



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:27 AM EDT

PDB ID : 5FB3
Title : Structure of glycerophosphate dehydrogenase in complex with NADPH
Authors : Sakuraba, H.; Hayashi, J.; Yamamoto, K.; Yoneda, K.; Ohshima, T.
Deposited on : 2015-12-14
Resolution : 2.45 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 : 2.37.1
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) : 2.37.1

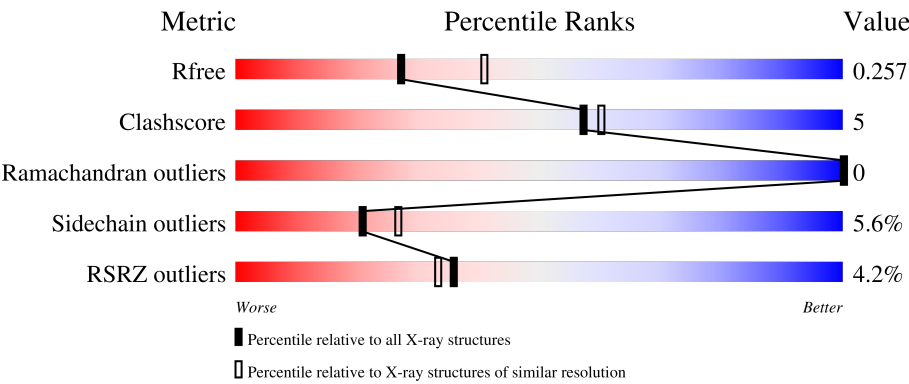
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	338	<div><div>5%</div><div>87%</div><div>10%</div><div>..</div></div>
1	B	338	<div><div>8%</div><div>77%</div><div>19%</div><div>..</div></div>
1	C	338	<div><div>7%</div><div>83%</div><div>14%</div><div>..</div></div>
1	D	338	<div><div>%</div><div>91%</div><div>8%</div><div>..</div></div>
1	E	338	<div><div>2%</div><div>83%</div><div>14%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	338	 <div>90%10%</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15870 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 Glycerol-1-phosphate dehydrogenase [NAD(P)+].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2597	1657	457	477	6			
1	B	329	Total	C	N	O	S	0	0	0
			2534	1620	443	465	6			
1	C	336	Total	C	N	O	S	0	1	0
			2597	1657	457	477	6			
1	D	336	Total	C	N	O	S	0	0	0
			2589	1652	454	477	6			
1	E	334	Total	C	N	O	S	0	0	0
			2571	1642	452	471	6			
1	F	337	Total	C	N	O	S	0	0	0
			2598	1658	456	478	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

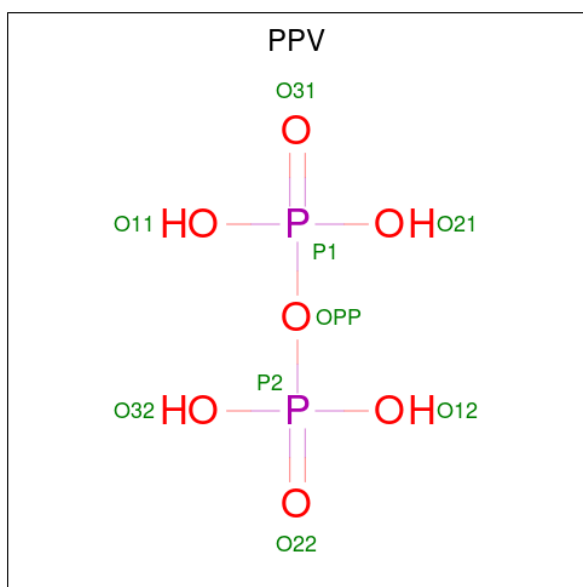
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



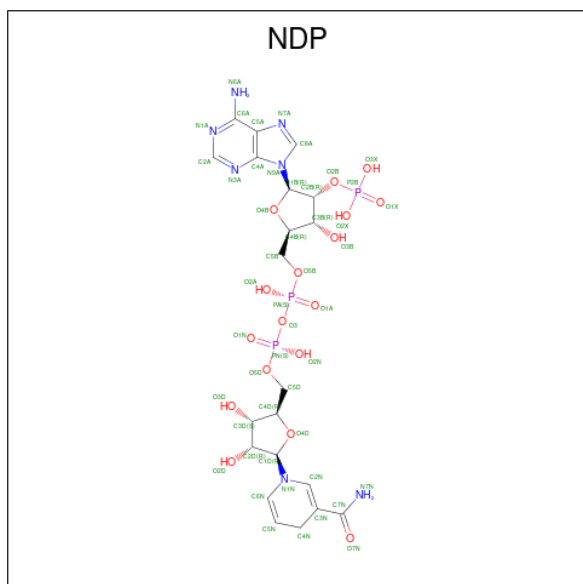
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total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

- Molecule 4 is PYROPHOSPHATE (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

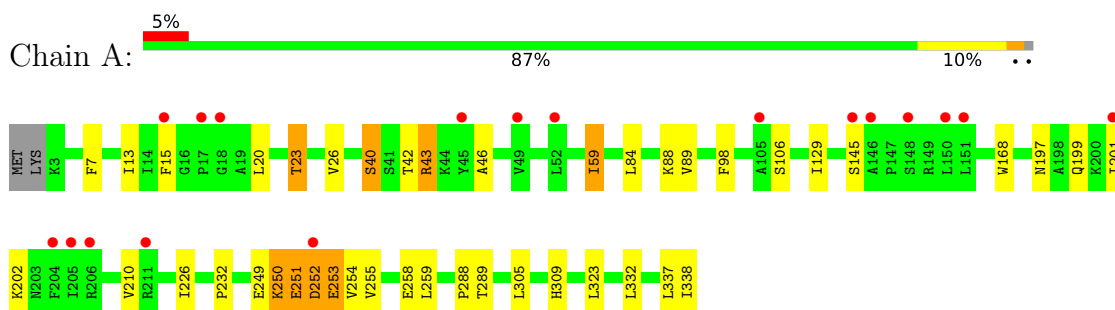
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	13	Total	O	0	0
			13	13		
6	C	19	Total	O	0	0
			19	19		
6	D	34	Total	O	0	0
			34	34		
6	E	29	Total	O	0	0
			29	29		
6	F	53	Total	O	0	0
			53	53		

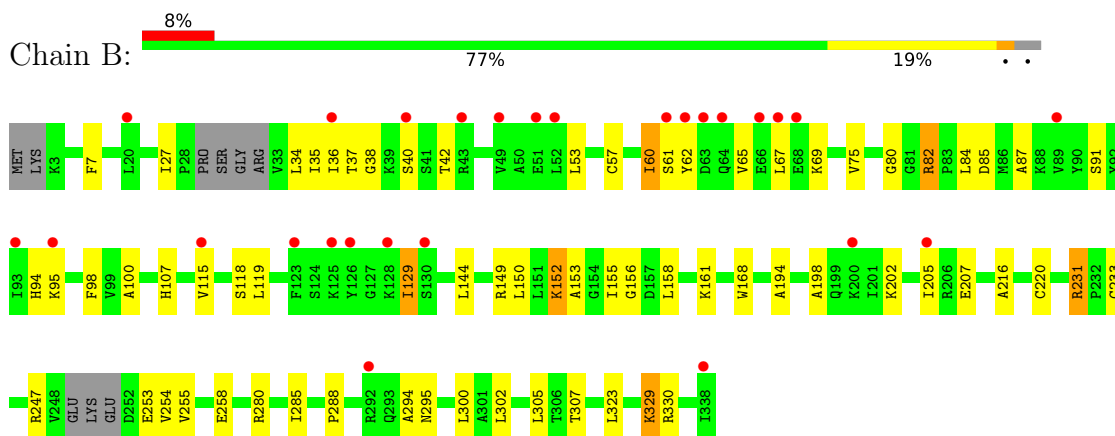
3 Residue-property plots

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.

