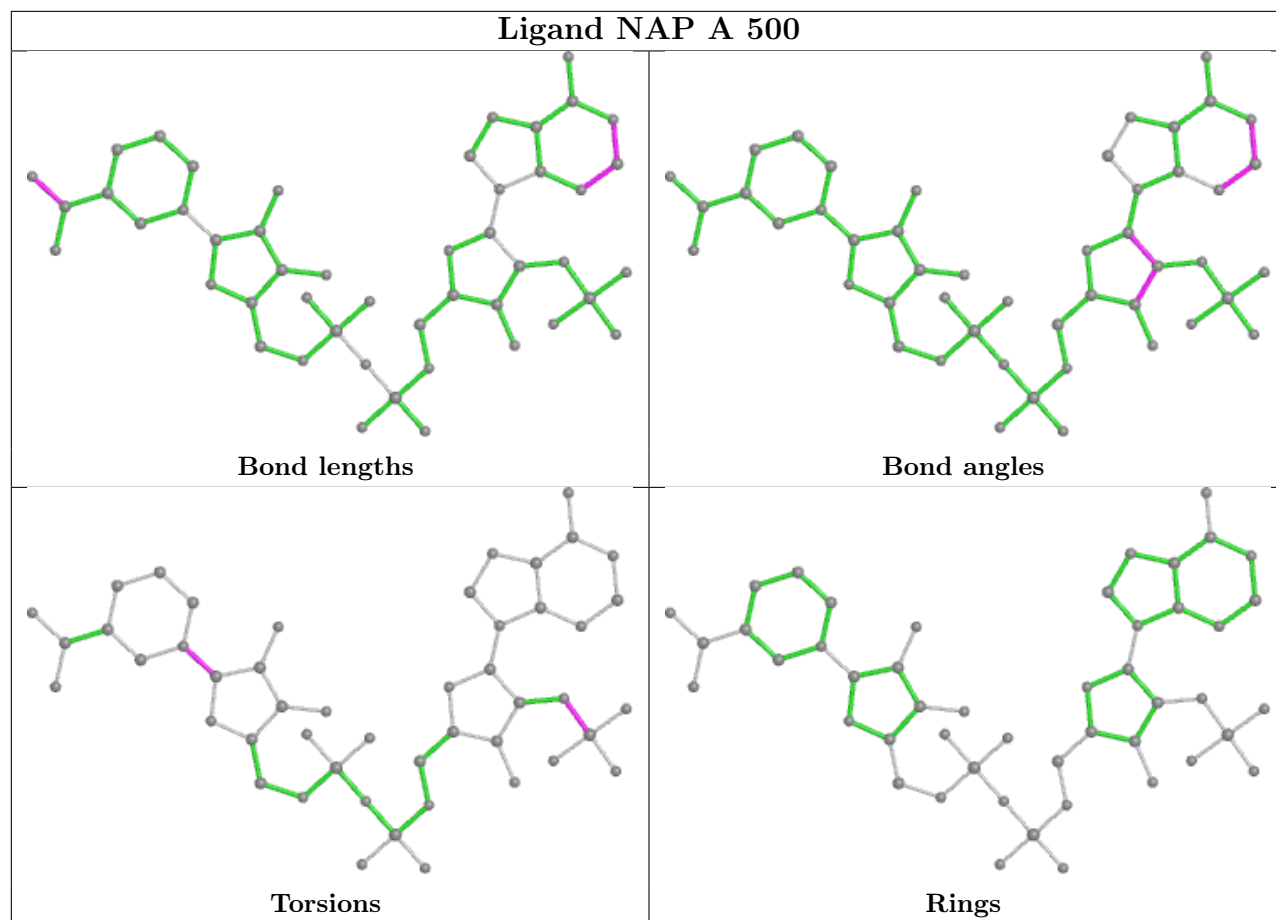
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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, 95th 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	482/505 (95%)	-0.46	3 (0%) 89 92	12, 30, 57, 83	0
1	B	482/505 (95%)	-0.35	4 (0%) 86 89	12, 29, 56, 84	0
1	C	482/505 (95%)	-0.24	10 (2%) 63 70	18, 34, 59, 84	0
1	D	482/505 (95%)	-0.21	11 (2%) 60 67	21, 35, 59, 85	0
1	E	482/505 (95%)	-0.44	2 (0%) 92 96	14, 31, 57, 83	0
1	F	471/505 (93%)	-0.42	6 (1%) 77 82	14, 29, 52, 88	0
All	All	2881/3030 (95%)	-0.35	36 (1%) 79 84	12, 31, 58, 88	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	472	HIS	5.3
1	D	472	HIS	4.8
1	F	471	GLY	4.0
1	B	2	ALA	3.8
1	D	245	THR	3.7
1	A	166	THR	3.4
1	C	245	THR	3.3
1	C	310	PHE	3.0
1	C	312	PHE	3.0
1	D	247	GLY	3.0
1	A	165	GLY	2.8
1	C	49	GLY	2.8
1	C	314	GLY	2.8
1	D	246	ASP	2.8
1	D	165	GLY	2.7
1	B	245	THR	2.5
1	A	167	GLY	2.5
1	F	165	GLY	2.5
1	B	308	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	2.4
1	D	243	GLN	2.4
1	F	166	THR	2.3
1	F	465	ILE	2.3
1	D	350	GLY	2.3
1	C	317	LYS	2.3
1	E	40	ASP	2.2
1	E	245	THR	2.2
1	C	44	ALA	2.2
1	D	475	THR	2.2
1	D	166	THR	2.2
1	C	480	SER	2.2
1	D	383	ASN	2.2
1	F	468	ASN	2.2
1	D	347	THR	2.1
1	C	244	ASP	2.0
1	C	315	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 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, 95th 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(\AA^2)	Q<0.9
3	CL	D	1486	1/1	0.81	0.82	81,81,81,81	0
3	CL	E	1486	1/1	0.88	0.10	67,67,67,67	0
4	SO4	C	1485	5/5	0.90	0.31	75,100,106,115	0
3	CL	A	1487	1/1	0.91	0.09	80,80,80,80	0
3	CL	E	1488	1/1	0.92	0.06	75,75,75,75	0
4	SO4	B	1487	5/5	0.93	0.22	46,67,92,99	0

