



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:44 AM UTC

PDB ID : 7CS6 / pdb_00007cs6
Title : IiPLR1 with NADP⁺ and (-)lariciresinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

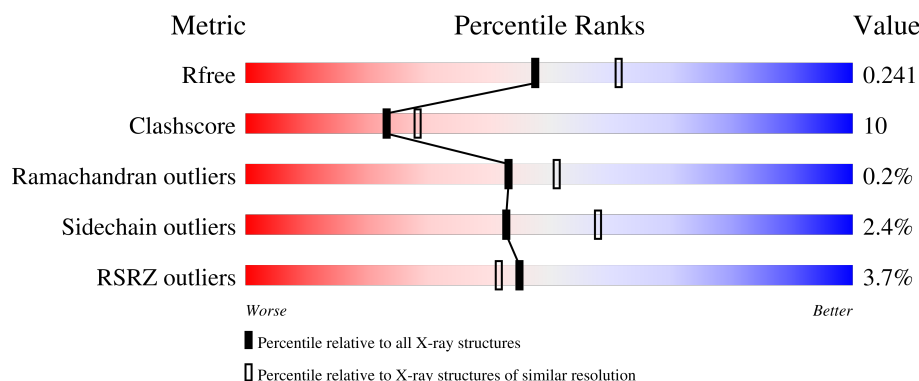
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	317	3% 73% 16% • 10%
1	B	317	7% 68% 21% • 9%
1	C	317	4% 69% 21% • 9%
1	D	317	2% 75% 16% • 9%
1	E	317	3% 78% 11% • 9%

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Mol	Chain	Length	Quality of chain
1	F	317	2% 84% 10% 5%

2 Entry composition [i](#)

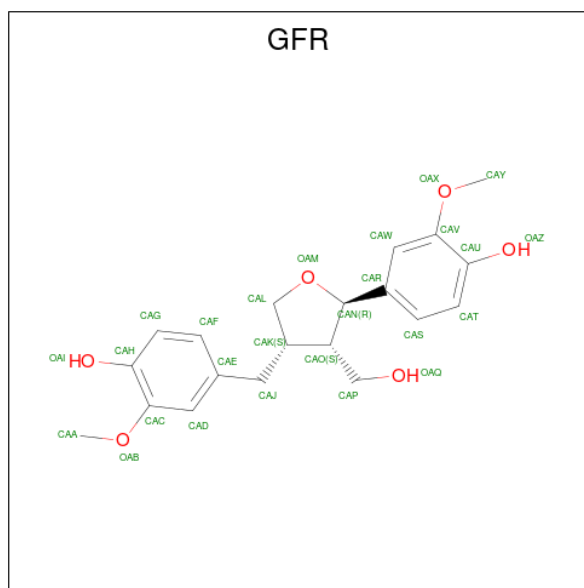
There are 4 unique types of molecules in this entry. The entry contains 14974 atoms, of which 156 are hydrogens and 0 are deuteriums.

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 Pinorensinol-lariciresinol reductase.

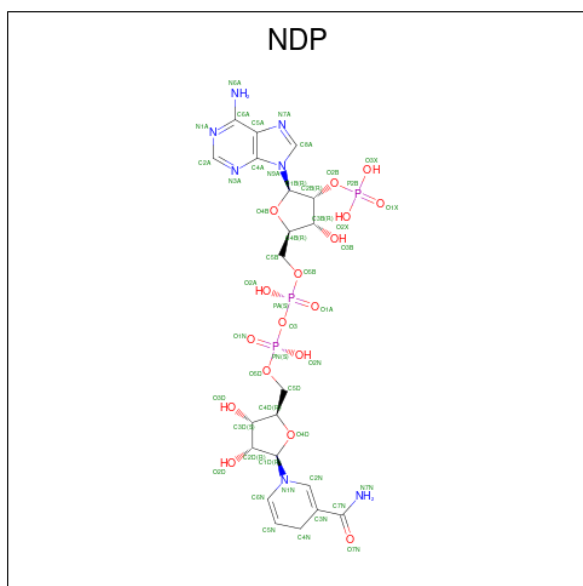
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2253	1434	379	430	10			
1	B	289	Total	C	N	O	S	0	0	0
			2278	1451	385	432	10			
1	C	287	Total	C	N	O	S	0	0	0
			2258	1435	381	432	10			
1	D	289	Total	C	N	O	S	0	0	0
			2270	1443	383	434	10			
1	E	287	Total	C	N	O	S	0	0	0
			2257	1436	380	431	10			
1	F	300	Total	C	N	O	S	0	0	0
			2371	1507	402	452	10			

- Molecule 2 is 4-[[[(3S,4S,5R)-4-(hydroxymethyl)-5-(3-methoxy-4-oxidanyl-phenyl)oxolan-3-yl]methyl]-2-methoxy-phenol (CCD ID: GFR) (formula: C₂₀H₂₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 26	C 20	O 6	0	0
2	B	1	Total 26	C 20	O 6	0	0
2	C	1	Total 26	C 20	O 6	0	0
2	D	1	Total 26	C 20	O 6	0	0
2	E	1	Total 26	C 20	O 6	0	0
2	F	1	Total 26	C 20	O 6	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	B	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	C	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	D	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	E	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	F	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

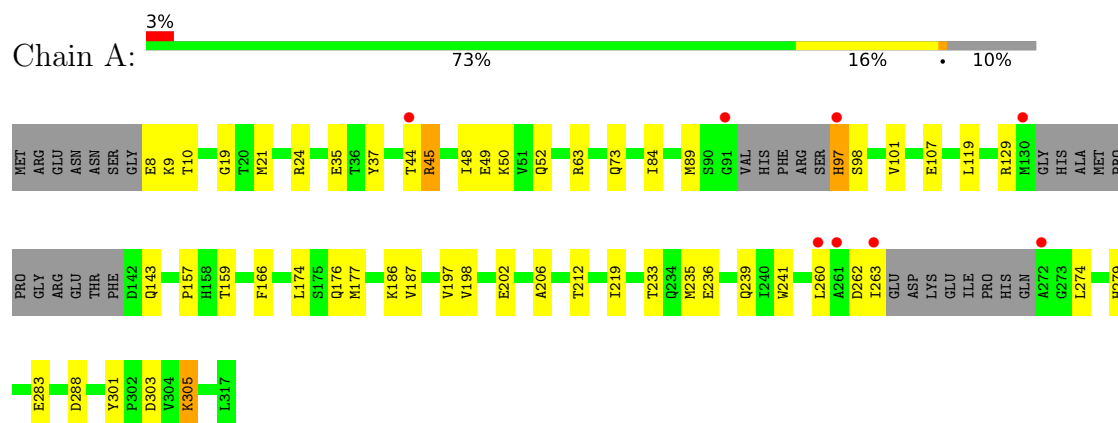
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		
4	B	122	Total	O	0	0
			122	122		
4	C	87	Total	O	0	0
			87	87		
4	D	88	Total	O	0	0
			88	88		
4	E	112	Total	O	0	0
			112	112		
4	F	167	Total	O	0	0
			167	167		

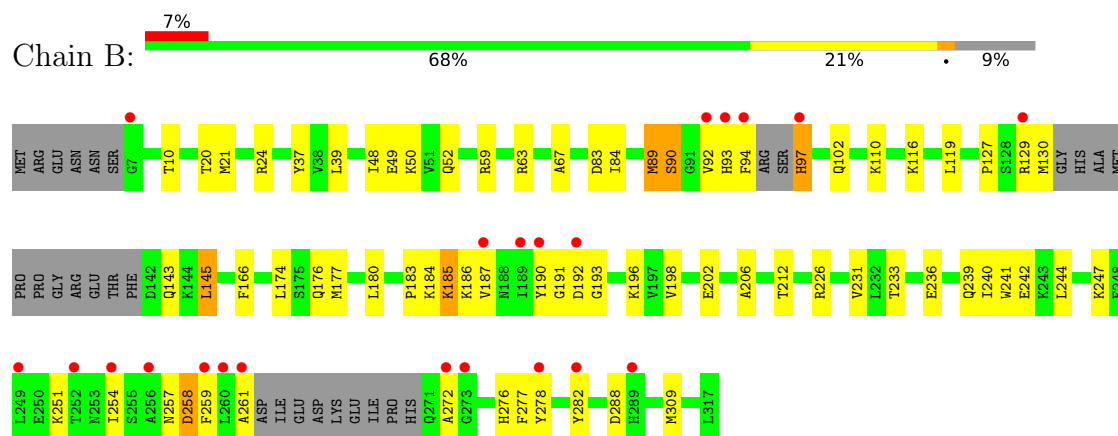
3 Residue-property plots

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.