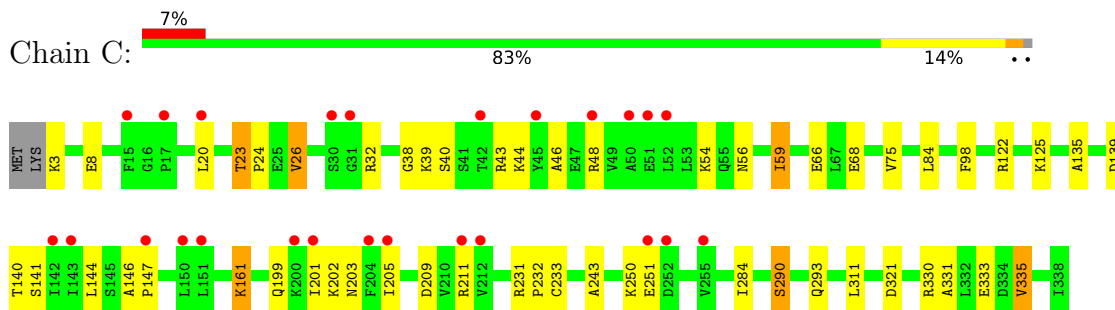
- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



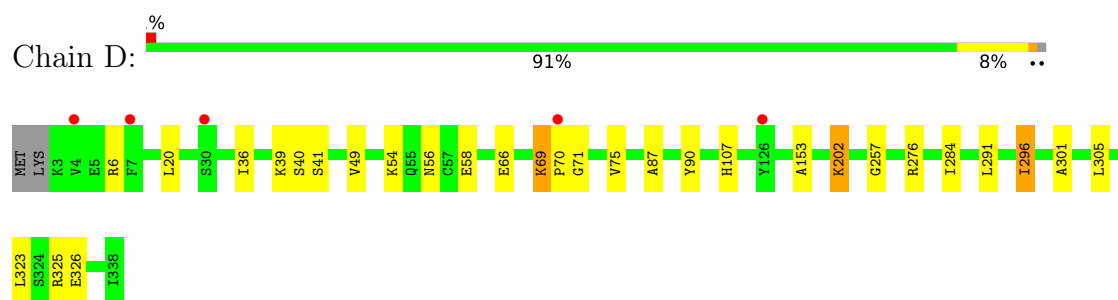
- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



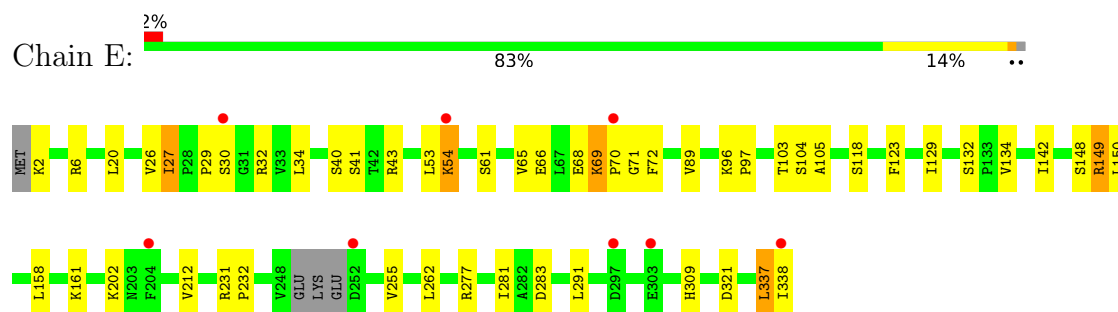
- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



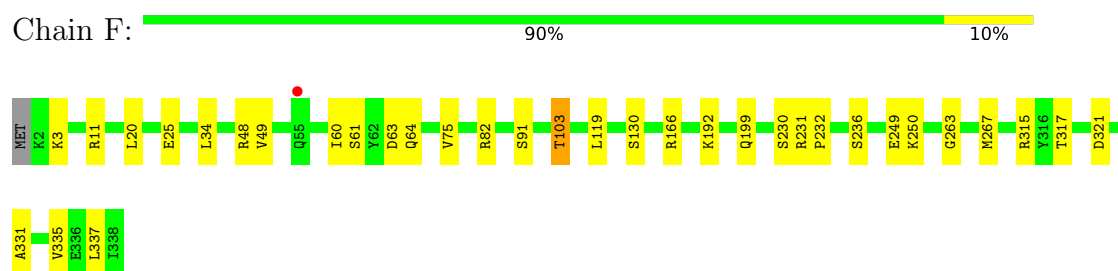
- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



- Molecule 1: Glycerol-1-phosphate dehydrogenase [NAD(P)+]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.18Å 123.33Å 166.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 49.58 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.45) 99.6 (49.58-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.207 , 0.260 0.210 , 0.257	Depositor DCC
R_{free} test set	3854 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtrriage
Anisotropy	0.455	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15870	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7547e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PPV, NDP, SO4, ZN

