Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 11:36 PM EDT

PDB ID	:	2PAF
Title	:	Crystal Structure of the Lactose Repressor bound to anti-inducer ONPF in induced state
Authors	:	Daber, R.
Deposited on	:	2007-03-27
Resolution	:	3.50 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:

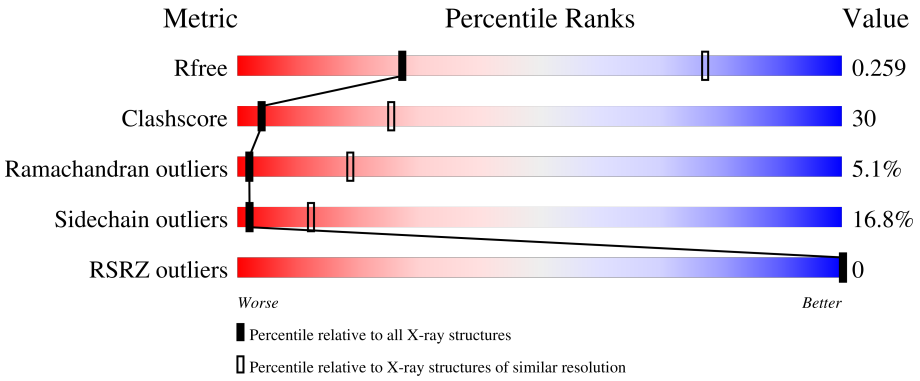
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	269	46% 39% 14% .
1	B	269	46% 44% 9% .

2 Entry composition

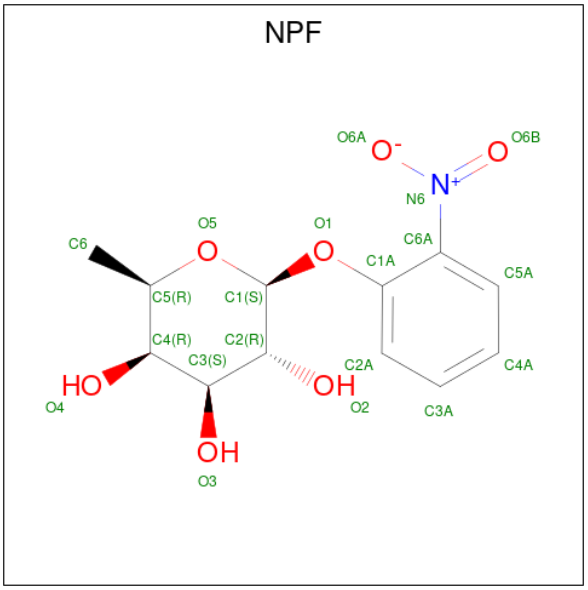
There are 2 unique types of molecules in this entry. The entry contains 4068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactose operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2014	1260	356	388	10			
1	B	269	Total	C	N	O	S	0	0	0
			2014	1260	356	388	10			

- Molecule 2 is 2-nitrophenyl beta-D-fucopyranoside (three-letter code: NPF) (formula: $C_{12}H_{15}NO_7$).



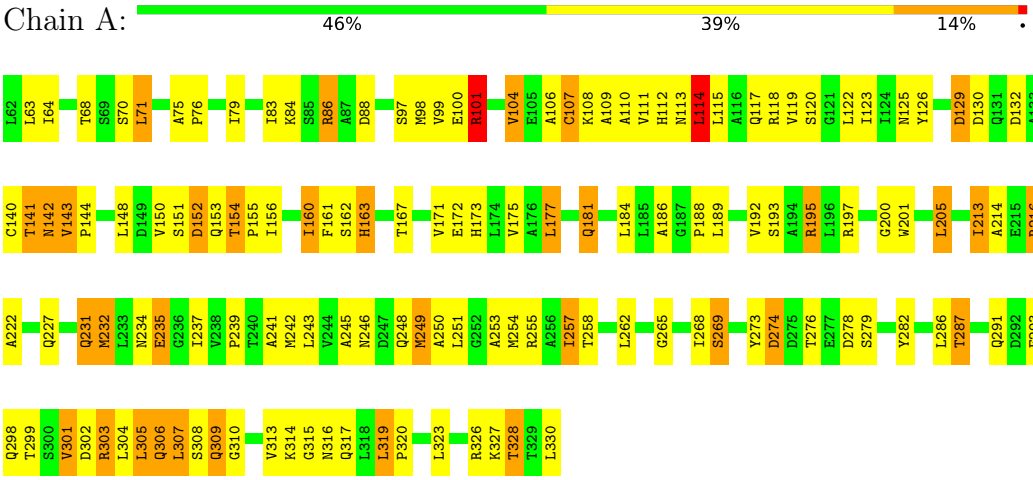
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	12	1	7		
2	B	1	Total	C	N	O	0	0
			20	12	1	7		

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.

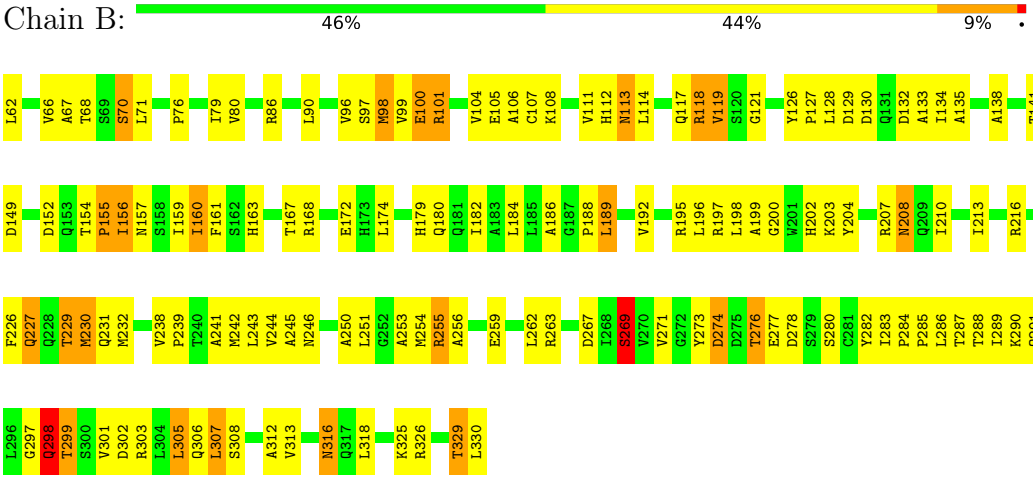
• Molecule 1: Lactose operon repressor

Chain A:



• Molecule 1: Lactose operon repressor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.54Å 77.54Å 212.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 3.50 19.81 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.81-3.50) 99.1 (19.81-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	5.13 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.265 0.190 , 0.259	Depositor DCC
R_{free} test set	413 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4068	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.99% 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: NPF

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	0.87	2/2041 (0.1%)	0.91	1/2773 (0.0%)
1	B	0.83	2/2041 (0.1%)	0.89	0/2773
All	All	0.85	4/4082 (0.1%)	0.90	1/5546 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	SER	CB-OG	6.84	1.51	1.42
1	B	280	SER	CB-OG	6.12	1.50	1.42
1	A	327	LYS	CE-NZ	5.69	1.63	1.49
1	A	235	GLU	CG-CD	5.31	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	LEU	CA-CB-CG	5.12	127.06	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ALA	Peptide
1	A	113	ASN	Peptide
1	B	278	ASP	Peptide

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	2014	0	2058	128	0
1	B	2014	0	2058	123	0
2	A	20	0	0	2	0
2	B	20	0	0	3	0
All	All	4068	0	4116	247	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 30.

All (247) 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:A:99:VAL:HG11	1:A:126:TYR:CE1	1.58	1.37
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.06	1.19
1:B:298:GLN:HG3	1:B:299:THR:N	1.57	1.07
1:A:99:VAL:CG1	1:A:126:TYR:CE1	2.38	1.06
1:A:86:ARG:HB3	1:A:301:VAL:HG11	1.38	1.04
1:B:312:ALA:HB1	1:B:313:VAL:HA	1.40	1.00
1:A:195:ARG:HH21	1:A:195:ARG:HG3	1.33	0.92
1:B:168:ARG:HG2	1:B:172:GLU:HG3	1.51	0.92
1:A:99:VAL:HG11	1:A:126:TYR:CD1	2.06	0.90
1:A:245:ALA:HB3	1:A:249:MET:HE1	1.54	0.89
1:B:216:ARG:HH12	1:B:231:GLN:HE21	0.92	0.89
1:A:216:ARG:HG2	1:A:216:ARG:NH1	1.84	0.87
1:B:216:ARG:NH1	1:B:231:GLN:HE21	1.75	0.84
1:B:216:ARG:HH12	1:B:231:GLN:NE2	1.75	0.84
1:A:144:PRO:HB3	1:A:307:LEU:HD12	1.61	0.83
1:A:255:ARG:HH21	1:B:285:PRO:HG2	1.46	0.81
1:A:110:ALA:O	1:A:111:VAL:HB	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:HIS:HB3	1:B:182:ILE:HD11	1.64	0.79
1:A:99:VAL:HG12	1:A:100:GLU:O	1.82	0.78
1:B:213:ILE:HD11	1:B:239:PRO:HB3	1.65	0.78
1:A:99:VAL:CG1	1:A:126:TYR:HE1	1.98	0.74
1:B:70:SER:CB	1:B:101:ARG:HH22	2.01	0.74
1:A:110:ALA:C	1:A:112:HIS:H	1.91	0.73
1:B:298:GLN:CG	1:B:299:THR:N	2.44	0.72
1:A:110:ALA:C	1:A:112:HIS:N	2.40	0.72
1:B:229:THR:HG21	1:B:253:ALA:HA	1.72	0.72
1:A:195:ARG:HG3	1:A:195:ARG:NH2	1.98	0.72
1:B:168:ARG:HG2	1:B:172:GLU:CG	2.19	0.72
1:B:188:PRO:HG3	1:B:219:ASP:HA	1.70	0.71
1:A:245:ALA:HB3	1:A:249:MET:CE	2.19	0.71
1:A:152:ASP:HB3	1:A:160:ILE:HD11	1.73	0.70
1:B:298:GLN:HG3	1:B:299:THR:H	1.55	0.69
1:B:100:GLU:HG3	1:B:101:ARG:H	1.57	0.69
1:A:241:ALA:HA	1:A:269:SER:O	1.92	0.69
1:B:263:ARG:O	1:B:267:ASP:HB2	1.93	0.69
1:A:245:ALA:O	1:A:273:TYR:HB3	1.93	0.68
1:A:140:CYS:O	1:A:141:THR:O	2.11	0.68
1:A:257:ILE:HG23	1:A:268:ILE:HD12	1.76	0.68
1:A:79:ILE:O	1:A:83:ILE:HG12	1.95	0.67
1:A:286:LEU:HA	1:A:328:THR:OG1	1.95	0.67
1:B:197:ARG:NH2	2:B:901:NPF:C2A	2.58	0.66
1:B:70:SER:HB2	1:B:101:ARG:HH22	1.59	0.66
1:A:144:PRO:HG2	1:A:308:SER:HB2	1.78	0.66
1:B:141:THR:O	1:B:141:THR:HG22	1.96	0.66
1:B:229:THR:CG2	1:B:256:ALA:HB3	2.26	0.65
1:A:141:THR:O	1:A:142:ASN:HB2	1.97	0.65
1:B:167:THR:HG21	1:B:200:GLY:HA3	1.76	0.65
1:A:86:ARG:HG3	1:A:298:GLN:HA	1.79	0.64
1:B:68:THR:HG23	1:B:71:LEU:HD11	1.78	0.64
1:B:294:ARG:HB3	1:B:294:ARG:HH11	1.63	0.64
1:A:111:VAL:O	1:A:115:LEU:HG	1.97	0.64
1:A:287:THR:OG1	1:A:326:ARG:N	2.24	0.64
1:A:298:GLN:O	1:A:302:ASP:HB2	1.97	0.64
1:A:163:HIS:O	1:A:167:THR:HG23	1.99	0.63
1:A:144:PRO:HB3	1:A:307:LEU:CD1	2.26	0.63
1:A:197:ARG:HH22	2:A:902:NPF:C2A	2.12	0.63
1:B:189:LEU:O	1:B:195:ARG:NH2	2.31	0.63
1:B:302:ASP:HA	1:B:305:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	2:A:902:NPF:C2A	2.63	0.62
1:A:154:THR:CG2	1:A:155:PRO:HD2	2.30	0.62
1:B:70:SER:HB2	1:B:101:ARG:NH2	2.15	0.61
1:A:86:ARG:HB3	1:A:301:VAL:CG1	2.22	0.61
1:B:161:PHE:HB2	1:B:291:GLN:HE21	1.66	0.61
1:B:250:ALA:O	1:B:254:MET:HG2	2.01	0.60
1:B:213:ILE:HD11	1:B:239:PRO:CB	2.32	0.60
1:A:201:TRP:O	1:A:205:LEU:HB2	2.02	0.60