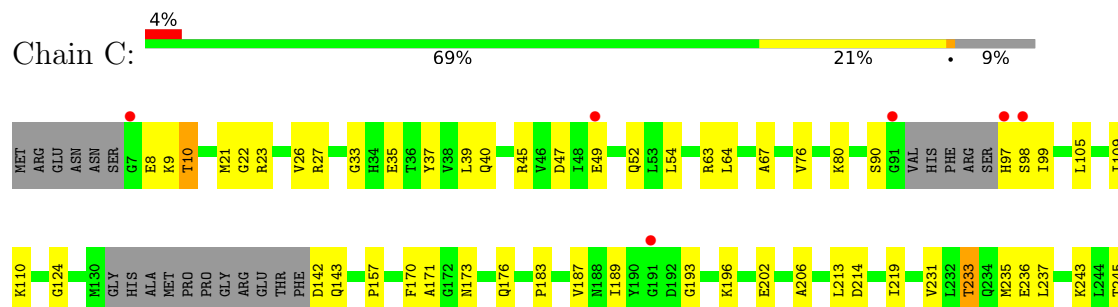
• Molecule 1: Pinoresinol-lariciresinol reductase

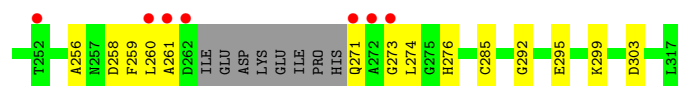


• Molecule 1: Pinoresinol-lariciresinol reductase

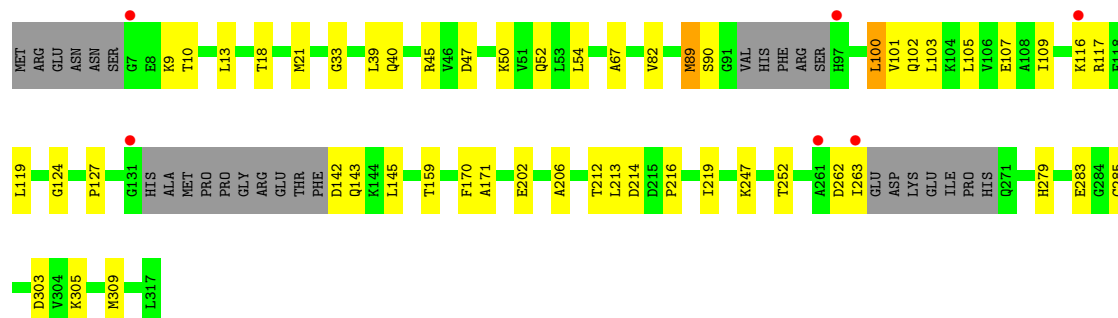
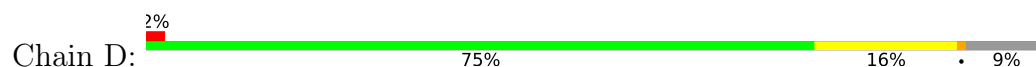


• Molecule 1: Pinoresinol-lariciresinol reductase

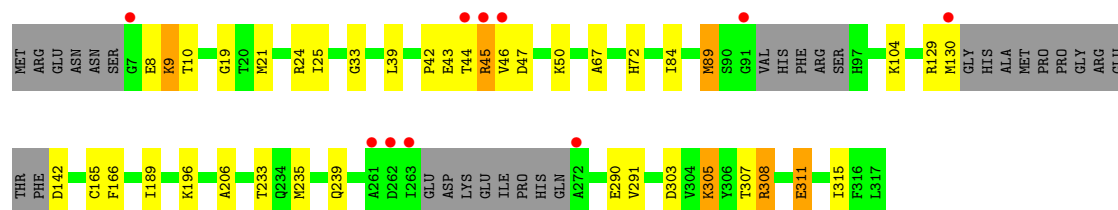
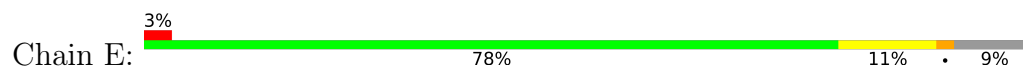




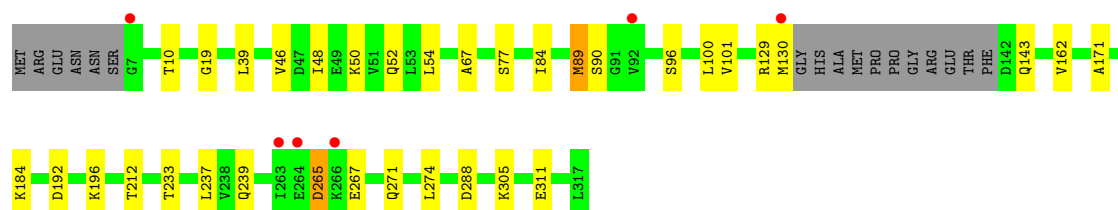
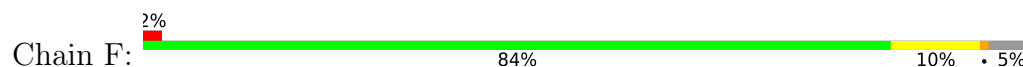
• Molecule 1: Pinoresinol-lariciresinol reductase



• Molecule 1: Pinoresinol-lariciresinol reductase



• Molecule 1: Pinoresinol-lariciresinol reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	244.44Å 244.44Å 75.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.34 – 2.20 42.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.34-2.20) 93.5 (42.34-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155, PHENIX 1.10_2155	Depositor
R, R_{free}	0.197 , 0.240 0.199 , 0.241	Depositor DCC
R_{free} test set	2006 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14974	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.85 % 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 7.4939e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GFR, NDP

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	0.32	0/2290	0.50	0/3093
1	B	0.33	0/2317	0.50	0/3129
1	C	0.33	1/2295 (0.0%)	0.49	0/3099
1	D	0.31	0/2307	0.48	0/3115
1	E	0.32	0/2294	0.53	0/3098
1	F	0.37	0/2414	0.53	0/3263
All	All	0.33	1/13917 (0.0%)	0.51	0/18797

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLN	C-N	-5.67	1.21	1.33

There are no bond angle outliers.