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	0.42	0/2646	0.59	0/3577
1	B	0.42	0/2577	0.62	0/3483
1	C	0.45	0/2646	0.63	0/3577
1	D	0.48	0/2635	0.66	1/3563 (0.0%)
1	E	0.48	0/2616	0.67	0/3536
1	F	0.53	0/2644	0.68	2/3574 (0.1%)
All	All	0.47	0/15764	0.64	3/21310 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	GLY	N-CA-C	5.80	127.59	113.10
1	F	321	ASP	CB-CG-OD1	5.31	123.08	118.30
1	F	166	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2597	0	2698	24	0
1	B	2534	0	2630	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2597	0	2698	30	0
1	D	2589	0	2685	15	0
1	E	2571	0	2672	37	0
1	F	2598	0	2698	15	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
2	F	1	0	0	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	15	0	0	0	0
4	B	9	0	0	0	0
5	D	48	0	26	1	0
5	E	48	0	26	1	0
5	F	48	0	26	3	0
6	A	17	0	0	0	0
6	B	13	0	0	0	0
6	C	19	0	0	0	0
6	D	34	0	0	1	0
6	E	29	0	0	0	0
6	F	53	0	0	0	0
All	All	15870	0	16159	157	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 (157) 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:331:ALA:O	1:C:335:VAL:HG22	1.49	1.10
1:E:66:GLU:HB2	1:E:69:LYS:HG2	1.34	1.08
1:C:290:SER:HB3	1:C:293:GLN:HG3	1.41	1.03
1:B:152:LYS:HE2	1:B:285:ILE:O	1.58	1.01
1:E:66:GLU:O	1:E:69:LYS:HG3	1.71	0.91
1:B:158:LEU:HD12	1:B:194:ALA:HB2	1.60	0.84
1:C:290:SER:CB	1:C:293:GLN:HG3	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:GLU:O	1:E:69:LYS:CG	2.31	0.78
1:B:27:ILE:HD11	1:B:53:LEU:HD22	1.68	0.76
1:C:331:ALA:O	1:C:335:VAL:CG2	2.31	0.76
1:C:140:THR:O	1:C:144:LEU:HB2	1.87	0.74
1:E:123:PHE:HB2	1:E:129:ILE:HD11	1.69	0.74
1:B:158:LEU:CD1	1:B:194:ALA:HB2	2.19	0.71
1:E:34:LEU:HB2	1:E:72:PHE:CD2	2.25	0.71
1:B:153:ALA:O	1:B:156:GLY:N	2.24	0.71
1:C:144:LEU:O	1:C:144:LEU:HD23	1.91	0.69
1:F:103:THR:HG22	5:F:402:NDP:N7A	2.07	0.69
1:D:296:ILE:HD11	1:D:301:ALA:HB2	1.77	0.67
1:A:250:LYS:O	1:A:253:GLU:HB2	1.94	0.66
1:B:37:THR:HG23	1:B:38:GLY:N	2.09	0.66
1:E:40:SER:OG	1:E:41:SER:N	2.29	0.64
1:B:38:GLY:O	1:B:61:SER:HB3	1.98	0.64
1:E:89:VAL:HG22	1:E:129:ILE:HD13	1.80	0.63
1:F:230:SER:OG	1:F:315:ARG:NH2	2.34	0.61
1:B:168:TRP:CD1	1:B:231:ARG:HG2	2.37	0.60
1:A:249:GLU:OE2	1:A:249:GLU:N	2.30	0.59
1:B:115:VAL:HB	1:B:129:ILE:HD11	1.85	0.59
1:A:254:VAL:HG21	1:A:259:LEU:HD21	1.85	0.59
1:A:40:SER:O	1:A:43:ARG:NE	2.35	0.58
1:B:149:ARG:O	1:B:152:LYS:HB2	2.04	0.57
1:C:20:LEU:O	1:C:23:THR:HG22	2.05	0.57
1:B:85:ASP:HB3	1:B:115:VAL:HG23	1.86	0.56
1:B:152:LYS:CE	1:B:285:ILE:O	2.45	0.55
1:E:26:VAL:HG23	1:E:27:ILE:CD1	2.37	0.54
1:D:296:ILE:CD1	1:D:301:ALA:HB2	2.37	0.54
1:D:291:LEU:HD22	1:D:296:ILE:HD12	1.90	0.54
1:A:168:TRP:CZ3	1:A:232:PRO:HB3	2.43	0.53
1:B:149:ARG:NH1	1:B:258:GLU:OE2	2.42	0.53
1:E:26:VAL:HG23	1:E:27:ILE:HD12	1.91	0.52
1:E:27:ILE:CD1	1:E:27:ILE:N	2.73	0.52
1:F:103:THR:CG2	5:F:402:NDP:N7A	2.72	0.52
1:C:290:SER:HB3	1:C:293:GLN:CG	2.28	0.51
1:C:203:ASN:HB2	1:C:205:ILE:HD12	1.92	0.51
1:E:277:ARG:O	1:E:281:ILE:HG12	2.10	0.51
1:E:291:LEU:HD12	1:E:338:ILE:CG2	2.41	0.51
1:B:60:ILE:HD11	1:B:65:VAL:HA	1.92	0.50
1:E:231:ARG:N	1:E:232:PRO:HD2	2.26	0.50
1:C:26:VAL:HG21	1:C:135:ALA:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:PRO:HG2	1:E:30:SER:H	1.75	0.50
1:B:38:GLY:HA2	1:B:62:TYR:CE2	2.47	0.50
1:C:59:ILE:HG12	1:C:59:ILE:O	2.12	0.50
1:F:34:LEU:HD11	1:F:60:ILE:HD11	1.93	0.50
1:A:250:LYS:HG2	1:A:252:ASP:OD1	2.11	0.50
1:C:161:LYS:HE2	1:C:233:CYS:O	2.11	0.50
1:C:231:ARG:N	1:C:232:PRO:HD2	2.27	0.49
1:C:144:LEU:HD23	1:C:144:LEU:C	2.32	0.49
1:A:89:VAL:HG22	1:A:129:ILE:HD13	1.93	0.49
1:E:71:GLY:C	1:E:72:PHE:CD1	2.85	0.49
1:C:201:ILE:HB	1:C:209:ASP:HB3	1.95	0.49
1:A:199:GLN:HG2	1:D:276:ARG:CZ	2.43	0.49
1:D:75:VAL:HG21	1:D:90:TYR:HD1	1.77	0.49
1:E:72:PHE:O	1:E:96:LYS:HE2	2.13	0.49
1:E:149:ARG:CZ	1:E:255:VAL:HG21	2.43	0.49
1:F:103:THR:HG23	5:F:402:NDP:H61A	1.77	0.49
1:B:247:ARG:HB3	1:B:300:LEU:HD11	1.94	0.48
1:F:75:VAL:HG11	1:F:91:SER:HB2	1.95	0.48
1:E:132:SER:OG	1:F:11:ARG:NH1	2.43	0.48
1:E:158:LEU:HA	1:E:161:LYS:HE2	1.94	0.48
1:A:88:LYS:HG2	1:A:98:PHE:CE2	2.48	0.48
1:E:97:PRO:HB3	1:E:134:VAL:HG21	1.94	0.48
1:A:197:ASN:O	1:A:201:ILE:HG12	2.14	0.48
1:E:26:VAL:C	1:E:27:ILE:HD12	2.34	0.47
1:A:46:ALA:CB	1:A:59:ILE:HD12	2.44	0.47
1:C:26:VAL:HG21	1:C:135:ALA:HB1	1.97	0.47