Continued on next page...

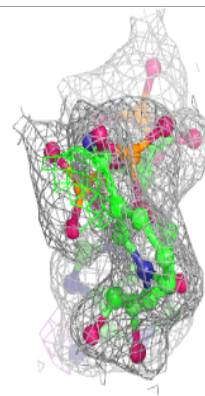
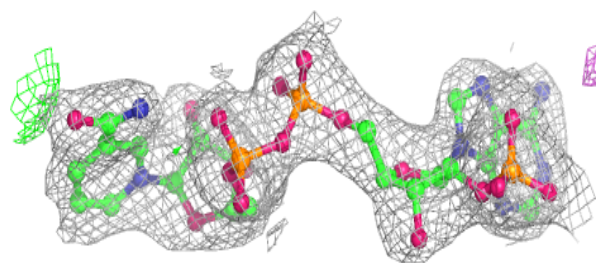
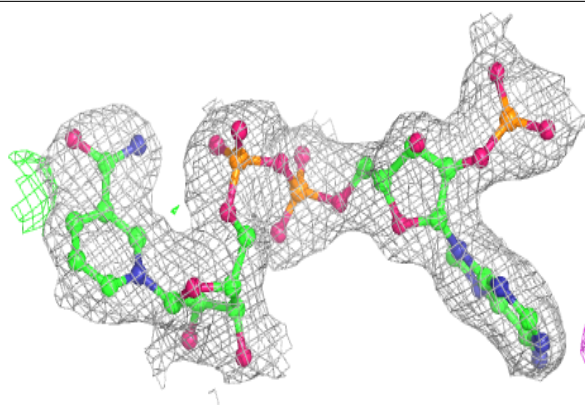
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	B	1485	1/1	0.94	0.05	56,56,56,56	0
4	SO4	D	1485	5/5	0.94	0.33	91,92,100,116	0
4	SO4	A	1486	5/5	0.95	0.17	68,70,83,92	0
2	NAP	C	500	48/48	0.95	0.13	40,42,44,54	0
4	SO4	F	1475	5/5	0.95	0.21	69,69,78,85	0
3	CL	A	1488	1/1	0.96	0.07	62,62,62,62	0
2	NAP	D	500	48/48	0.96	0.12	28,33,42,46	0
3	CL	F	1476	1/1	0.96	0.06	62,62,62,62	0
4	SO4	E	1484	5/5	0.96	0.23	58,97,106,106	0
2	NAP	A	500	48/48	0.96	0.13	19,29,40,44	0
2	NAP	E	500	48/48	0.97	0.12	13,27,36,48	0
2	NAP	B	500	48/48	0.97	0.11	23,31,42,50	0
3	CL	A	1484	1/1	0.98	0.19	37,37,37,37	0
4	SO4	E	1485	5/5	0.98	0.12	17,25,35,36	0
3	CL	B	1488	1/1	0.98	0.05	61,61,61,61	0
3	CL	B	1484	1/1	0.99	0.22	34,34,34,34	0
4	SO4	C	1484	5/5	0.99	0.15	16,25,42,44	0
3	CL	F	1473	1/1	0.99	0.14	35,35,35,35	0
4	SO4	F	1474	5/5	0.99	0.14	12,15,20,32	0
4	SO4	D	1484	5/5	0.99	0.16	21,27,35,36	0
4	SO4	B	1486	5/5	1.00	0.14	12,19,21,24	0
4	SO4	A	1485	5/5	1.00	0.11	10,18,24,25	0