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	2253	0	2261	40	1
1	B	2278	0	2282	76	0
1	C	2258	0	2261	54	2
1	D	2270	0	2275	48	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2257	0	2264	42	0
1	F	2371	0	2371	28	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	1	0
2	D	26	0	0	1	0
2	E	26	0	0	0	0
2	F	26	0	0	0	0
3	A	48	26	23	6	0
3	B	48	26	24	5	0
3	C	48	26	24	3	0
3	D	48	26	23	5	0
3	E	48	26	24	9	0
3	F	48	26	23	5	0
4	A	111	0	0	0	0
4	B	122	0	0	13	0
4	C	87	0	0	8	0
4	D	88	0	0	5	0
4	E	112	0	0	4	0
4	F	167	0	0	5	0
All	All	14818	156	13855	287	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (287) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:HG23	1:B:236:GLU:H	1.20	1.04
1:D:202:GLU:OE2	4:D:501:HOH:O	1.84	0.96
1:E:45:ARG:NH2	1:E:47:ASP:OD1	1.98	0.96
1:B:129:ARG:NH1	1:B:288:ASP:OD2	1.99	0.94
1:C:271:GLN:NE2	4:C:501:HOH:O	2.03	0.91
1:B:143:GLN:NE2	4:B:503:HOH:O	2.11	0.83
1:B:183:PRO:O	4:B:501:HOH:O	1.97	0.83
1:B:257:ASN:O	4:B:502:HOH:O	1.97	0.83
1:A:8:GLU:N	1:A:8:GLU:OE1	2.11	0.82
1:B:185:LYS:HE3	1:B:185:LYS:HA	1.62	0.82
1:F:129:ARG:NH1	1:F:288:ASP:OD2	2.13	0.82
1:F:96:SER:H	1:F:143:GLN:HG3	1.44	0.81
1:B:193:GLY:O	1:B:233:THR:OG1	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ALA:HB1	1:D:309:MET:HE2	1.64	0.80
1:E:45:ARG:O	4:E:501:HOH:O	2.00	0.78
1:E:21:MET:HE1	1:E:206:ALA:HB2	1.66	0.78
1:C:8:GLU:HG3	1:C:9:LYS:H	1.49	0.78
1:C:233:THR:HG22	1:C:236:GLU:OE1	1.84	0.77
1:E:43:GLU:OE2	4:E:501:HOH:O	2.03	0.76
1:D:171:ALA:HB1	1:D:309:MET:CE	2.16	0.76
1:C:193:GLY:O	1:C:233:THR:OG1	2.01	0.76
1:C:233:THR:HG23	1:C:236:GLU:H	1.50	0.76
1:D:116:LYS:HZ3	1:D:117:ARG:HH21	1.32	0.75
1:D:262:ASP:O	1:D:263:ILE:HG13	1.87	0.75
1:B:233:THR:HG22	1:B:236:GLU:OE2	1.87	0.74
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.68	0.74
1:B:233:THR:CG2	1:B:236:GLU:HG3	2.18	0.73
1:B:184:LYS:O	1:B:185:LYS:HD2	1.89	0.73
1:C:245:THR:OG1	4:C:502:HOH:O	2.06	0.73
1:A:233:THR:OG1	1:A:236:GLU:HG3	1.89	0.72
1:C:142:ASP:OD2	4:C:503:HOH:O	2.08	0.71
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.72	0.71
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.72	0.70
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.73	0.70
1:D:116:LYS:NZ	1:D:117:ARG:HH21	1.90	0.69
1:E:9:LYS:HG2	1:E:33:GLY:O	1.93	0.69
1:E:290:GLU:OE2	1:E:291:VAL:N	2.19	0.69
1:E:308:ARG:O	1:E:311:GLU:HG2	1.92	0.69
1:B:21:MET:HE1	1:B:206:ALA:HB2	1.76	0.68
1:A:129:ARG:NH1	1:A:288:ASP:OD2	2.24	0.68
1:C:110:LYS:NZ	4:C:508:HOH:O	2.25	0.68
1:E:239:GLN:OE1	4:E:502:HOH:O	2.10	0.68
1:C:259:PHE:CZ	1:C:274:LEU:HD23	2.28	0.68
1:B:92:VAL:HG22	4:B:514:HOH:O	1.93	0.67
1:B:21:MET:CE	1:B:206:ALA:HB2	2.24	0.67
1:A:177:MET:HE1	1:A:274:LEU:HD13	1.77	0.66
1:D:116:LYS:HD3	1:D:116:LYS:C	2.18	0.66
1:B:186:LYS:HD2	1:B:186:LYS:C	2.20	0.66
1:D:9:LYS:HD2	1:D:33:GLY:O	1.95	0.66
1:B:129:ARG:HH11	1:B:288:ASP:CG	2.03	0.66
1:B:202:GLU:OE1	4:B:504:HOH:O	2.14	0.66
1:D:21:MET:HE1	1:D:206:ALA:HB2	1.77	0.65
1:D:252:THR:HG21	1:F:271:GLN:HG3	1.77	0.65
1:B:89:MET:HE1	1:B:102:GLN:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LYS:HE2	4:D:574:HOH:O	1.96	0.65
1:A:97:HIS:N	1:A:143:GLN:HE22	1.95	0.65
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.78	0.65
1:E:21:MET:CE	1:E:206:ALA:HB2	2.27	0.65
1:F:39:LEU:CD1	1:F:67:ALA:HB3	2.28	0.64
1:D:50:LYS:HE3	3:D:402:NDP:O3X	1.98	0.64
1:E:10:THR:HG21	1:E:84:ILE:HD12	1.80	0.63
1:B:309:MET:HE2	1:B:309:MET:HA	1.81	0.63
1:D:116:LYS:HD3	1:D:116:LYS:O	1.98	0.63
1:E:50:LYS:HE3	3:E:402:NDP:O3X	1.98	0.63
1:C:299:LYS:HE3	4:C:549:HOH:O	1.98	0.62
1:B:10:THR:HG21	1:B:84:ILE:HD12	1.82	0.61
1:D:127:PRO:HB2	1:D:145:LEU:HD13	1.82	0.61
1:A:235:MET:O	1:A:239:GLN:HG3	2.00	0.61
1:F:192:ASP:HB2	4:F:550:HOH:O	2.00	0.61
1:D:21:MET:CE	1:D:206:ALA:HB2	2.30	0.61
1:C:35:GLU:OE1	1:C:37:TYR:OH	2.16	0.60
1:B:184:LYS:C	1:B:185:LYS:HD2	2.27	0.60
1:A:50:LYS:HE3	3:A:402:NDP:O3X	2.02	0.59
1:A:8:GLU:HG2	1:A:9:LYS:H	1.66	0.59
1:C:233:THR:CG2	1:C:236:GLU:HG3	2.33	0.59
1:E:45:ARG:HH22	1:E:50:LYS:HD2	1.66	0.59
1:E:44:THR:OG1	1:E:45:ARG:HD3	2.02	0.59
1:B:185:LYS:HA	1:B:185:LYS:CE	2.25	0.58
1:D:89:MET:HE1	1:D:102:GLN:HG3	1.84	0.58
3:C:402:NDP:O5D	3:C:402:NDP:H6N	2.04	0.58
1:B:90:SER:HB3	3:B:402:NDP:H8A	1.85	0.58
1:E:307:THR:HG23	1:E:311:GLU:HG3	1.86	0.57
1:D:52:GLN:OE1	1:E:24:ARG:NH2	2.38	0.57
1:B:37:TYR:CE2	1:B:63:ARG:HD2	2.40	0.57
1:B:83:ASP:HB3	1:B:116:LYS:HD2	1.86	0.57
1:B:49:GLU:HG2	1:B:50:LYS:N	2.20	0.56
1:B:191:GLY:N	1:B:254:ILE:O	2.35	0.56
1:B:233:THR:HG22	1:B:236:GLU:CG	2.36	0.56
1:F:311:GLU:OE2	4:F:501:HOH:O	2.17	0.56
1:B:261:ALA:N	4:B:502:HOH:O	2.39	0.56
1:C:9:LYS:O	1:C:10:THR:HB	2.05	0.56
1:D:279:HIS:ND1	1:D:283:GLU:OE2	2.31	0.56
1:A:305:LYS:HA	1:A:305:LYS:CE	2.35	0.56
1:D:39:LEU:CD1	1:D:67:ALA:HB3	2.36	0.56
1:E:305:LYS:CE	1:E:305:LYS:HA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:HG22	1:B:236:GLU:HG3	1.88	0.55
1:B:254:ILE:HG13	1:B:258:ASP:HB3	1.88	0.55
1:C:124:GLY:HA3	2:C:401:GFR:OAZ	2.06	0.55
3:F:402:NDP:O5D	3:F:402:NDP:H6N	2.06	0.55
1:C:8:GLU:HG3	1:C:9:LYS:N	2.20	0.55
1:C:47:ASP:OD2	4:C:504:HOH:O	2.18	0.55
1:F:50:LYS:HE3	3:F:402:NDP:O3X	2.06	0.55
1:A:8:GLU:HG2	1:A:9:LYS:N	2.23	0.54
1:C:256:ALA:O	1:C:260:LEU:HD12	2.07	0.54
1:D:171:ALA:CB	1:D:309:MET:CE	2.86	0.54
1:E:19:GLY:HA3	3:E:402:NDP:H52A	1.90	0.54
1:E:72:HIS:ND1	4:E:506:HOH:O	2.33	0.54
1:C:9:LYS:HD2	1:C:33:GLY:O	2.08	0.53
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.90	0.53
1:D:116:LYS:NZ	1:D:117:ARG:HE	2.06	0.53
1:D:279:HIS:HD1	1:D:283:GLU:CD	2.15	0.53
1:E:10:THR:CG2	1:E:84:ILE:HD12	2.39	0.53
3:B:402:NDP:O5D	3:B:402:NDP:H6N	2.07	0.53
1:B:89:MET:HE1	1:B:102:GLN:HG3	1.90	0.53
1:C:259:PHE:CE2	1:C:274:LEU:HD23	2.44	0.53
1:D:303:ASP:OD1	1:D:303:ASP:N	2.42	0.53
1:E:45:ARG:NH2	1:E:50:LYS:HD2	2.24	0.53
1:C:157:PRO:HB3	1:C:219:ILE:HD11	1.91	0.52
1:B:177:MET:HG2	1:B:277:PHE:CZ	2.45	0.52
1:B:278:TYR:HD2	1:B:282:TYR:CD2	2.28	0.52
1:B:196:LYS:HD2	1:B:231:VAL:HG12	1.91	0.52
1:A:166:PHE:HB3	1:A:202:GLU:OE1	2.10	0.52
1:B:233:THR:HG23	1:B:236:GLU:N	2.05	0.52
1:C:49:GLU:HA	1:C:49:GLU:OE1	2.08	0.52
1:C:189:ILE:HD12	1:C:235:MET:CE	2.40	0.52
1:B:166:PHE:H	3:B:402:NDP:H72N	1.57	0.51
1:B:236:GLU:O	1:B:240:ILE:HG13	2.11	0.51
1:D:40:GLN:HG3	1:D:54:LEU:HD21	1.92	0.51
1:C:54:LEU:HD22	1:C:64:LEU:HD22	1.93	0.51
1:D:47:ASP:OD2	4:D:503:HOH:O	2.19	0.51
1:E:196:LYS:HD3	1:E:233:THR:HG23	1.93	0.51
1:D:13:LEU:HB2	1:D:82:VAL:HG11	1.93	0.51
1:D:171:ALA:HB1	1:D:309:MET:HE1	1.93	0.51
1:B:278:TYR:HD2	1:B:282:TYR:HD2	1.58	0.51
1:F:184:LYS:HE2	4:F:540:HOH:O	2.11	0.50
1:C:9:LYS:O	1:C:10:THR:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PHE:H	3:A:402:NDP:H72N	1.60	0.50
1:C:176:GLN:CD	1:C:187:VAL:HG23	2.36	0.50
1:F:48:ILE:O	1:F:52:GLN:HG3	2.12	0.50
1:A:21:MET:CE	1:A:206:ALA:HB2	2.42	0.49
1:A:35:GLU:HG2	1:A:37:TYR:CE2	2.46	0.49