1:B:247:ARG:HH12	1:B:307:THR:HG21	1.80	0.47
1:C:46:ALA:HB1	1:C:59:ILE:HD12	1.97	0.47
1:C:75:VAL:O	1:C:98:PHE:HA	2.14	0.47
1:E:72:PHE:CD1	1:E:72:PHE:N	2.82	0.47
1:D:202:LYS:HD3	1:D:284:ILE:O	2.15	0.47
1:B:35:ILE:HD12	1:B:57:CYS:HB3	1.97	0.46
1:E:68:GLU:O	1:E:70:PRO:HD3	2.15	0.46
1:F:335:VAL:HG23	1:F:337:LEU:HD13	1.96	0.46
1:D:20:LEU:HD11	1:D:49:VAL:CG2	2.46	0.46
1:D:153:ALA:O	1:D:257:GLY:HA3	2.15	0.46
1:D:36:ILE:HD12	1:D:87:ALA:HA	1.96	0.46
1:A:20:LEU:O	1:A:23:THR:CG2	2.64	0.46
1:B:220:CYS:HB3	1:B:233:CYS:SG	2.56	0.46
1:C:199:GLN:HG3	1:C:284:ILE:HG21	1.98	0.46
1:F:236:SER:HB3	1:F:317:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:HD3	1:B:119:LEU:HD11	1.98	0.46
1:D:296:ILE:C	1:D:296:ILE:HD13	2.36	0.46
1:B:155:ILE:O	1:B:158:LEU:HB2	2.17	0.45
1:B:288:PRO:CB	1:B:294:ALA:HB2	2.46	0.45
1:E:309:HIS:CE1	1:E:321:ASP:O	2.68	0.45
1:A:332:LEU:HB3	1:A:338:ILE:HG12	1.98	0.45
1:B:80:GLY:O	1:B:84:LEU:HD13	2.15	0.45
1:B:302:LEU:HD21	1:B:329:LYS:HG2	1.99	0.45
1:D:40:SER:OG	1:D:41:SER:N	2.49	0.45
1:C:38:GLY:O	1:C:39:LYS:HD2	2.16	0.45
1:F:263:GLY:O	1:F:267:MET:HG2	2.17	0.45
1:B:158:LEU:O	1:B:161:LYS:HG2	2.17	0.44
1:C:144:LEU:C	1:C:144:LEU:CD2	2.85	0.44
1:E:123:PHE:HB2	1:E:129:ILE:CD1	2.42	0.44
1:F:331:ALA:O	1:F:335:VAL:HG22	2.18	0.44
1:D:325:ARG:NH1	6:D:1102:HOH:O	2.50	0.44
1:F:61:SER:OG	1:F:63:ASP:OD1	2.27	0.44
1:C:39:LYS:HA	1:C:40:SER:HA	1.80	0.44
1:A:46:ALA:HB3	1:A:59:ILE:HD12	1.99	0.43
1:B:305:LEU:HB3	1:B:323:LEU:HD23	1.99	0.43
1:C:23:THR:N	1:C:24:PRO:CD	2.81	0.43
1:A:13:ILE:HD12	1:B:7:PHE:CE2	2.53	0.43
1:A:20:LEU:O	1:A:23:THR:HG23	2.18	0.43
1:A:84:LEU:O	1:A:88:LYS:HG3	2.18	0.43
1:A:251:GLU:O	1:A:254:VAL:O	2.35	0.43
1:C:59:ILE:O	1:C:59:ILE:CG1	2.65	0.43
1:E:66:GLU:HB2	1:E:69:LYS:CG	2.23	0.43
1:A:305:LEU:HB3	1:A:323:LEU:HD23	2.00	0.43
1:B:37:THR:HG23	1:B:38:GLY:O	2.19	0.42
1:B:82:ARG:CD	1:B:119:LEU:HD11	2.49	0.42
1:C:161:LYS:N	1:C:161:LYS:HD2	2.34	0.42
1:A:289:THR:O	1:A:337:LEU:HD23	2.18	0.42
1:B:34:LEU:HD11	1:B:60:ILE:HG23	2.00	0.42
1:B:40:SER:HB3	1:B:42:THR:HG22	2.00	0.42
1:B:61:SER:O	1:B:65:VAL:HG23	2.20	0.42
1:E:262:LEU:HD22	1:E:337:LEU:HD21	2.01	0.42
1:E:6:ARG:NH1	1:F:25:GLU:OE1	2.52	0.42
1:A:309:HIS:H	1:A:309:HIS:CD2	2.36	0.42
1:B:198:ALA:O	1:B:202:LYS:HB2	2.20	0.42
1:B:288:PRO:HB2	1:B:294:ALA:HB2	2.01	0.42
1:E:26:VAL:CG2	1:E:27:ILE:CD1	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:CE2	1:A:226:ILE:HG12	2.55	0.41
1:E:61:SER:O	1:E:65:VAL:HG23	2.20	0.41
1:B:98:PHE:CZ	1:B:100:ALA:HB2	2.55	0.41
1:A:250:LYS:CB	1:A:253:GLU:OE1	2.69	0.41
1:A:258:GLU:HG2	1:A:288:PRO:HD2	2.03	0.41
1:C:211[A]:ARG:HE	1:C:211[A]:ARG:HB2	1.68	0.41
1:B:34:LEU:CD1	1:B:60:ILE:HG23	2.50	0.41
1:E:150:LEU:HD11	5:E:1001:NDP:H51A	2.03	0.41
1:D:305:LEU:HB3	1:D:323:LEU:HD23	2.02	0.41
1:E:53:LEU:O	1:E:54:LYS:C	2.59	0.41
1:B:158:LEU:HD11	1:B:216:ALA:CB	2.51	0.41
1:F:231:ARG:N	1:F:232:PRO:HD2	2.36	0.41
1:B:91:SER:O	1:B:94:HIS:O	2.38	0.41
1:D:107:HIS:CE1	5:D:1001:NDP:C2N	3.04	0.41
1:E:69:LYS:HA	1:E:70:PRO:HD2	1.76	0.41
1:F:20:LEU:HD11	1:F:49:VAL:CG2	2.51	0.41
1:B:36:ILE:HD12	1:B:87:ALA:HA	2.03	0.41
1:C:243:ALA:HB2	1:C:311:LEU:HD11	2.02	0.41
1:E:43:ARG:HE	1:E:43:ARG:HB2	1.78	0.41
1:B:150:LEU:HD23	1:B:255:VAL:HG13	2.03	0.40
1:D:69:LYS:HG3	1:D:70:PRO:N	2.35	0.40
1:E:20:LEU:HD22	1:E:142:ILE:CD1	2.50	0.40
1:E:103:THR:HG23	1:E:142:ILE:CG2	2.51	0.40
1:E:104:SER:OG	1:E:105:ALA:N	2.54	0.40
1:C:139:ASP:OD1	1:C:141:SER:OG	2.39	0.40
1:C:330:ARG:NH2	1:C:333:GLU:OE1	2.54	0.40
1:C:146:ALA:O	1:C:147:PRO:C	2.59	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	335/338 (99%)	325 (97%)	10 (3%)	0	100	100
1	B	323/338 (96%)	311 (96%)	12 (4%)	0	100	100
1	C	335/338 (99%)	322 (96%)	13 (4%)	0	100	100
1	D	334/338 (99%)	324 (97%)	10 (3%)	0	100	100
1	E	330/338 (98%)	319 (97%)	11 (3%)	0	100	100
1	F	335/338 (99%)	328 (98%)	7 (2%)	0	100	100
All	All	1992/2028 (98%)	1929 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	278/279 (100%)	262 (94%)	16 (6%)	20	25
1	B	271/279 (97%)	251 (93%)	20 (7%)	13	16
1	C	278/279 (100%)	255 (92%)	23 (8%)	11	12
1	D	277/279 (99%)	267 (96%)	10 (4%)	35	46
1	E	275/279 (99%)	263 (96%)	12 (4%)	28	37
1	F	278/279 (100%)	267 (96%)	11 (4%)	31	41
All	All	1657/1674 (99%)	1565 (94%)	92 (6%)	21	27