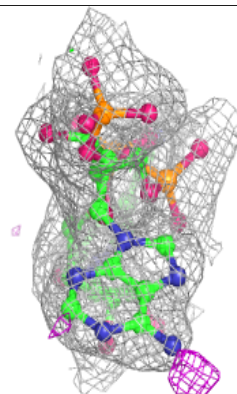
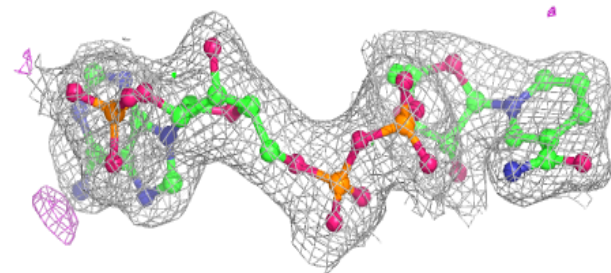
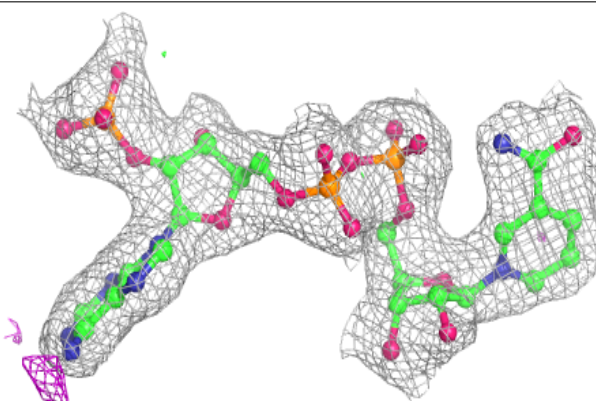
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 500:

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

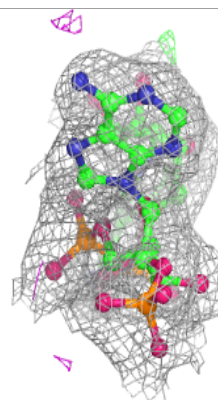
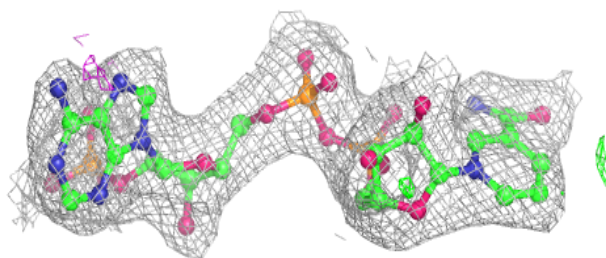
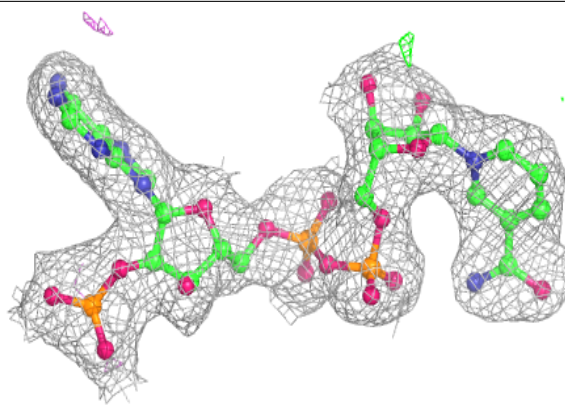
**Electron density around NAP D 500:**