1:E:165:CYS:HA	3:E:402:NDP:H72N	1.77	0.49
1:E:307:THR:CG2	1:E:311:GLU:HG3	2.42	0.49
1:F:196:LYS:HD3	1:F:233:THR:HG23	1.94	0.49
1:A:49:GLU:HA	1:A:49:GLU:OE1	2.12	0.49
1:D:214:ASP:OD2	4:D:502:HOH:O	2.18	0.49
1:A:44:THR:O	1:A:45:ARG:HB2	2.13	0.49
1:A:35:GLU:HG2	1:A:37:TYR:HE2	1.77	0.49
1:B:272:ALA:N	4:B:512:HOH:O	2.45	0.49
1:D:213:LEU:HD12	1:D:214:ASP:N	2.27	0.49
1:E:44:THR:C	1:E:45:ARG:HD3	2.37	0.49
1:F:265:ASP:OD2	1:F:265:ASP:N	2.46	0.49
1:B:92:VAL:HG23	1:B:93:HIS:CG	2.48	0.49
1:B:129:ARG:O	1:B:129:ARG:HG2	2.13	0.49
1:D:90:SER:HA	3:D:402:NDP:O3	2.12	0.49
1:F:305:LYS:HG3	1:F:305:LYS:O	2.12	0.49
1:A:260:LEU:N	1:A:260:LEU:HD12	2.28	0.48
1:B:59:ARG:NH2	4:B:507:HOH:O	2.34	0.48
1:E:303:ASP:OD1	1:E:303:ASP:N	2.46	0.48
1:A:157:PRO:HB3	1:A:219:ILE:HD11	1.96	0.48
1:F:10:THR:HG21	1:F:84:ILE:HD12	1.95	0.48
1:B:233:THR:CG2	1:B:236:GLU:CG	2.90	0.48
1:B:272:ALA:HB1	1:B:276:HIS:CE1	2.48	0.48
1:F:239:GLN:OE1	4:F:502:HOH:O	2.20	0.48
1:B:94:PHE:HB3	4:B:503:HOH:O	2.13	0.48
1:D:89:MET:HE1	1:D:102:GLN:CG	2.43	0.48
1:B:92:VAL:HG23	1:B:93:HIS:ND1	2.28	0.48
1:C:171:ALA:HA	1:C:237:LEU:HD21	1.96	0.48
1:C:196:LYS:HD2	1:C:231:VAL:HG12	1.96	0.48
1:C:21:MET:CE	1:C:206:ALA:HB2	2.44	0.47
1:C:176:GLN:NE2	1:C:187:VAL:HG23	2.30	0.47
1:B:24:ARG:NH2	1:F:52:GLN:OE1	2.47	0.47
1:C:76:VAL:O	1:C:80:LYS:HG3	2.14	0.47
1:E:19:GLY:CA	3:E:402:NDP:H52A	2.45	0.47
1:B:89:MET:HB2	1:B:89:MET:HE3	1.23	0.47
1:E:19:GLY:HA3	3:E:402:NDP:C5B	2.45	0.47
1:E:46:VAL:HG12	1:E:46:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD11	1:A:241:TRP:CD1	2.50	0.47
1:F:129:ARG:O	1:F:130:MET:HB2	2.14	0.47
1:F:100:LEU:HG	1:F:143:GLN:OE1	2.14	0.46
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.31	0.46
1:C:233:THR:CG2	1:C:236:GLU:CG	2.94	0.46
1:D:252:THR:HG21	1:F:271:GLN:CG	2.43	0.46
1:B:110:LYS:NZ	4:B:515:HOH:O	2.48	0.46
1:D:216:PRO:O	1:D:219:ILE:HG22	2.15	0.46
1:B:20:THR:HG21	1:F:48:ILE:HD13	1.97	0.46
1:C:90:SER:HB3	3:C:402:NDP:O1A	2.16	0.46
1:C:183:PRO:O	4:C:505:HOH:O	2.21	0.46
1:A:48:ILE:O	1:A:52:GLN:HG3	2.16	0.46
1:B:127:PRO:HB2	1:B:145:LEU:HD13	1.97	0.46
1:C:22:GLY:O	1:C:26:VAL:HG23	2.16	0.46
1:C:173:ASN:O	1:C:176:GLN:HG2	2.16	0.46
1:B:48:ILE:O	1:B:52:GLN:HG3	2.15	0.45
1:D:100:LEU:HD13	1:D:143:GLN:HB3	1.99	0.45
1:A:10:THR:CG2	1:A:84:ILE:HD12	2.46	0.45
1:B:247:LYS:NZ	4:B:517:HOH:O	2.50	0.45
1:C:285:CYS:HB3	4:C:518:HOH:O	2.16	0.45
1:D:116:LYS:HZ3	1:D:117:ARG:NH2	2.06	0.45
1:E:166:PHE:H	3:E:402:NDP:H72N	1.62	0.45
1:F:89:MET:HB3	1:F:89:MET:HE3	1.49	0.45
1:B:202:GLU:CD	1:B:202:GLU:H	2.25	0.45
1:E:189:ILE:HG13	1:E:235:MET:HE1	1.98	0.45
1:A:89:MET:HE1	3:A:402:NDP:N3A	2.30	0.45
1:C:21:MET:HE1	1:C:206:ALA:HB2	1.98	0.45
1:C:273:GLY:O	1:C:276:HIS:HB2	2.17	0.45
1:B:233:THR:HG22	1:B:236:GLU:CD	2.42	0.45
1:E:50:LYS:CE	3:E:402:NDP:O3X	2.64	0.45
1:B:174:LEU:HD11	1:B:241:TRP:CD1	2.52	0.45
1:C:170:PHE:HE1	3:C:402:NDP:N7N	2.14	0.44
1:D:171:ALA:CB	1:D:309:MET:HE2	2.40	0.44
1:D:103:LEU:O	1:D:107:GLU:HG3	2.18	0.44
1:D:119:LEU:HD12	1:D:119:LEU:N	2.33	0.44
3:D:402:NDP:O5D	3:D:402:NDP:H6N	2.17	0.44
1:A:98:SER:O	1:A:101:VAL:HG22	2.18	0.44
1:B:259:PHE:CD1	1:B:282:TYR:HE2	2.36	0.44
1:A:8:GLU:CG	1:A:9:LYS:H	2.30	0.44
1:B:278:TYR:CD2	1:B:282:TYR:CD2	3.06	0.43
1:F:171:ALA:HA	1:F:237:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:HD12	1:C:235:MET:HE2	2.01	0.43
1:D:202:GLU:CD	1:D:202:GLU:H	2.26	0.43
1:A:89:MET:HE3	1:A:89:MET:HB3	1.89	0.43
1:A:176:GLN:NE2	1:A:187:VAL:HG22	2.32	0.43
1:D:171:ALA:CB	1:D:309:MET:HE1	2.48	0.43
1:A:37:TYR:CE1	1:A:63:ARG:HD2	2.53	0.43
1:B:242:GLU:OE2	1:B:251:LYS:NZ	2.44	0.43
1:A:197:VAL:HG12	1:A:198:VAL:N	2.34	0.43
1:B:10:THR:CG2	1:B:84:ILE:HD12	2.46	0.43
1:B:90:SER:HB2	3:B:402:NDP:O1A	2.19	0.43
1:D:116:LYS:HZ2	1:D:117:ARG:HE	1.66	0.43
1:A:303:ASP:OD1	1:A:303:ASP:N	2.51	0.43
1:E:129:ARG:O	1:E:130:MET:HB2	2.19	0.43
1:A:119:LEU:HG	1:A:159:THR:HB	2.00	0.43
1:B:190:TYR:HA	1:B:254:ILE:HG23	2.01	0.43
1:D:105:LEU:O	1:D:109:ILE:HG13	2.19	0.43
1:F:196:LYS:HD3	1:F:233:THR:CG2	2.49	0.43
1:A:305:LYS:HA	1:A:305:LYS:HE3	2.01	0.43
1:B:239:GLN:NE2	4:B:519:HOH:O	2.51	0.43
1:E:196:LYS:HD3	1:E:233:THR:CG2	2.48	0.43
1:B:176:GLN:NE2	1:B:187:VAL:HG23	2.34	0.42
1:B:241:TRP:O	1:B:244:LEU:N	2.52	0.42
1:F:89:MET:HA	3:F:402:NDP:O4B	2.19	0.42
1:B:272:ALA:HB1	1:B:276:HIS:HE1	1.85	0.42
3:E:402:NDP:H6N	3:E:402:NDP:O5D	2.20	0.42
1:F:90:SER:HB3	3:F:402:NDP:O1A	2.19	0.42
1:A:176:GLN:NE2	1:A:187:VAL:CG2	2.82	0.42
1:B:198:VAL:HG11	1:B:226:ARG:HA	2.02	0.42
1:E:45:ARG:HH21	1:E:47:ASP:CG	2.18	0.42
1:A:262:ASP:O	1:A:263:ILE:HB	2.20	0.42
1:B:309:MET:HA	1:B:309:MET:CE	2.47	0.42
1:C:105:LEU:O	1:C:109:ILE:HG13	2.19	0.42
1:D:170:PHE:HE2	3:D:402:NDP:N7N	2.17	0.42
1:A:212:THR:HA	1:A:301:TYR:OH	2.19	0.42
1:C:23:ARG:O	1:C:27:ARG:HG3	2.20	0.42
1:C:235:MET:HE2	1:C:235:MET:HB2	1.94	0.42
1:A:166:PHE:CD2	3:A:402:NDP:C7N	3.03	0.42
1:B:192:ASP:O	1:B:192:ASP:OD2	2.38	0.42
1:C:202:GLU:H	1:C:202:GLU:CD	2.27	0.42
1:E:44:THR:O	1:E:45:ARG:HG3	2.19	0.42
3:A:402:NDP:O5D	3:A:402:NDP:H6N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:THR:OG1	3:D:402:NDP:O1X	2.24	0.41
1:D:124:GLY:HA3	2:D:401:GFR:OAZ	2.20	0.41
1:E:39:LEU:HD11	1:E:67:ALA:HB3	2.02	0.41
1:C:63:ARG:NH2	1:E:8:GLU:HB3	2.34	0.41
1:D:285:CYS:HB3	4:D:528:HOH:O	2.20	0.41
1:E:315:ILE:HD12	1:E:315:ILE:HA	1.87	0.41
1:E:89:MET:O	3:E:402:NDP:H3D	2.20	0.41
1:E:45:ARG:HE	1:E:45:ARG:HB2	1.71	0.41
1:C:99:ILE:HD13	1:C:99:ILE:HA	1.93	0.41
1:C:213:LEU:HD12	1:C:214:ASP:N	2.36	0.41
1:B:59:ARG:NE	4:B:507:HOH:O	2.42	0.41
1:B:97:HIS:N	1:B:143:GLN:OE1	2.54	0.41
1:B:180:LEU:HD21	1:F:46:VAL:HG13	2.02	0.41
1:C:243:LYS:O	1:C:243:LYS:HG3	2.18	0.41
1:C:292:GLY:O	1:C:295:GLU:HG2	2.21	0.41
1:B:48:ILE:HG22	4:F:542:HOH:O	2.21	0.41
1:B:89:MET:HG2	3:B:402:NDP:H1B	2.02	0.41
1:B:119:LEU:HD12	1:B:119:LEU:N	2.35	0.41
1:C:99:ILE:HB	1:C:143:GLN:HG3	2.01	0.41
1:A:279:HIS:HA	1:A:283:GLU:HG3	2.02	0.41
1:C:233:THR:HG22	1:C:236:GLU:CD	2.44	0.41
1:C:97:HIS:O	1:C:98:SER:C	2.65	0.40
1:D:117:ARG:HD3	1:D:159:THR:OG1	2.20	0.40
1:A:107:GLU:OE2	1:A:107:GLU:HA	2.22	0.40
1:C:303:ASP:OD2	1:C:303:ASP:N	2.47	0.40
1:E:21:MET:HE3	1:E:25:ILE:HG13	2.04	0.40
1:E:42:PRO:O	1:E:43:GLU:C	2.63	0.40
1:F:265:ASP:O	1:F:267:GLU:N	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASP:OD1	1:D:45:ARG:NH2[5_554]	2.05	0.15
1:A:24:ARG:NH2	1:C:52:GLN:OE1[3_454]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	278/317 (88%)	270 (97%)	7 (2%)	1 (0%)	30	34
1	B	281/317 (89%)	270 (96%)	11 (4%)	0	100	100
1	C	279/317 (88%)	268 (96%)	9 (3%)	2 (1%)	18	19
1	D	281/317 (89%)	275 (98%)	6 (2%)	0	100	100
1	E	279/317 (88%)	271 (97%)	8 (3%)	0	100	100
1	F	296/317 (93%)	286 (97%)	10 (3%)	0	100	100
All	All	1694/1902 (89%)	1640 (97%)	51 (3%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	261	ALA
1	A	45	ARG
1	C	10	THR