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	23	THR
1	A	26	VAL
1	A	40	SER
1	A	42	THR
1	A	43	ARG
1	A	59	ILE

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Mol	Chain	Res	Type
1	A	106	SER
1	A	145	SER
1	A	202	LYS
1	A	210	VAL
1	A	250	LYS
1	A	251	GLU
1	A	252	ASP
1	A	253	GLU
1	A	255	VAL
1	B	60	ILE
1	B	67	LEU
1	B	69	LYS
1	B	75	VAL
1	B	82	ARG
1	B	95	LYS
1	B	107	HIS
1	B	118	SER
1	B	129	ILE
1	B	144	LEU
1	B	152	LYS
1	B	205	ILE
1	B	207	GLU
1	B	231	ARG
1	B	253	GLU
1	B	254	VAL
1	B	280	ARG
1	B	295	ASN
1	B	329	LYS
1	B	330	ARG
1	C	3	LYS
1	C	8	GLU
1	C	23	THR
1	C	26	VAL
1	C	32	ARG
1	C	43	ARG
1	C	44	LYS
1	C	48	ARG
1	C	54	LYS
1	C	56	ASN
1	C	59	ILE
1	C	66	GLU
1	C	68	GLU

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Mol	Chain	Res	Type
1	C	84	LEU
1	C	122	ARG
1	C	125	LYS
1	C	161	LYS
1	C	202	LYS
1	C	250	LYS
1	C	251	GLU
1	C	290	SER
1	C	321	ASP
1	C	335	VAL
1	D	6	ARG
1	D	39	LYS
1	D	54	LYS
1	D	56	ASN
1	D	58	GLU
1	D	66	GLU
1	D	69	LYS
1	D	202	LYS
1	D	296	ILE
1	D	326	GLU
1	E	2	LYS
1	E	27	ILE
1	E	32	ARG
1	E	54	LYS
1	E	69	LYS
1	E	118	SER
1	E	148	SER
1	E	149	ARG
1	E	202	LYS
1	E	212	VAL
1	E	283	ASP
1	E	337	LEU
1	F	3	LYS
1	F	48	ARG
1	F	64	GLN
1	F	82	ARG
1	F	103	THR
1	F	119	LEU
1	F	130	SER
1	F	192	LYS
1	F	199	GLN
1	F	249	GLU

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Mol	Chain	Res	Type
1	F	250	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	309	HIS
1	B	55	GLN
1	B	64	GLN
1	C	309	HIS
1	E	242	HIS
1	F	197	ASN
1	F	293	GLN
1	F	309	HIS

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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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
3	SO4	B	2002	-	4,4,4	0.33	0	6,6,6	0.23	0
3	SO4	C	2003	-	4,4,4	0.42	0	6,6,6	0.21	0
3	SO4	F	404	-	4,4,4	0.37	0	6,6,6	0.31	0
4	PPV	B	2004	-	6,8,8	0.64	0	13,13,13	1.11	2 (15%)
3	SO4	B	2003	-	4,4,4	0.35	0	6,6,6	0.09	0
5	NDP	D	1001	-	45,52,52	1.00	4 (8%)	53,80,80	1.10	3 (5%)
3	SO4	F	401	-	4,4,4	0.41	0	6,6,6	0.20	0
5	NDP	E	1001	-	45,52,52	0.97	2 (4%)	53,80,80	1.36	8 (15%)
3	SO4	A	2004	-	4,4,4	0.32	0	6,6,6	0.25	0
3	SO4	C	2002	-	4,4,4	0.33	0	6,6,6	0.37	0
3	SO4	A	2003	-	4,4,4	0.35	0	6,6,6	0.34	0
3	SO4	D	1003	-	4,4,4	0.32	0	6,6,6	0.23	0
3	SO4	F	405	-	4,4,4	0.37	0	6,6,6	0.39	0
5	NDP	F	402	-	45,52,52	1.09	2 (4%)	53,80,80	1.26	6 (11%)
3	SO4	E	1003	-	4,4,4	0.39	0	6,6,6	0.23	0
3	SO4	A	2002	-	4,4,4	0.36	0	6,6,6	0.36	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
4	PPV	B	2004	-	-	0/6/6/6	-
5	NDP	F	402	-	-	7/30/77/77	0/5/5/5
5	NDP	D	1001	-	-	5/30/77/77	0/5/5/5
5	NDP	E	1001	-	-	7/30/77/77	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	NDP	C6N-C5N	3.17	1.39	1.33
5	E	1001	NDP	C6N-C5N	3.03	1.38	1.33
5	D	1001	NDP	C6N-C5N	2.75	1.38	1.33
5	F	402	NDP	C5A-C4A	2.63	1.47	1.40
5	E	1001	NDP	C5A-C4A	2.58	1.47	1.40
5	D	1001	NDP	C2A-N3A	2.48	1.36	1.32
5	D	1001	NDP	C5A-C4A	2.37	1.47	1.40
5	D	1001	NDP	O4B-C1B	2.20	1.44	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1001	NDP	N3A-C2A-N1A	-3.72	122.86	128.68
5	E	1001	NDP	PN-O3-PA	-3.52	120.76	132.83
5	F	402	NDP	N3A-C2A-N1A	-3.44	123.30	128.68
5	E	1001	NDP	C4A-C5A-N7A	-3.34	105.92	109.40
5	D	1001	NDP	N3A-C2A-N1A	-3.25	123.60	128.68
5	F	402	NDP	C3N-C7N-N7N	2.86	122.75	117.67
5	E	1001	NDP	C3N-C7N-N7N	2.69	122.45	117.67
5	F	402	NDP	O4B-C1B-C2B	-2.67	101.96	106.59
5	E	1001	NDP	C1B-N9A-C4A	-2.62	122.03	126.64
5	F	402	NDP	C1D-N1N-C2N	-2.58	116.81	121.11
5	D	1001	NDP	C4A-C5A-N7A	-2.55	106.75	109.40
4	B	2004	PPV	O21-P1-O11	2.41	116.86	107.64
5	F	402	NDP	PN-O3-PA	-2.40	124.60	132.83
5	F	402	NDP	C4A-C5A-N7A	-2.39	106.90	109.40
5	E	1001	NDP	C2A-N1A-C6A	2.31	122.70	118.75
5	D	1001	NDP	O2B-P2B-O1X	-2.30	100.53	109.39
5	E	1001	NDP	C1D-N1N-C2N	-2.28	117.31	121.11
4	B	2004	PPV	P2-OPP-P1	-2.06	125.76	132.83
5	E	1001	NDP	C5A-C6A-N6A	2.06	123.47	120.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

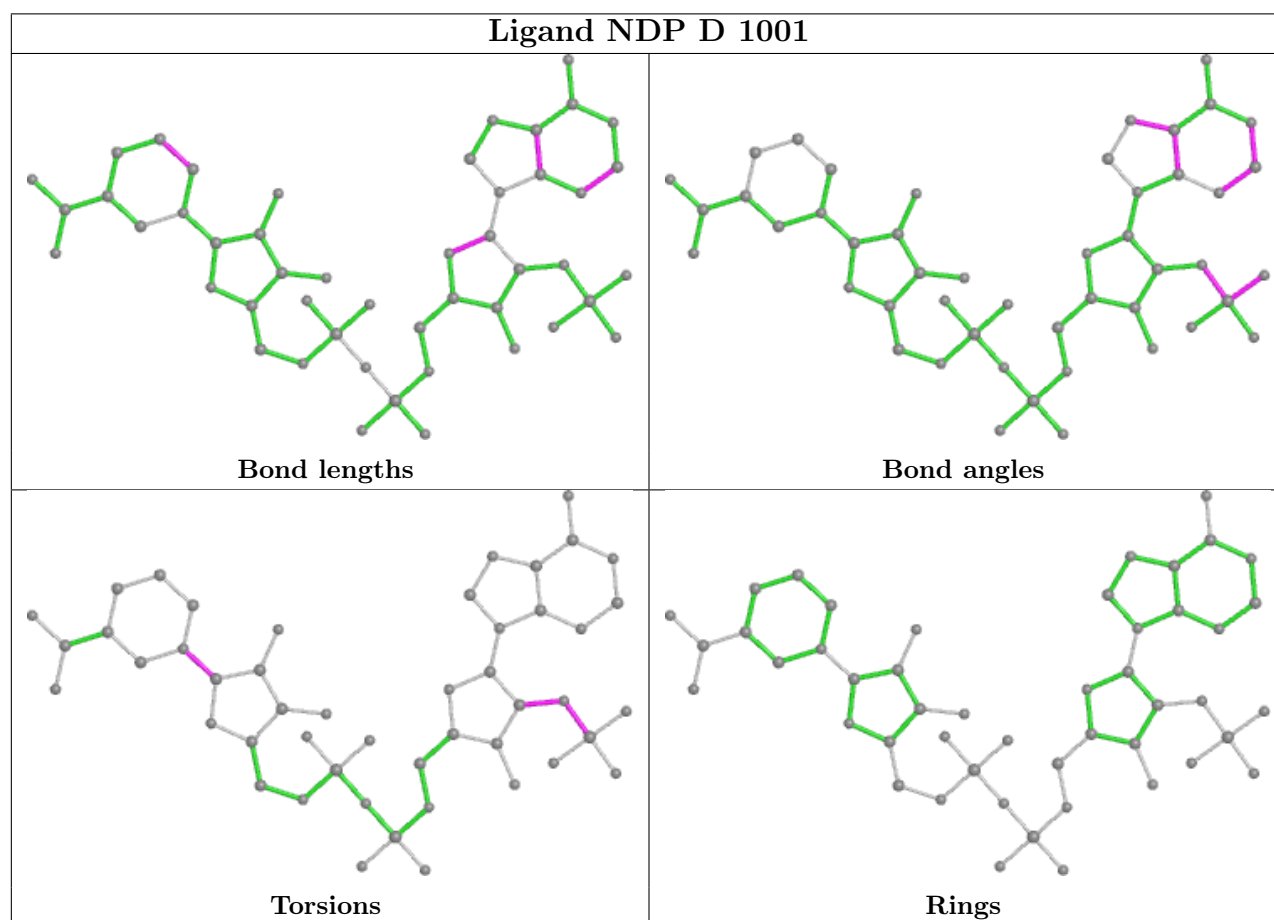
Mol	Chain	Res	Type	Atoms
5	D	1001	NDP	C3B-C2B-O2B-P2B
5	E	1001	NDP	C3B-C2B-O2B-P2B
5	F	402	NDP	C3B-C2B-O2B-P2B
5	D	1001	NDP	C1B-C2B-O2B-P2B
5	E	1001	NDP	C3D-C4D-C5D-O5D
5	F	402	NDP	C2D-C1D-N1N-C2N
5	F	402	NDP	O4D-C1D-N1N-C2N
5	E	1001	NDP	C2D-C1D-N1N-C2N
5	E	1001	NDP	O4D-C1D-N1N-C2N
5	D	1001	NDP	O4D-C1D-N1N-C2N
5	F	402	NDP	C1B-C2B-O2B-P2B
5	E	1001	NDP	C2D-C1D-N1N-C6N
5	F	402	NDP	C2D-C1D-N1N-C6N
5	E	1001	NDP	O4D-C1D-N1N-C6N
5	F	402	NDP	O4D-C1D-N1N-C6N
5	D	1001	NDP	C2B-O2B-P2B-O2X
5	E	1001	NDP	C2B-O2B-P2B-O3X
5	F	402	NDP	C2B-O2B-P2B-O2X
5	D	1001	NDP	C2D-C1D-N1N-C2N