1:A:250:ALA:O	1:A:253:ALA:HB3	2.02	0.60
1:A:132:ASP:HA	1:A:135:ALA:HB3	1.84	0.60
1:A:117:GLN:HG3	1:B:117:GLN:HB3	1.83	0.59
1:A:134:ILE:HD13	1:A:134:ILE:H	1.67	0.59
1:B:294:ARG:HB3	1:B:294:ARG:NH1	2.18	0.59
1:B:242:MET:HE1	1:B:253:ALA:HB1	1.84	0.59
1:B:297:GLY:O	1:B:301:VAL:HG23	2.03	0.59
1:A:75:ALA:N	1:A:76:PRO:HD2	2.18	0.59
1:A:154:THR:HG22	1:A:155:PRO:HD2	1.85	0.59
1:B:68:THR:CG2	1:B:71:LEU:HD11	2.33	0.59
1:B:255:ARG:HE	1:B:259:GLU:CD	2.06	0.59
1:A:141:THR:O	1:A:142:ASN:CB	2.51	0.58
1:B:276:THR:CG2	1:B:277:GLU:N	2.66	0.58
1:A:306:GLN:HE22	1:A:313:VAL:HG12	1.68	0.58
1:A:231:GLN:O	1:A:235:GLU:HG3	2.04	0.58
1:A:151:SER:C	1:A:153:GLN:H	2.07	0.58
1:A:188:PRO:HD2	1:A:220:TRP:CE2	2.38	0.58
1:A:296:LEU:HA	1:A:299:THR:HG22	1.87	0.57
1:A:101:ARG:H	1:A:101:ARG:HD3	1.69	0.56
1:B:99:VAL:CG1	1:B:106:ALA:HB1	2.34	0.56
1:B:119:VAL:HG23	1:B:121:GLY:H	1.70	0.56
1:B:230:MET:HG2	1:B:256:ALA:HB1	1.87	0.56
1:B:243:LEU:HD23	1:B:271:VAL:HB	1.86	0.56
1:B:287:THR:HG23	1:B:325:LYS:HA	1.87	0.56
1:A:258:THR:HG21	1:B:283:ILE:HG21	1.87	0.56
1:A:279:SER:HA	1:A:282:TYR:CE1	2.40	0.56
1:B:104:VAL:CG2	1:B:132:ASP:HB3	2.35	0.56
1:B:179:HIS:HB3	1:B:182:ILE:CD1	2.34	0.56
1:B:288:THR:OG1	1:B:289:ILE:N	2.38	0.56
1:A:83:ILE:HD13	1:A:297:GLY:HA2	1.88	0.56
1:B:312:ALA:CB	1:B:313:VAL:HA	2.22	0.56
1:B:79:ILE:HD11	1:B:293:PHE:HD1	1.72	0.55
1:B:86:ARG:HG2	1:B:298:GLN:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PRO:HD3	1:B:149:ASP:OD2	2.05	0.55
1:B:251:LEU:HB2	1:B:282:TYR:CE2	2.41	0.55
1:B:70:SER:CB	1:B:101:ARG:NH2	2.70	0.55
1:B:303:ARG:O	1:B:307:LEU:HB2	2.06	0.55
1:B:80:VAL:HG13	1:B:96:VAL:HG21	1.89	0.54
1:A:68:THR:HG21	1:A:71:LEU:CD2	2.37	0.54
1:B:135:ALA:O	1:B:138:ALA:HB3	2.07	0.54
1:A:110:ALA:O	1:A:112:HIS:N	2.32	0.54
1:B:192:VAL:HG22	1:B:196:LEU:HD11	1.90	0.54
1:B:254:MET:HE1	1:B:284:PRO:O	2.07	0.54
1:A:216:ARG:HD2	1:A:232:MET:HB2	1.89	0.54
1:B:79:ILE:HD13	1:B:293:PHE:HB3	1.90	0.53
1:B:163:HIS:H	1:B:163:HIS:CD2	2.27	0.53
1:A:195:ARG:HH21	1:A:195:ARG:CG	2.09	0.53
1:A:167:THR:O	1:A:171:VAL:HG23	2.08	0.53
1:B:269:SER:HB3	1:B:329:THR:HA	1.90	0.53
1:A:222:ALA:HA	1:A:248:GLN:O	2.08	0.52
1:A:161:PHE:HB2	1:A:291:GLN:HE21	1.75	0.52
1:A:115:LEU:C	1:A:117:GLN:H	2.13	0.52
1:B:146:LEU:HD11	1:B:303:ARG:HH11	1.75	0.51
1:A:160:ILE:O	1:A:319:LEU:HD23	2.10	0.51
1:A:134:ILE:C	1:A:136:VAL:N	2.63	0.51
1:A:148:LEU:HD13	1:A:296:LEU:HD21	1.93	0.51
1:B:184:LEU:HD23	1:B:243:LEU:HB2	1.93	0.51
1:B:241:ALA:HA	1:B:269:SER:O	2.11	0.50
1:A:125:ASN:HB2	1:A:148:LEU:HD12	1.93	0.50
1:A:173:HIS:O	1:A:177:LEU:HB2	2.11	0.50
1:B:161:PHE:HB2	1:B:291:GLN:NE2	2.26	0.50
1:B:66:VAL:HB	1:B:96:VAL:HG22	1.93	0.50
1:B:298:GLN:HG3	1:B:299:THR:CA	2.38	0.50
1:B:262:LEU:HD22	1:B:267:ASP:HB3	1.94	0.49
1:A:104:VAL:O	1:A:107:CYS:N	2.45	0.49
1:B:128:LEU:HD13	1:B:133:ALA:HA	1.94	0.49
1:A:97:SER:HB3	1:A:114:LEU:HD23	1.94	0.49
1:A:253:ALA:O	1:A:257:ILE:HG12	2.12	0.49
1:A:64:ILE:HD13	1:A:301:VAL:CG2	2.42	0.49
1:A:251:LEU:HB2	1:A:282:TYR:CE2	2.48	0.49
1:A:123:ILE:HG13	1:A:304:LEU:HD22	1.95	0.48
1:B:104:VAL:HG21	1:B:132:ASP:HB3	1.96	0.48
1:B:286:LEU:O	1:B:326:ARG:HD2	2.14	0.47
1:A:269:SER:HB3	1:A:328:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:HB1	1:B:313:VAL:CA	2.29	0.47
1:B:67:ALA:HA	1:B:97:SER:O	2.15	0.47
1:A:63:LEU:O	1:A:120:SER:N	2.47	0.47
1:A:273:TYR:O	1:A:274:ASP:CB	2.61	0.47
1:A:303:ARG:HH12	1:A:317:GLN:HB2	1.80	0.47
1:B:229:THR:CG2	1:B:256:ALA:CB	2.92	0.47
1:B:97:SER:OG	1:B:113:ASN:ND2	2.48	0.47
1:B:197:ARG:HH22	2:B:901:NPF:C2A	2.27	0.47
1:A:114:LEU:O	1:A:119:VAL:HG13	2.15	0.47
1:B:159:ILE:HD11	1:B:303:ARG:HD2	1.96	0.47
1:B:295:LEU:HD12	1:B:298:GLN:HG2	1.96	0.47
1:B:273:TYR:O	1:B:274:ASP:CB	2.63	0.47
1:B:246:ASN:HA	1:B:273:TYR:O	2.14	0.46
1:B:295:LEU:O	1:B:299:THR:OG1	2.33	0.46
1:A:148:LEU:HD22	1:A:296:LEU:HD11	1.97	0.46
1:A:86:ARG:HH12	1:A:298:GLN:HE21	1.63	0.46
1:A:257:ILE:HG12	1:A:257:ILE:H	1.58	0.46
1:A:306:GLN:NE2	1:A:313:VAL:HG12	2.31	0.46
1:B:213:ILE:HD11	1:B:239:PRO:CA	2.45	0.46
1:A:134:ILE:O	1:A:136:VAL:N	2.49	0.46
1:A:99:VAL:HG21	1:A:126:TYR:CD1	2.52	0.45
1:B:76:PRO:HA	1:B:79:ILE:HG12	1.98	0.45
1:B:152:ASP:HB2	1:B:316:ASN:ND2	2.31	0.45
1:B:105:GLU:HA	1:B:108:LYS:HD3	1.98	0.45
1:B:198:LEU:O	1:B:199:ALA:C	2.53	0.45
1:B:273:TYR:O	1:B:274:ASP:HB2	2.16	0.45