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	244/271 (90%)	241 (99%)	3 (1%)	63	78
1	B	246/271 (91%)	238 (97%)	8 (3%)	33	45
1	C	244/271 (90%)	242 (99%)	2 (1%)	73	85
1	D	245/271 (90%)	238 (97%)	7 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	244/271 (90%)	236 (97%)	8 (3%)	33	45
1	F	257/271 (95%)	249 (97%)	8 (3%)	35	48
All	All	1480/1626 (91%)	1444 (98%)	36 (2%)	43	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	97	HIS
1	A	305	LYS
1	B	89	MET
1	B	90	SER
1	B	97	HIS
1	B	130	MET
1	B	145	LEU
1	B	185	LYS
1	B	212	THR
1	B	258	ASP
1	C	45	ARG
1	C	233	THR
1	D	10	THR
1	D	89	MET
1	D	100	LEU
1	D	101	VAL
1	D	142	ASP
1	D	212	THR
1	D	247	LYS
1	E	9	LYS
1	E	45	ARG
1	E	89	MET
1	E	104	LYS
1	E	142	ASP
1	E	305	LYS
1	E	308	ARG
1	E	311	GLU
1	F	54	LEU
1	F	77	SER
1	F	89	MET
1	F	101	VAL
1	F	162	VAL
1	F	212	THR