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

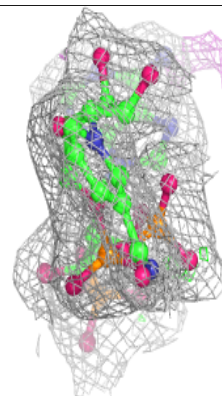
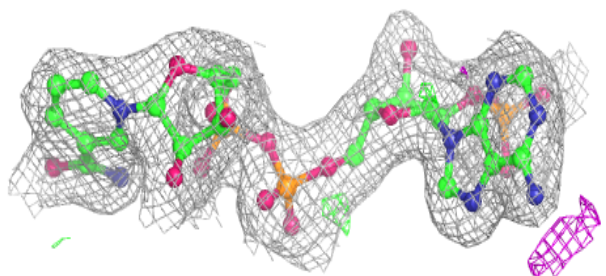
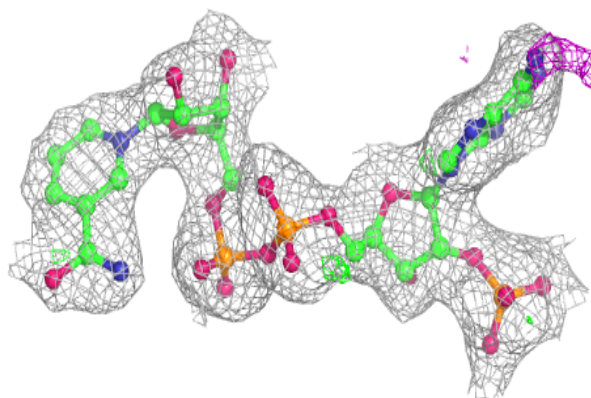


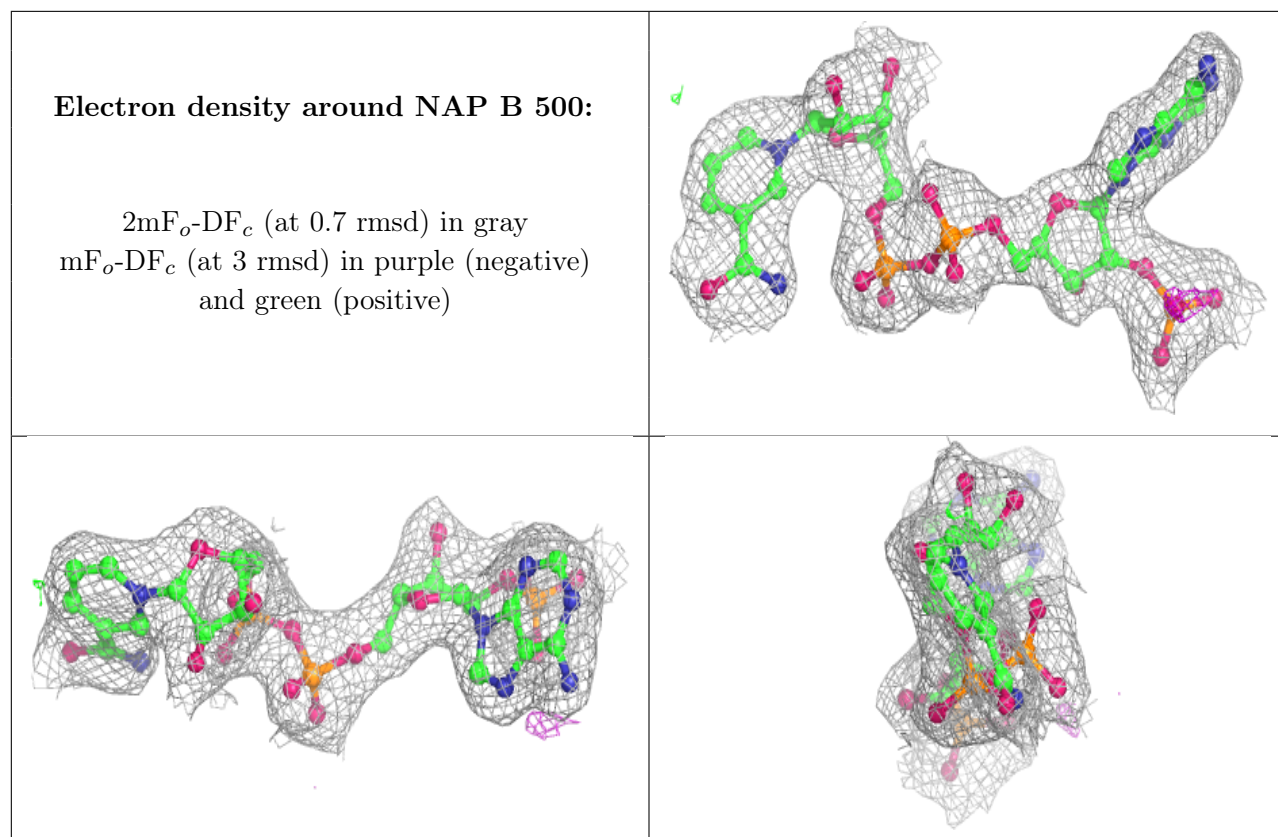
Electron density around NAP A 500:

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

**Electron density around NAP E 500:**

$2mF_o-DF_c$ (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.