1:A:161:PHE:CB	1:A:291:GLN:HE21	2.29	0.45
1:B:226:PHE:O	1:B:227:GLN:C	2.55	0.45
1:B:100:GLU:CG	1:B:101:ARG:H	2.27	0.45
1:B:203:LYS:HD2	1:B:204:TYR:CE2	2.51	0.45
1:A:213:ILE:HD11	1:A:239:PRO:HA	1.99	0.45
1:A:114:LEU:HD12	1:A:122:LEU:CD2	2.47	0.44
1:A:161:PHE:HB2	1:A:291:GLN:NE2	2.32	0.44
1:A:152:ASP:N	1:A:152:ASP:OD1	2.50	0.44
1:B:246:ASN:OD1	1:B:246:ASN:C	2.55	0.44
1:A:265:GLY:HA2	1:A:269:SER:HA	2.00	0.44
1:A:184:LEU:HD23	1:A:243:LEU:HB2	1.98	0.44
1:B:112:HIS:O	1:B:113:ASN:C	2.56	0.44
1:A:319:LEU:HD23	1:A:319:LEU:H	1.83	0.43
1:B:204:TYR:O	1:B:208:ASN:HB2	2.18	0.43
1:A:151:SER:C	1:A:153:GLN:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASP:HB2	1:B:316:ASN:HD21	1.83	0.43
1:B:192:VAL:HG22	1:B:196:LEU:CD1	2.47	0.43
1:A:140:CYS:HB3	1:A:143:VAL:HG11	1.99	0.43
1:B:147:PHE:CD1	1:B:156:ILE:HD12	2.53	0.43
1:B:99:VAL:HG11	1:B:126:TYR:CE1	2.53	0.43
1:B:160:ILE:HG13	1:B:161:PHE:N	2.32	0.43
1:A:201:TRP:CD1	1:A:243:LEU:HD13	2.53	0.43
1:B:71:LEU:HD13	1:B:98:MET:HB3	2.00	0.43
1:B:126:TYR:HA	1:B:127:PRO:HD2	1.77	0.43
1:A:282:TYR:N	1:A:282:TYR:CD1	2.87	0.43
1:A:319:LEU:HB2	1:A:320:PRO:CD	2.48	0.43
1:B:154:THR:HA	1:B:155:PRO:HD3	1.74	0.43
1:A:142:ASN:N	1:A:143:VAL:HB	2.34	0.43
1:A:152:ASP:HB3	1:A:160:ILE:CD1	2.47	0.42
1:B:157:ASN:HD22	1:B:157:ASN:HA	1.63	0.42
1:A:186:ALA:HB3	1:A:217:GLU:HA	2.01	0.42
1:A:254:MET:HA	1:A:257:ILE:HG13	2.01	0.42
1:A:257:ILE:HG22	1:A:262:LEU:HB2	2.01	0.42
1:A:134:ILE:C	1:A:136:VAL:H	2.21	0.42
1:A:171:VAL:O	1:A:175:VAL:HG23	2.19	0.42
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.18	0.42
1:A:308:SER:O	1:A:309:GLN:HB2	2.20	0.42
1:A:79:ILE:CG1	1:A:293:PHE:HD1	2.33	0.42
1:A:213:ILE:CD1	1:A:239:PRO:HA	2.50	0.42
1:A:246:ASN:OD1	1:A:249:MET:HB2	2.19	0.42
1:A:282:TYR:N	1:A:282:TYR:HD1	2.16	0.42
1:B:112:HIS:C	1:B:114:LEU:N	2.72	0.42
1:A:108:LYS:HB3	1:A:136:VAL:HG22	2.02	0.42
1:B:104:VAL:CG1	1:B:105:GLU:N	2.83	0.42
1:B:99:VAL:HG12	1:B:100:GLU:N	2.34	0.42
1:B:160:ILE:HD12	2:B:901:NPF:C4A	2.50	0.42
1:B:232:MET:HE1	1:B:242:MET:SD	2.60	0.42
1:A:99:VAL:CG1	1:A:126:TYR:CD1	2.88	0.41
1:B:107:CYS:O	1:B:111:VAL:HG23	2.20	0.41
1:B:186:ALA:HA	1:B:245:ALA:HB2	2.02	0.41
1:B:219:ASP:OD1	1:B:224:SER:HB3	2.20	0.41
1:A:150:VAL:HG21	1:A:156:ILE:HD11	2.01	0.41
1:B:192:VAL:O	1:B:196:LEU:HD12	2.19	0.41
1:B:156:ILE:HB	1:B:157:ASN:H	1.66	0.41
1:A:84:LYS:HD3	1:B:98:MET:HG2	2.03	0.41
1:A:305:LEU:O	1:A:307:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD12	1:B:243:LEU:HD21	2.03	0.41
1:A:140:CYS:HB3	1:A:143:VAL:CG1	2.51	0.41
1:A:181:GLN:HB3	1:A:213:ILE:HD11	2.02	0.41
1:A:279:SER:HA	1:A:282:TYR:CD1	2.55	0.41
1:A:167:THR:HG21	1:A:200:GLY:HA3	2.03	0.41
1:A:303:ARG:O	1:A:303:ARG:HG3	2.18	0.41
1:B:100:GLU:CG	1:B:101:ARG:N	2.84	0.41
1:B:325:LYS:H	1:B:325:LYS:HG2	1.69	0.41
1:A:305:LEU:HD23	1:A:306:GLN:N	2.36	0.41
1:B:202:HIS:O	1:B:203:LYS:C	2.59	0.41
1:B:244:VAL:HG11	1:B:250:ALA:N	2.36	0.41
1:B:276:THR:HG23	1:B:277:GLU:N	2.35	0.41
1:A:189:LEU:O	1:A:195:ARG:NH2	2.53	0.41
1:A:241:ALA:CA	1:A:269:SER:O	2.65	0.41
1:B:79:ILE:CD1	1:B:293:PHE:HD1	2.33	0.41
1:B:100:GLU:HG3	1:B:101:ARG:N	2.31	0.41
1:A:214:ALA:HB2	1:A:237:ILE:HG21	2.02	0.41
1:A:242:MET:N	1:A:269:SER:O	2.53	0.41
1:A:305:LEU:O	1:A:306:GLN:C	2.59	0.40
1:B:112:HIS:O	1:B:114:LEU:N	2.54	0.40
1:B:242:MET:CE	1:B:253:ALA:HB1	2.50	0.40
1:A:75:ALA:HB1	1:A:293:PHE:CE1	2.56	0.40
1:A:273:TYR:O	1:A:274:ASP:HB2	2.21	0.40
1:B:118:ARG:HH11	1:B:118:ARG:HB3	1.87	0.40
1:A:64:ILE:HD13	1:A:301:VAL:HG23	2.03	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	267/269 (99%)	206 (77%)	44 (16%)	17 (6%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	267/269 (99%)	216 (81%)	41 (15%)	10 (4%)	3 26
All	All	534/538 (99%)	422 (79%)	85 (16%)	27 (5%)	2 19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	141	THR
1	A	142	ASN
1	A	274	ASP
1	A	309	GLN
1	B	130	ASP
1	A	101	ARG
1	A	129	ASP
1	A	162	SER
1	A	310	GLY
1	B	156	ILE
1	B	274	ASP
1	A	135	ALA
1	A	152	ASP
1	A	306	GLN
1	B	70	SER
1	B	113	ASN
1	B	295	LEU
1	A	217	GLU
1	A	232	MET
1	A	315	GLY
1	B	101	ARG
1	B	227	GLN
1	B	298	GLN
1	A	106	ALA
1	A	143	VAL
1	B	155	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	220/220 (100%)	177 (80%)	43 (20%)	1 7
1	B	220/220 (100%)	189 (86%)	31 (14%)	3 19
All	All	440/440 (100%)	366 (83%)	74 (17%)	2 12