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Mol	Chain	Res	Type
1	F	265	ASP
1	F	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	GLN
1	B	81	GLN
1	C	40	GLN
1	C	97	HIS
1	D	34	HIS
1	D	41	GLN
1	D	73	GLN
1	E	81	GLN
1	F	41	GLN
1	F	93	HIS
1	F	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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
3	NDP	D	402	-	51,52,52	3.50	24 (47%)	71,80,80	1.97	16 (22%)
3	NDP	A	402	-	51,52,52	3.61	24 (47%)	71,80,80	1.90	15 (21%)
2	GFR	B	401	-	28,28,28	1.61	3 (10%)	37,39,39	5.32	13 (35%)
3	NDP	B	402	-	51,52,52	3.47	22 (43%)	71,80,80	1.87	14 (19%)
2	GFR	E	401	-	28,28,28	1.93	4 (14%)	37,39,39	5.40	16 (43%)
2	GFR	A	401	-	28,28,28	1.85	3 (10%)	37,39,39	5.52	17 (45%)
3	NDP	C	402	-	51,52,52	3.51	23 (45%)	71,80,80	1.98	12 (16%)
3	NDP	E	402	-	51,52,52	3.56	24 (47%)	71,80,80	1.91	16 (22%)
2	GFR	C	401	-	28,28,28	1.84	3 (10%)	37,39,39	5.45	15 (40%)
2	GFR	D	401	-	28,28,28	1.65	3 (10%)	37,39,39	5.47	12 (32%)
2	GFR	F	401	-	28,28,28	2.14	5 (17%)	37,39,39	5.44	17 (45%)
3	NDP	F	402	-	51,52,52	3.53	23 (45%)	71,80,80	1.95	14 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	402	-	-	6/34/77/77	0/5/5/5
3	NDP	A	402	-	-	2/34/77/77	0/5/5/5
2	GFR	B	401	-	-	7/14/27/27	0/3/3/3
3	NDP	B	402	-	-	6/34/77/77	0/5/5/5
2	GFR	E	401	-	-	7/14/27/27	0/3/3/3
2	GFR	A	401	-	-	7/14/27/27	0/3/3/3
3	NDP	C	402	-	-	7/34/77/77	0/5/5/5
3	NDP	E	402	-	-	5/34/77/77	0/5/5/5
2	GFR	C	401	-	-	7/14/27/27	0/3/3/3
2	GFR	D	401	-	-	7/14/27/27	0/3/3/3
2	GFR	F	401	-	-	7/14/27/27	0/3/3/3
3	NDP	F	402	-	-	4/34/77/77	0/5/5/5