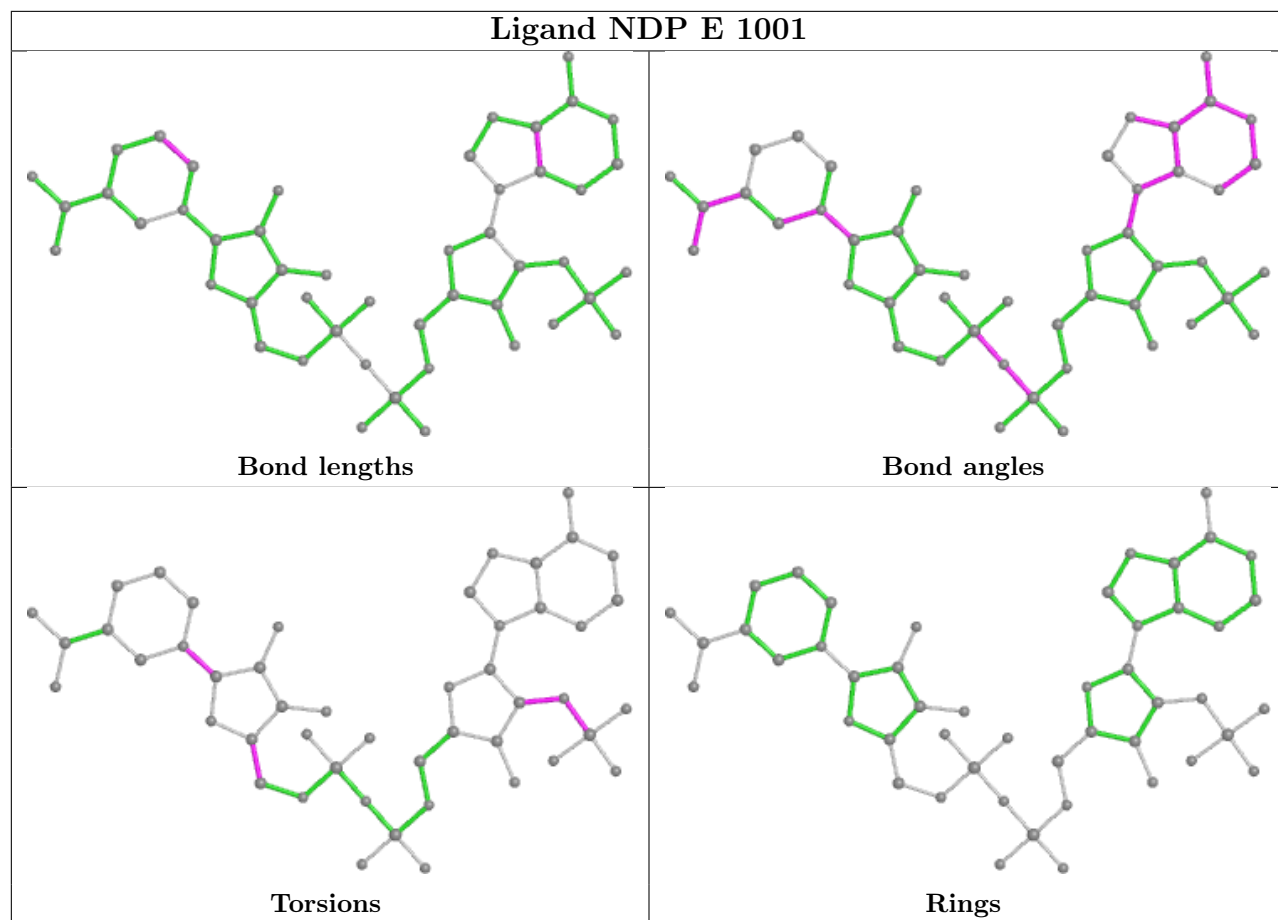
There are no ring outliers.