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	71	LEU
1	A	86	ARG
1	A	88	ASP
1	A	98	MET
1	A	101	ARG
1	A	104	VAL
1	A	107	CYS
1	A	114	LEU
1	A	118	ARG
1	A	129	ASP
1	A	130	ASP
1	A	134	ILE
1	A	154	THR
1	A	160	ILE
1	A	163	HIS
1	A	172	GLU
1	A	177	LEU
1	A	181	GLN
1	A	192	VAL
1	A	193	SER
1	A	195	ARG
1	A	205	LEU
1	A	213	ILE
1	A	216	ARG
1	A	231	GLN
1	A	234	ASN
1	A	249	MET
1	A	257	ILE
1	A	269	SER
1	A	276	THR
1	A	278	ASP
1	A	287	THR
1	A	294	ARG
1	A	301	VAL

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Mol	Chain	Res	Type
1	A	303	ARG
1	A	305	LEU
1	A	307	LEU
1	A	314	LYS
1	A	316	ASN
1	A	319	LEU
1	A	323	LEU
1	A	328	THR
1	B	62	LEU
1	B	90	LEU
1	B	98	MET
1	B	100	GLU
1	B	118	ARG
1	B	119	VAL
1	B	129	ASP
1	B	134	ILE
1	B	160	ILE
1	B	180	GLN
1	B	189	LEU
1	B	207	ARG
1	B	208	ASN
1	B	210	ILE
1	B	229	THR
1	B	230	MET
1	B	238	VAL
1	B	255	ARG
1	B	269	SER
1	B	276	THR
1	B	290	LYS
1	B	298	GLN
1	B	299	THR
1	B	305	LEU
1	B	306	GLN
1	B	307	LEU
1	B	308	SER
1	B	316	ASN
1	B	318	LEU
1	B	329	THR
1	B	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	113	ASN
1	A	157	ASN
1	A	181	GLN
1	A	209	GLN
1	A	234	ASN
1	A	291	GLN
1	A	298	GLN
1	A	306	GLN
1	B	113	ASN
1	B	157	ASN
1	B	163	HIS
1	B	227	GLN
1	B	231	GLN
1	B	291	GLN
1	B	306	GLN
1	B	316	ASN