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NDP	O4B-C1B	9.02	1.62	1.42
3	C	402	NDP	O4B-C1B	8.89	1.62	1.42
3	E	402	NDP	O4B-C1B	8.84	1.62	1.42
3	B	402	NDP	O4B-C1B	8.78	1.62	1.42
3	C	402	NDP	C2B-C1B	-8.71	1.31	1.53
3	A	402	NDP	C2B-C1B	-8.68	1.31	1.53
3	B	402	NDP	C2B-C1B	-8.68	1.31	1.53
3	A	402	NDP	O4B-C1B	8.66	1.62	1.42
3	A	402	NDP	O4D-C1D	8.66	1.62	1.42
3	E	402	NDP	C2B-C1B	-8.66	1.31	1.53
3	D	402	NDP	C2B-C1B	-8.58	1.32	1.53
3	C	402	NDP	O4D-C1D	8.56	1.61	1.42
3	E	402	NDP	O4D-C1D	8.55	1.61	1.42
3	F	402	NDP	O4B-C1B	8.45	1.61	1.42
3	D	402	NDP	O4D-C1D	8.23	1.61	1.42
3	F	402	NDP	C2B-C1B	-8.13	1.33	1.53
3	F	402	NDP	O4D-C1D	7.97	1.60	1.42
3	B	402	NDP	O4D-C1D	7.95	1.60	1.42
3	F	402	NDP	C2D-C1D	-7.27	1.30	1.53
3	B	402	NDP	C2D-C1D	-7.21	1.30	1.53
3	E	402	NDP	C2D-C1D	-7.20	1.30	1.53
3	C	402	NDP	C2D-C1D	-7.11	1.31	1.53
3	C	402	NDP	C6N-C5N	7.02	1.54	1.33
3	D	402	NDP	C2D-C1D	-6.99	1.31	1.53
3	A	402	NDP	C2D-C1D	-6.97	1.31	1.53
3	A	402	NDP	C6N-C5N	6.94	1.54	1.33
3	D	402	NDP	C6N-C5N	6.93	1.54	1.33
3	E	402	NDP	C6N-C5N	6.92	1.54	1.33
2	C	401	GFR	CAR-CAN	-6.75	1.39	1.51
3	B	402	NDP	C6N-C5N	6.74	1.53	1.33
3	D	402	NDP	O4D-C4D	-6.69	1.30	1.45
3	A	402	NDP	PA-O3	6.62	1.66	1.59
3	F	402	NDP	PA-O3	6.59	1.66	1.59
3	F	402	NDP	C6N-C5N	6.59	1.53	1.33
3	F	402	NDP	O4B-C4B	-6.51	1.30	1.45
3	E	402	NDP	O4B-C4B	-6.47	1.30	1.45
3	E	402	NDP	O4D-C4D	-6.44	1.30	1.45
3	F	402	NDP	O4D-C4D	-6.39	1.30	1.45
3	B	402	NDP	O4B-C4B	-6.30	1.31	1.45
3	D	402	NDP	O4B-C4B	-6.30	1.31	1.45
3	C	402	NDP	O4D-C4D	-6.27	1.31	1.45
3	A	402	NDP	O4B-C4B	-6.25	1.31	1.45
3	B	402	NDP	O4D-C4D	-6.22	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	O4D-C4D	-6.20	1.31	1.45
3	C	402	NDP	O4B-C4B	-6.14	1.31	1.45
2	E	401	GFR	CAR-CAN	-6.07	1.40	1.51
2	D	401	GFR	CAR-CAN	-6.03	1.40	1.51
2	F	401	GFR	CAJ-CAE	-5.99	1.37	1.51
2	F	401	GFR	CAR-CAN	-5.83	1.41	1.51
3	A	402	NDP	C2N-C3N	5.81	1.51	1.35
2	C	401	GFR	CAJ-CAE	-5.73	1.37	1.51
2	A	401	GFR	CAR-CAN	-5.71	1.41	1.51
3	C	402	NDP	C2N-C3N	5.60	1.50	1.35
3	E	402	NDP	PA-O3	5.60	1.65	1.59
3	E	402	NDP	C2N-C3N	5.57	1.50	1.35
2	A	401	GFR	CAJ-CAE	-5.56	1.38	1.51
3	D	402	NDP	C2N-C3N	5.47	1.50	1.35
3	E	402	NDP	C6A-N6A	5.46	1.48	1.34
3	B	402	NDP	C2N-C3N	5.44	1.50	1.35
3	F	402	NDP	PN-O3	5.39	1.65	1.59
2	E	401	GFR	CAJ-CAE	-5.34	1.38	1.51
3	B	402	NDP	C6A-N6A	5.29	1.47	1.34
3	A	402	NDP	C6A-N6A	5.28	1.47	1.34
3	B	402	NDP	PA-O3	5.23	1.65	1.59
3	D	402	NDP	C6A-N6A	5.22	1.47	1.34
2	B	401	GFR	CAR-CAN	-5.22	1.42	1.51
3	A	402	NDP	PN-O3	5.17	1.65	1.59
3	C	402	NDP	C6A-N6A	5.13	1.47	1.34
3	F	402	NDP	C2N-C3N	5.13	1.49	1.35
2	F	401	GFR	OAM-CAN	5.12	1.52	1.43
3	C	402	NDP	PA-O3	5.07	1.65	1.59
3	D	402	NDP	PA-O3	5.03	1.64	1.59
2	D	401	GFR	CAJ-CAE	-5.00	1.39	1.51
3	F	402	NDP	C6A-N6A	4.88	1.46	1.34
2	B	401	GFR	CAJ-CAE	-4.70	1.40	1.51
3	E	402	NDP	PN-O3	4.59	1.64	1.59
2	E	401	GFR	OAM-CAN	4.30	1.51	1.43
2	A	401	GFR	OAM-CAN	4.26	1.51	1.43
3	E	402	NDP	C7N-N7N	4.21	1.45	1.33
3	C	402	NDP	C7N-N7N	4.16	1.45	1.33
3	B	402	NDP	C7N-N7N	3.96	1.44	1.33
3	C	402	NDP	PN-O3	3.94	1.63	1.59
3	A	402	NDP	C7N-N7N	3.93	1.44	1.33
3	D	402	NDP	C7N-N7N	3.82	1.44	1.33
3	D	402	NDP	PN-O3	3.63	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	NDP	C7N-N7N	3.56	1.43	1.33
2	B	401	GFR	OAM-CAN	3.53	1.49	1.43
3	A	402	NDP	P2B-O2B	3.42	1.65	1.59
3	E	402	NDP	O3D-C3D	-3.39	1.34	1.43
2	F	401	GFR	OAM-CAL	-3.38	1.36	1.43
3	C	402	NDP	C4N-C5N	3.26	1.57	1.49
3	D	402	NDP	C4N-C5N	3.07	1.57	1.49
3	F	402	NDP	C4N-C5N	3.06	1.56	1.49
3	D	402	NDP	O3D-C3D	-3.05	1.35	1.43
3	F	402	NDP	O3B-C3B	-3.01	1.35	1.43
3	B	402	NDP	C5A-C4A	-3.01	1.33	1.39
3	C	402	NDP	O3D-C3D	-2.99	1.35	1.43
3	B	402	NDP	O3B-C3B	-2.95	1.35	1.43
3	F	402	NDP	C5A-C4A	-2.89	1.33	1.39
3	D	402	NDP	C6N-N1N	2.88	1.44	1.37
3	B	402	NDP	PN-O3	2.88	1.62	1.59
3	B	402	NDP	C5A-N7A	-2.86	1.33	1.39
3	D	402	NDP	O7N-C7N	-2.86	1.17	1.24
3	F	402	NDP	C6N-N1N	2.85	1.44	1.37
3	B	402	NDP	C6N-N1N	2.84	1.44	1.37
3	B	402	NDP	O3D-C3D	-2.83	1.35	1.43
3	B	402	NDP	C4N-C3N	2.82	1.55	1.50
3	F	402	NDP	P2B-O2B	2.82	1.64	1.59
3	C	402	NDP	O3B-C3B	-2.79	1.36	1.43
3	A	402	NDP	O3D-C3D	-2.78	1.36	1.43
3	A	402	NDP	O3B-C3B	-2.78	1.36	1.43
3	F	402	NDP	O3D-C3D	-2.77	1.36	1.43
3	A	402	NDP	O2D-C2D	2.76	1.49	1.43
3	E	402	NDP	O3B-C3B	-2.75	1.36	1.43
3	A	402	NDP	C6N-N1N	2.74	1.43	1.37
3	F	402	NDP	C5A-N7A	-2.74	1.34	1.39
3	D	402	NDP	O3B-C3B	-2.72	1.36	1.43
2	F	401	GFR	CAO-CAN	-2.70	1.48	1.54
3	B	402	NDP	C4N-C5N	2.70	1.56	1.49
3	C	402	NDP	C6N-N1N	2.69	1.43	1.37
3	F	402	NDP	C8A-N9A	-2.69	1.33	1.37
3	C	402	NDP	C5A-C4A	-2.68	1.34	1.39
3	A	402	NDP	C5A-C4A	-2.68	1.34	1.39
3	C	402	NDP	C7N-C3N	2.67	1.54	1.48
3	A	402	NDP	C8A-N9A	-2.66	1.33	1.37
3	E	402	NDP	C6N-N1N	2.63	1.43	1.37
3	B	402	NDP	C8A-N9A	-2.60	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C7N-C3N	2.59	1.54	1.48
3	A	402	NDP	C4N-C3N	2.58	1.54	1.50
3	A	402	NDP	C4N-C5N	2.56	1.55	1.49
2	E	401	GFR	OAM-CAL	-2.55	1.38	1.43
3	D	402	NDP	C5A-C4A	-2.53	1.34	1.39
3	A	402	NDP	C5A-N7A	-2.52	1.34	1.39
3	D	402	NDP	C4N-C3N	2.52	1.54	1.50
3	F	402	NDP	C7N-C3N	2.51	1.54	1.48
3	E	402	NDP	C4N-C5N	2.49	1.55	1.49
3	B	402	NDP	O2D-C2D	2.49	1.49	1.43
3	D	402	NDP	O2D-C2D	2.49	1.49	1.43
2	D	401	GFR	OAM-CAN	2.48	1.48	1.43
3	D	402	NDP	P2B-O2B	2.46	1.63	1.59
3	A	402	NDP	C7N-C3N	2.46	1.54	1.48
3	E	402	NDP	C8A-N9A	-2.45	1.33	1.37
3	C	402	NDP	O2D-C2D	2.44	1.49	1.43
3	C	402	NDP	O7N-C7N	-2.43	1.18	1.24
3	E	402	NDP	C5A-C4A	-2.41	1.34	1.39
3	E	402	NDP	O2D-C2D	2.41	1.48	1.43
3	E	402	NDP	C5A-N7A	-2.32	1.34	1.39
2	C	401	GFR	OAM-CAN	2.31	1.47	1.43
3	D	402	NDP	C7N-C3N	2.28	1.53	1.48
3	E	402	NDP	O7N-C7N	-2.25	1.19	1.24
3	C	402	NDP	C4N-C3N	2.24	1.54	1.50
3	D	402	NDP	C5A-N7A	-2.23	1.35	1.39
3	F	402	NDP	C4N-C3N	2.23	1.54	1.50
3	C	402	NDP	C8A-N9A	-2.22	1.33	1.37
3	E	402	NDP	C7N-C3N	2.17	1.53	1.48
3	F	402	NDP	O2D-C2D	2.16	1.48	1.43
3	A	402	NDP	O7N-C7N	-2.12	1.19	1.24
3	D	402	NDP	C8A-N9A	-2.09	1.34	1.37
3	E	402	NDP	C4N-C3N	2.08	1.54	1.50
3	C	402	NDP	C5A-N7A	-2.07	1.35	1.39
3	E	402	NDP	P2B-O2B	2.03	1.63	1.59