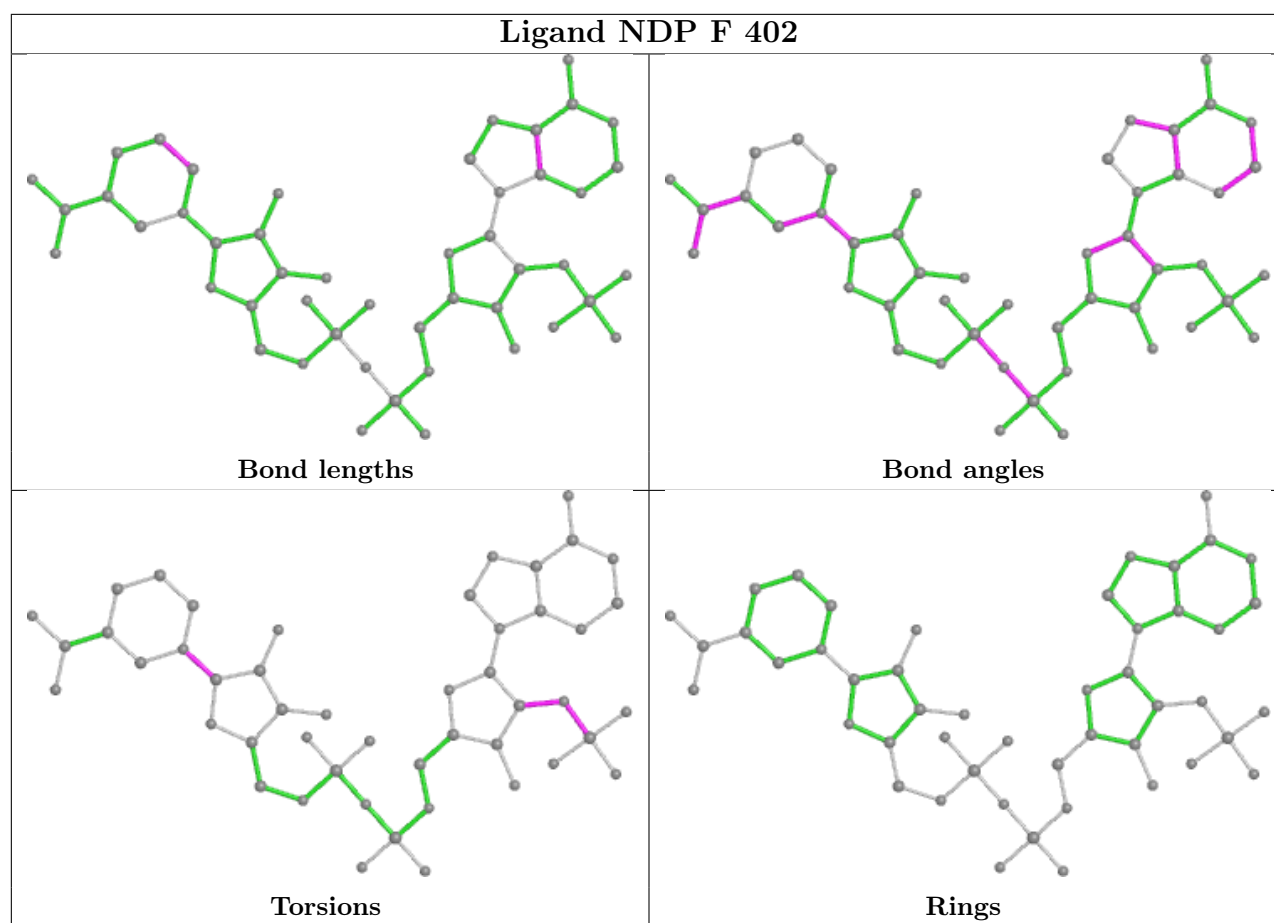
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	NDP	1	0
5	E	1001	NDP	1	0
5	F	402	NDP	3	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	336/338 (99%)	0.12	18 (5%) 25 23	42, 60, 99, 126	0
1	B	329/338 (97%)	0.43	27 (8%) 11 8	39, 76, 120, 138	0
1	C	336/338 (99%)	0.34	25 (7%) 14 11	35, 66, 110, 129	0
1	D	336/338 (99%)	-0.15	5 (1%) 73 71	32, 48, 85, 103	0
1	E	334/338 (98%)	0.10	8 (2%) 59 54	41, 62, 94, 115	0
1	F	337/338 (99%)	-0.25	1 (0%) 94 94	30, 44, 69, 99	0
All	All	2008/2028 (99%)	0.10	84 (4%) 36 33	30, 58, 103, 138	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	ASP	8.0
1	A	205	ILE	6.8
1	C	204	PHE	5.6
1	C	50	ALA	5.5
1	B	52	LEU	5.4
1	E	252	ASP	5.4
1	A	204	PHE	5.1
1	B	62	TYR	4.7
1	C	201	ILE	4.6
1	A	148	SER	4.3
1	B	51	GLU	4.2
1	B	67	LEU	4.2
1	C	151	LEU	4.2
1	D	70	PRO	4.2
1	E	70	PRO	4.2
1	C	30	SER	3.9
1	C	150	LEU	3.8
1	A	252	ASP	3.7
1	A	17	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	128	LYS	3.6
1	B	130	SER	3.6
1	B	205	ILE	3.5
1	A	52	LEU	3.5
1	C	15	PHE	3.5
1	B	64	GLN	3.5
1	E	54	LYS	3.4
1	D	30	SER	3.3
1	B	89	VAL	3.3
1	C	52	LEU	3.2
1	C	17	PRO	3.2
1	B	126	TYR	3.2
1	C	45	TYR	3.1
1	C	251	GLU	3.1
1	C	211[A]	ARG	3.0
1	A	49	VAL	3.0
1	B	115	VAL	3.0
1	A	206	ARG	3.0
1	B	123	PHE	3.0
1	B	338	ILE	3.0
1	B	43	ARG	3.0
1	B	93	ILE	2.9
1	A	201	ILE	2.8
1	C	42	THR	2.8
1	A	45	TYR	2.8
1	C	205	ILE	2.8
1	B	68	GLU	2.8
1	A	105	ALA	2.7
1	B	36	ILE	2.7
1	B	61	SER	2.7
1	C	255	VAL	2.7
1	A	15	PHE	2.7
1	B	292	ARG	2.6
1	A	211[A]	ARG	2.6
1	E	297	ASP	2.5
1	B	125	LYS	2.5
1	B	20	LEU	2.5
1	C	143	ILE	2.5
1	A	18	GLY	2.5
1	C	142	ILE	2.5
1	C	200	LYS	2.5
1	C	31	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	LEU	2.4
1	E	30	SER	2.4
1	C	20	LEU	2.4
1	A	146	ALA	2.4
1	B	66	GLU	2.4
1	B	200	LYS	2.4
1	C	212	VAL	2.3
1	B	95	LYS	2.3
1	B	40	SER	2.3
1	C	48	ARG	2.3
1	A	145	SER	2.3
1	B	49	VAL	2.2
1	E	303	GLU	2.2
1	D	126	TYR	2.1
1	E	338	ILE	2.1
1	E	204	PHE	2.1
1	C	147	PRO	2.1
1	D	4	VAL	2.1
1	B	63	ASP	2.1
1	A	151	LEU	2.0
1	F	55	GLN	2.0
1	D	7	PHE	2.0
1	C	51	GLU	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.