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)

2 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	NPF	B	901	1	20,21,21	3.60	4 (20%)	27,30,30	2.53	13 (48%)
2	NPF	A	902	-	20,21,21	3.99	4 (20%)	27,30,30	2.83	13 (48%)

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	NPF	B	901	1	-	1/6/28/28	0/2/2/2
2	NPF	A	902	-	-	1/6/28/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NPF	O6B-N6	13.17	1.45	1.22
2	B	901	NPF	O6B-N6	11.71	1.42	1.22
2	A	902	NPF	C6A-C1A	8.03	1.54	1.40
2	B	901	NPF	C6A-C1A	7.70	1.54	1.40
2	B	901	NPF	C6A-N6	-6.31	1.34	1.45
2	A	902	NPF	C6A-N6	-5.57	1.35	1.45
2	A	902	NPF	O1-C1A	5.31	1.46	1.37
2	B	901	NPF	O1-C1A	3.35	1.43	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	NPF	C1A-O1-C1	-8.16	102.50	118.09
2	A	902	NPF	C1A-O1-C1	-7.94	102.92	118.09
2	A	902	NPF	O1-C1A-C6A	-5.63	110.52	117.31
2	A	902	NPF	O5-C5-C6	4.39	116.17	106.70
2	B	901	NPF	O1-C1A-C2A	-4.07	114.30	123.87
2	A	902	NPF	O1-C1A-C2A	-3.62	115.37	123.87
2	A	902	NPF	C3A-C2A-C1A	3.42	126.00	119.71
2	B	901	NPF	O5-C5-C4	-3.33	103.54	109.52
2	A	902	NPF	C4-C3-C2	3.31	116.60	110.82
2	B	901	NPF	O1-C1A-C6A	-3.29	113.34	117.31
2	A	902	NPF	C3-C4-C5	3.27	114.87	109.77
2	B	901	NPF	C1-O5-C5	-3.27	108.05	113.67
2	A	902	NPF	C5A-C6A-N6	3.06	119.74	116.47
2	B	901	NPF	C3A-C2A-C1A	2.97	125.18	119.71
2	A	902	NPF	C1-O5-C5	-2.82	108.82	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	NPF	C2A-C1A-C6A	-2.68	112.23	118.81
2	A	902	NPF	C4A-C5A-C6A	2.56	122.97	118.61
2	B	901	NPF	O3-C3-C4	-2.54	104.48	110.35
2	A	902	NPF	O1-C1-C2	2.53	110.81	107.14
2	B	901	NPF	C2A-C1A-C6A	-2.46	112.77	118.81
2	A	902	NPF	O5-C5-C4	-2.33	105.33	109.52
2	B	901	NPF	O5-C5-C6	2.25	111.55	106.70
2	B	901	NPF	C3-C4-C5	2.15	113.13	109.77
2	B	901	NPF	O1-C1-C2	2.13	110.22	107.14
2	B	901	NPF	O4-C4-C3	-2.10	105.48	110.35
2	B	901	NPF	C4A-C5A-C6A	2.10	122.19	118.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	NPF	C2A-C1A-O1-C1
2	A	902	NPF	C2A-C1A-O1-C1

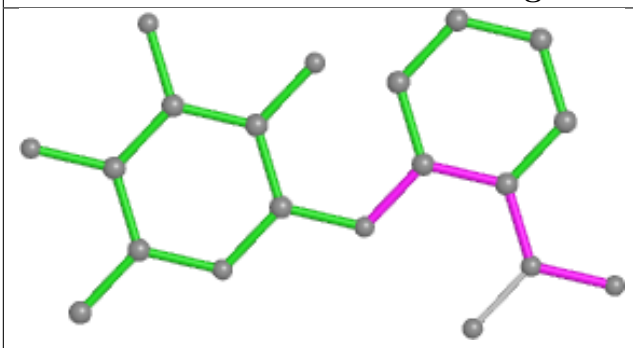
There are no ring outliers.

2 monomers are involved in 5 short contacts:

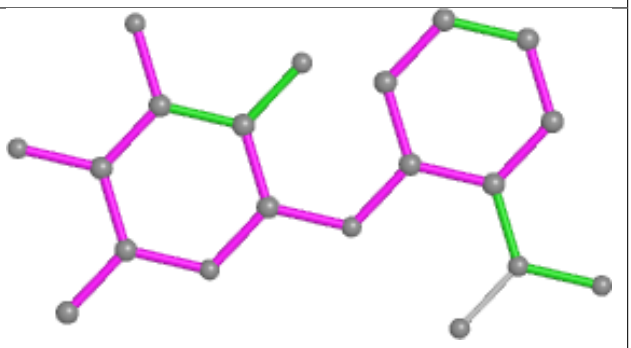
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	NPF	3	0
2	A	902	NPF	2	0

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.

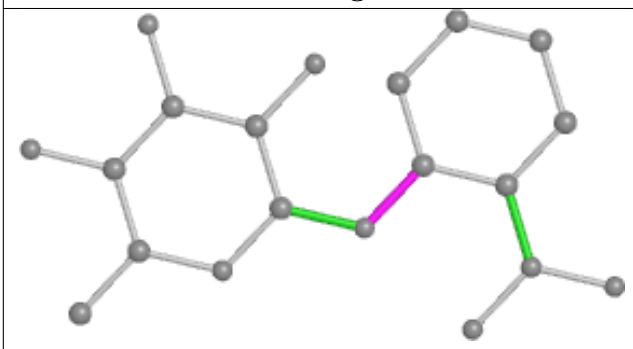
Ligand NPF B 901



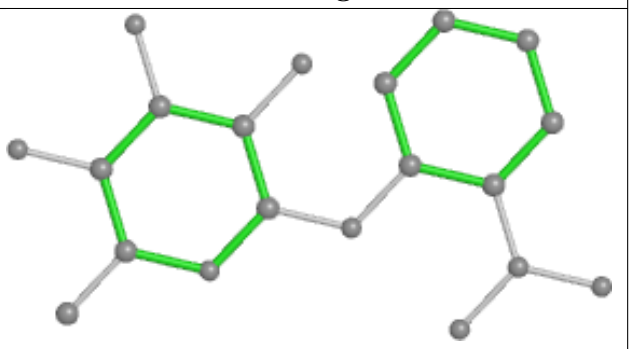
Bond lengths



Bond angles

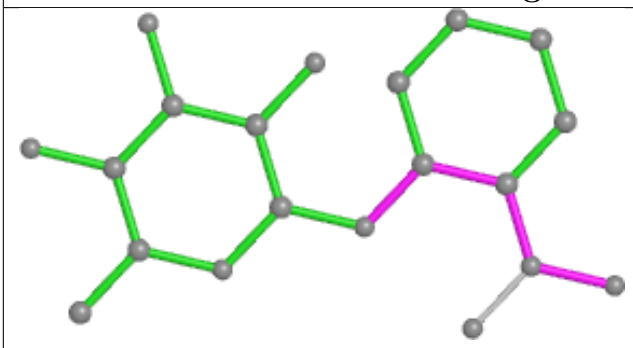


Torsions

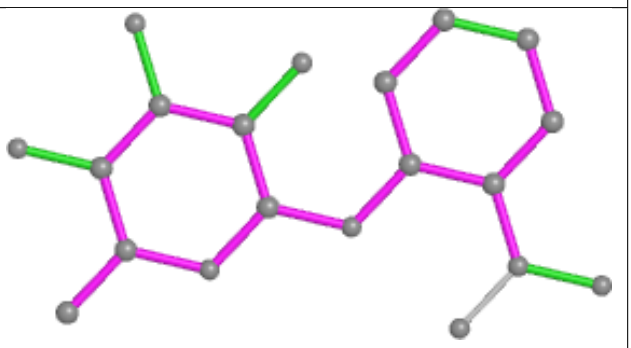


Rings

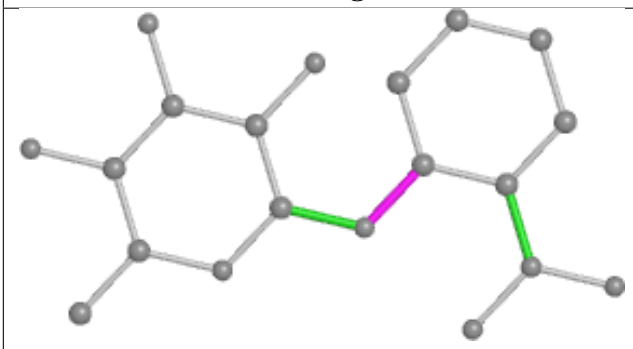
Ligand NPF A 902



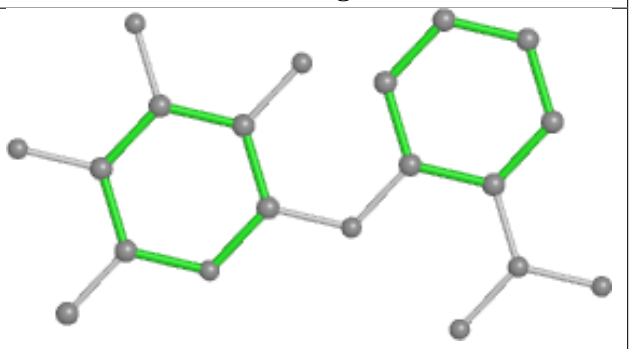
Bond lengths



Bond angles



Torsions



Rings

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	269/269 (100%)	-0.81	0	100	100	7, 26, 51, 69	0
1	B	269/269 (100%)	-0.78	0	100	100	8, 26, 50, 65	0
All	All	538/538 (100%)	-0.79	0	100	100	7, 26, 51, 69	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