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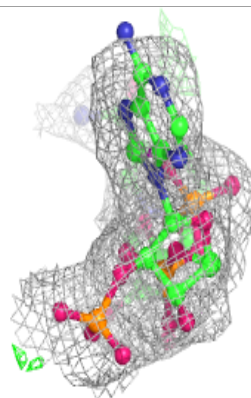
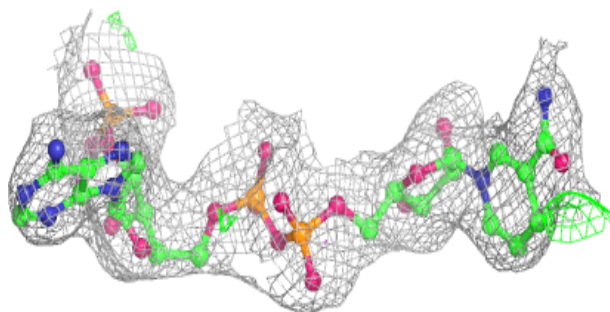
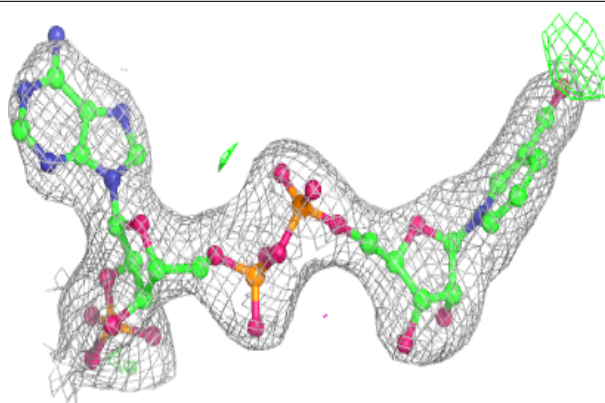
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	2003	5/5	0.82	0.21	120,121,127,128	0
4	PPV	B	2004	9/9	0.85	0.14	80,92,99,105	0
3	SO4	F	401	5/5	0.86	0.17	85,87,94,96	0
3	SO4	A	2003	5/5	0.87	0.21	86,93,101,102	0
3	SO4	C	2003	5/5	0.89	0.13	85,88,100,102	0
3	SO4	E	1003	5/5	0.90	0.14	79,85,92,96	0
3	SO4	A	2004	5/5	0.91	0.26	111,115,123,124	0
3	SO4	F	404	5/5	0.92	0.10	77,83,88,89	0
2	ZN	C	2001	1/1	0.95	0.08	96,96,96,96	0
5	NDP	E	1001	48/48	0.95	0.12	52,66,88,93	0
3	SO4	B	2002	5/5	0.96	0.11	65,66,72,72	0
5	NDP	D	1001	48/48	0.96	0.12	44,52,58,63	0
2	ZN	B	2001	1/1	0.96	0.17	77,77,77,77	0
5	NDP	F	402	48/48	0.97	0.11	35,38,43,46	0
2	ZN	A	2001	1/1	0.98	0.06	82,82,82,82	0
2	ZN	F	403	1/1	0.99	0.14	40,40,40,40	0
3	SO4	A	2002	5/5	0.99	0.08	50,54,59,60	0
3	SO4	F	405	5/5	0.99	0.07	59,62,66,68	0
3	SO4	C	2002	5/5	0.99	0.10	55,59,59,61	0
2	ZN	D	1002	1/1	0.99	0.13	47,47,47,47	0
3	SO4	D	1003	5/5	0.99	0.13	62,63,66,68	0
2	ZN	E	1002	1/1	0.99	0.12	57,57,57,57	0

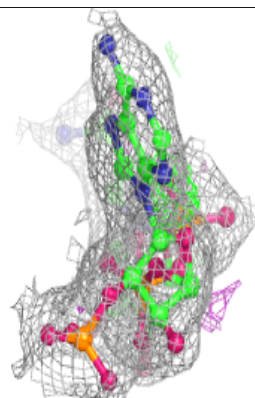
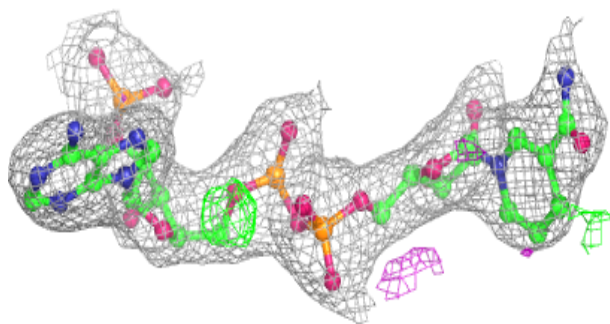
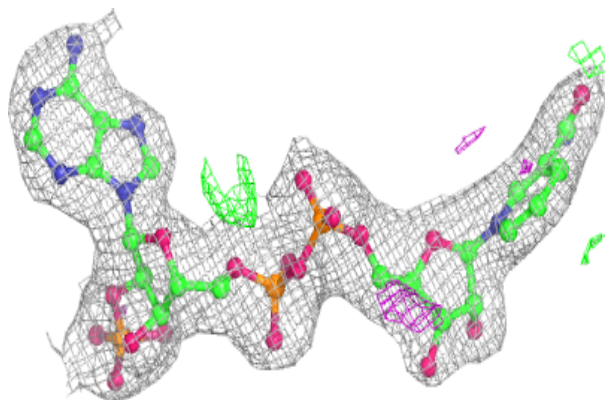
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

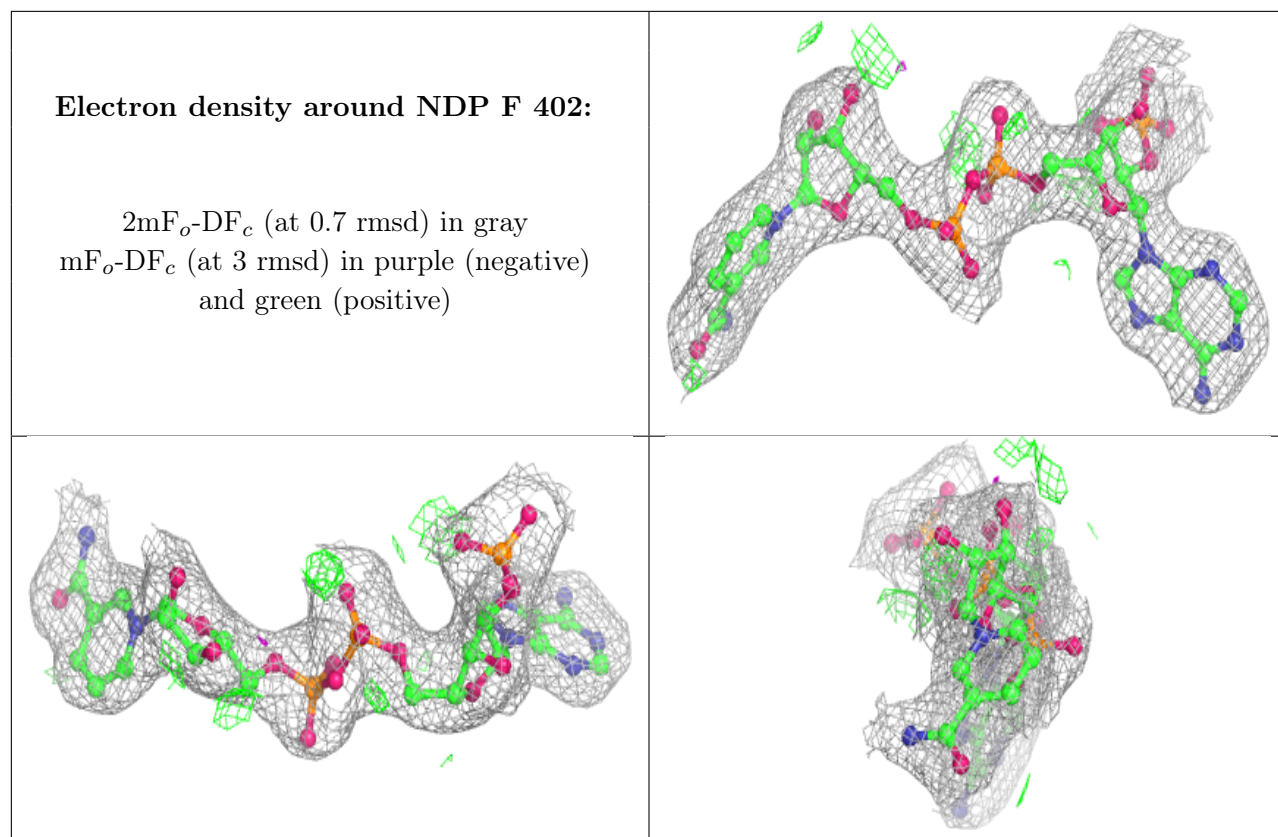
Electron density around NDP E 1001:

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

**Electron density around NDP D 1001:**

$2mF_o-DF_c$ (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.