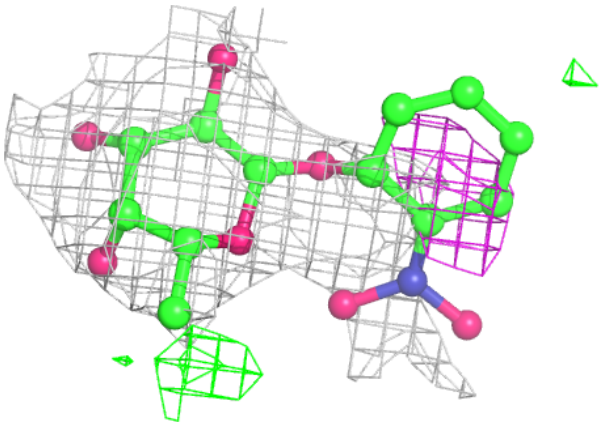
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

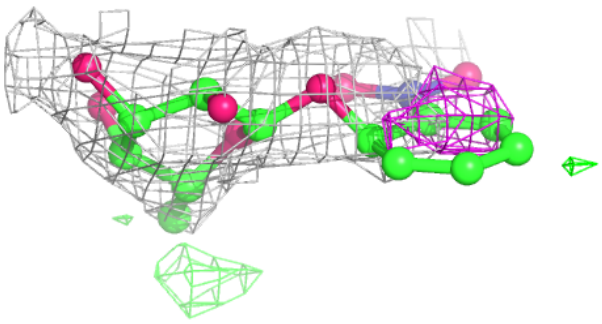
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NPF	A	902	20/20	0.88	0.27	38,46,61,63	0
2	NPF	B	901	20/20	0.94	0.18	31,35,56,57	0

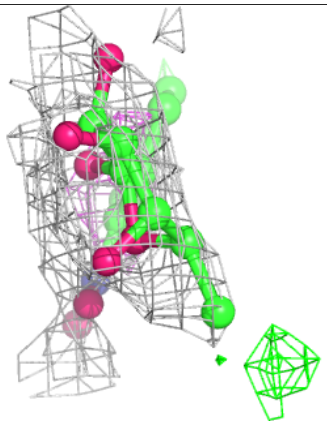
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NPF A 902:

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

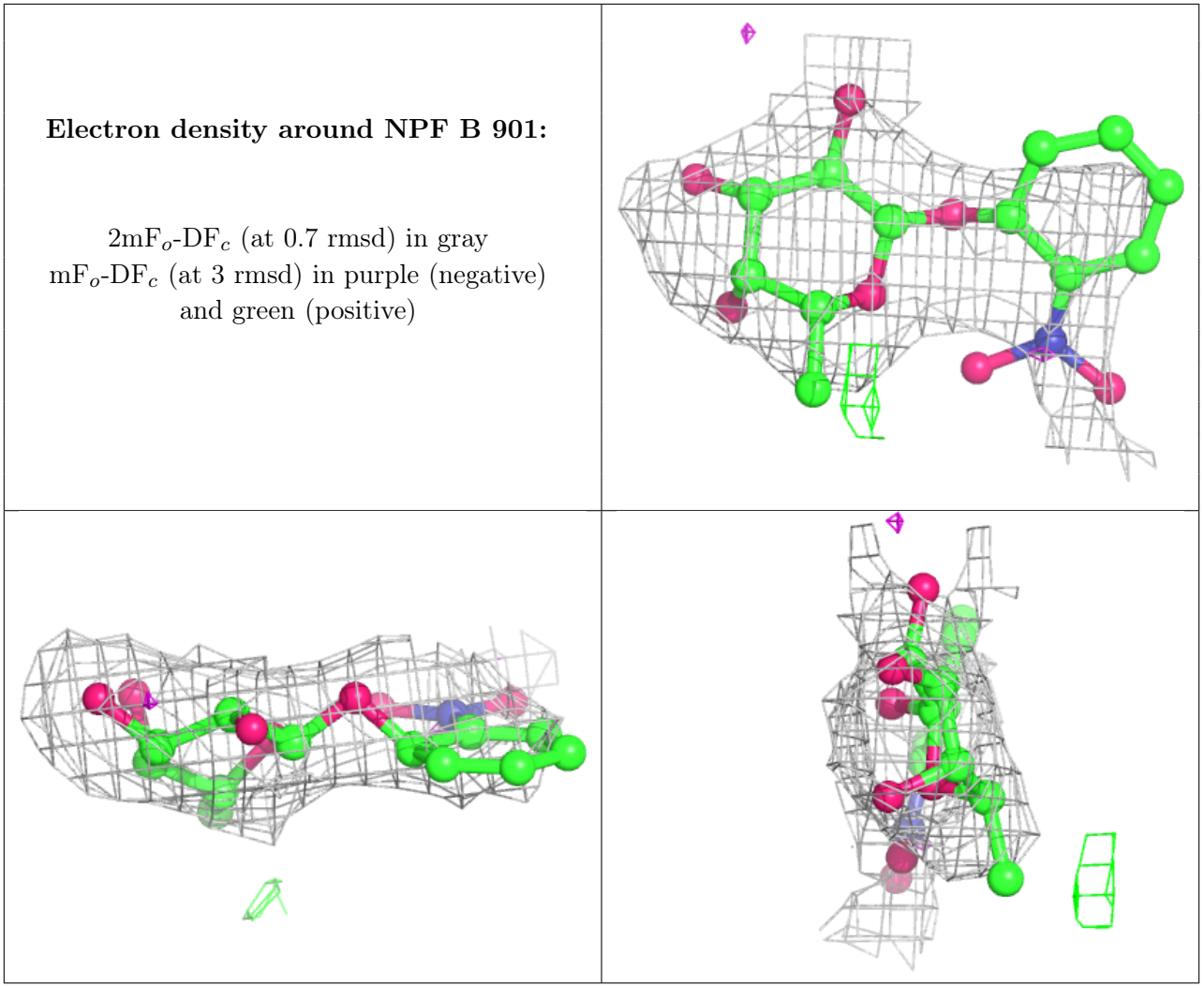






Electron density around NPF B 901:

$2mF_o$-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.