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	GFR	CAJ-CAK-CAL	-23.40	80.35	112.66
2	C	401	GFR	CAJ-CAK-CAL	-23.01	80.89	112.66
2	D	401	GFR	CAJ-CAK-CAL	-22.83	81.14	112.66
2	B	401	GFR	CAJ-CAK-CAL	-22.50	81.59	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GFR	CAJ-CAK-CAL	-22.40	81.74	112.66
2	A	401	GFR	CAJ-CAK-CAL	-21.92	82.39	112.66
2	A	401	GFR	CAL-CAK-CAO	-12.31	87.02	101.71
2	D	401	GFR	CAL-CAK-CAO	-12.07	87.31	101.71
2	B	401	GFR	CAL-CAK-CAO	-11.82	87.60	101.71
2	A	401	GFR	CAL-OAM-CAN	-11.66	82.56	106.43
2	F	401	GFR	CAL-OAM-CAN	-11.56	82.77	106.43
2	C	401	GFR	CAL-OAM-CAN	-11.54	82.80	106.43
2	C	401	GFR	CAL-CAK-CAO	-11.46	88.04	101.71
2	E	401	GFR	CAL-OAM-CAN	-11.44	83.00	106.43
2	D	401	GFR	CAL-OAM-CAN	-11.37	83.16	106.43
2	B	401	GFR	CAL-OAM-CAN	-11.03	83.85	106.43
2	E	401	GFR	CAL-CAK-CAO	-10.92	88.67	101.71
2	F	401	GFR	CAL-CAK-CAO	-10.09	89.67	101.71
2	B	401	GFR	OAM-CAN-CAR	9.44	120.89	110.39
2	D	401	GFR	OAM-CAN-CAR	9.19	120.61	110.39
2	A	401	GFR	OAM-CAL-CAK	9.12	117.86	105.91
2	F	401	GFR	OAM-CAN-CAR	9.07	120.48	110.39
2	C	401	GFR	OAM-CAN-CAR	8.83	120.21	110.39
2	D	401	GFR	OAM-CAL-CAK	8.62	117.20	105.91
2	E	401	GFR	OAM-CAL-CAK	8.58	117.15	105.91
2	A	401	GFR	OAM-CAN-CAR	8.51	119.85	110.39
2	B	401	GFR	OAM-CAL-CAK	8.51	117.06	105.91
2	E	401	GFR	OAM-CAN-CAR	8.50	119.84	110.39
2	F	401	GFR	OAM-CAL-CAK	7.86	116.21	105.91
2	C	401	GFR	OAM-CAL-CAK	7.85	116.19	105.91
2	D	401	GFR	CAA-OAB-CAC	-7.02	107.22	117.51
2	E	401	GFR	CAA-OAB-CAC	-6.92	107.36	117.51
2	C	401	GFR	CAA-OAB-CAC	-6.82	107.50	117.51
2	A	401	GFR	CAA-OAB-CAC	-6.43	108.09	117.51
2	F	401	GFR	OAM-CAN-CAO	-6.02	98.29	104.73
3	D	402	NDP	C5A-C4A-N3A	-5.76	118.78	126.72
3	D	402	NDP	N6A-C6A-N1A	-5.69	105.71	118.38
3	C	402	NDP	N6A-C6A-N1A	-5.63	105.84	118.38
2	E	401	GFR	OAM-CAN-CAO	-5.63	98.71	104.73
3	C	402	NDP	C4A-N9A-C1B	-5.52	113.73	126.63
3	F	402	NDP	C4A-N9A-C1B	-5.46	113.87	126.63
2	A	401	GFR	OAM-CAN-CAO	-5.46	98.89	104.73
3	B	402	NDP	N3A-C2A-N1A	-5.45	120.33	128.58
3	B	402	NDP	C5A-C4A-N3A	-5.39	119.29	126.72
2	A	401	GFR	CAP-CAO-CAK	-5.37	102.06	113.56
3	E	402	NDP	C5A-C4A-N3A	-5.35	119.35	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NDP	N3A-C2A-N1A	-5.30	120.56	128.58
3	F	402	NDP	N3A-C2A-N1A	-5.26	120.63	128.58
2	B	401	GFR	OAM-CAN-CAO	-5.25	99.11	104.73
3	A	402	NDP	C4A-N9A-C1B	-5.25	114.36	126.63
3	D	402	NDP	N3A-C2A-N1A	-5.21	120.69	128.58
3	E	402	NDP	N3A-C2A-N1A	-5.19	120.72	128.58
3	A	402	NDP	N6A-C6A-N1A	-5.17	106.87	118.38
3	C	402	NDP	C5A-C4A-N3A	-5.11	119.68	126.72
3	F	402	NDP	O4B-C1B-N9A	-4.94	98.61	108.09
3	A	402	NDP	C5A-C4A-N3A	-4.91	119.96	126.72
3	A	402	NDP	N3A-C2A-N1A	-4.85	121.24	128.58
2	A	401	GFR	CAY-OAX-CAV	-4.78	110.50	117.51
3	E	402	NDP	N6A-C6A-N1A	-4.74	107.83	118.38
3	B	402	NDP	N6A-C6A-N1A	-4.65	108.02	118.38
3	C	402	NDP	C1B-N9A-C8A	4.62	137.34	127.09
3	D	402	NDP	C4A-N9A-C1B	-4.57	115.95	126.63
3	E	402	NDP	C4A-N9A-C1B	-4.53	116.05	126.63
3	F	402	NDP	N6A-C6A-N1A	-4.52	108.31	118.38
2	F	401	GFR	CAP-CAO-CAK	-4.48	103.96	113.56
2	F	401	GFR	CAJ-CAE-CAD	-4.41	112.85	120.43
3	B	402	NDP	N3A-C4A-N9A	4.39	134.63	127.17
3	B	402	NDP	C4A-N9A-C1B	-4.38	116.38	126.63
3	E	402	NDP	N3A-C4A-N9A	4.36	134.57	127.17
3	F	402	NDP	N9A-C8A-N7A	-4.33	107.80	113.94
2	D	401	GFR	OAM-CAN-CAO	-4.28	100.15	104.73
3	F	402	NDP	C5A-C4A-N3A	-4.23	120.89	126.72
3	A	402	NDP	C1B-N9A-C8A	4.21	136.44	127.09
3	D	402	NDP	N3A-C4A-N9A	4.21	134.33	127.17
3	C	402	NDP	N9A-C8A-N7A	-4.18	108.01	113.94
2	C	401	GFR	OAM-CAN-CAO	-4.15	100.29	104.73
3	D	402	NDP	C5A-C6A-N6A	4.14	133.53	123.29
3	A	402	NDP	N9A-C8A-N7A	-4.13	108.08	113.94
3	F	402	NDP	C4A-N9A-C8A	4.13	110.07	105.74
2	B	401	GFR	CAA-OAB-CAC	-4.09	111.51	117.51
3	C	402	NDP	C5A-C6A-N6A	4.09	133.41	123.29
3	E	402	NDP	N9A-C8A-N7A	-4.06	108.18	113.94
3	B	402	NDP	N9A-C8A-N7A	-4.04	108.20	113.94
3	F	402	NDP	C1B-N9A-C8A	4.02	136.03	127.09
3	F	402	NDP	N3A-C4A-N9A	4.02	134.00	127.17
2	C	401	GFR	CAY-OAX-CAV	-4.01	111.64	117.51
2	D	401	GFR	CAP-CAO-CAK	-3.97	105.07	113.56
3	D	402	NDP	C1B-N9A-C8A	3.92	135.79	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	C5A-C6A-N6A	3.92	132.98	123.29
2	C	401	GFR	CAR-CAN-CAO	-3.88	110.29	115.90
3	D	402	NDP	N9A-C8A-N7A	-3.83	108.50	113.94
3	A	402	NDP	N3A-C4A-N9A	3.79	133.61	127.17
3	C	402	NDP	N3A-C4A-N9A	3.78	133.59	127.17
2	E	401	GFR	CAP-CAO-CAK	-3.74	105.56	113.56
2	E	401	GFR	CAY-OAX-CAV	-3.68	112.11	117.51
2	A	401	GFR	CAS-CAR-CAN	3.56	127.26	120.62
3	D	402	NDP	C2A-N3A-C4A	3.53	120.46	111.83
3	E	402	NDP	C5A-C6A-N6A	3.50	131.95	123.29
2	C	401	GFR	CAP-CAO-CAK	-3.49	106.08	113.56
3	E	402	NDP	C1B-N9A-C8A	3.47	134.80	127.09
3	B	402	NDP	C1B-N9A-C8A	3.46	134.77	127.09
3	C	402	NDP	C5B-C4B-C3B	-3.44	102.82	115.21
3	B	402	NDP	C5A-C6A-N6A	3.44	131.80	123.29
3	A	402	NDP	O4B-C1B-N9A	-3.42	101.53	108.09
2	E	401	GFR	CAJ-CAE-CAD	-3.41	114.58	120.43
3	B	402	NDP	C2A-N3A-C4A	3.40	120.14	111.83
3	C	402	NDP	C2A-N3A-C4A	3.33	119.95	111.83
2	F	401	GFR	CAR-CAN-CAO	-3.26	111.18	115.90
3	F	402	NDP	C5A-C6A-N6A	3.24	131.32	123.29
3	A	402	NDP	C4A-N9A-C8A	3.23	109.13	105.74
2	B	401	GFR	CAP-CAO-CAK	-3.23	106.64	113.56
3	E	402	NDP	C4A-N9A-C8A	3.22	109.12	105.74
3	E	402	NDP	C2A-N3A-C4A	3.22	119.69	111.83
3	E	402	NDP	C4B-O4B-C1B	-3.14	102.54	109.47
2	A	401	GFR	CAW-CAR-CAN	-3.12	113.00	119.88
3	B	402	NDP	C5B-C4B-C3B	-3.10	104.05	115.21
3	C	402	NDP	C4A-N9A-C8A	3.01	108.90	105.74
2	D	401	GFR	CAJ-CAE-CAD	-2.96	115.34	120.43
3	A	402	NDP	C2A-N3A-C4A	2.94	119.01	111.83
2	D	401	GFR	CAR-CAN-CAO	-2.93	111.65	115.90
2	E	401	GFR	CAR-CAN-CAO	-2.91	111.68	115.90
3	B	402	NDP	C4A-N9A-C8A	2.91	108.80	105.74
3	F	402	NDP	C4B-O4B-C1B	-2.84	103.19	109.47
2	B	401	GFR	CAR-CAN-CAO	-2.84	111.79	115.90
2	B	401	GFR	CAS-CAR-CAN	2.83	125.90	120.62
2	C	401	GFR	CAJ-CAE-CAD	-2.82	115.58	120.43
2	D	401	GFR	OAB-CAC-CAH	2.81	118.76	114.55
2	E	401	GFR	CAS-CAR-CAN	2.79	125.83	120.62
3	F	402	NDP	C2A-N3A-C4A	2.77	118.59	111.83
2	F	401	GFR	CAW-CAR-CAN	-2.77	113.77	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GFR	CAJ-CAE-CAD	-2.76	115.70	120.43
2	F	401	GFR	CAA-OAB-CAC	-2.72	113.52	117.51
3	B	402	NDP	O4B-C1B-N9A	-2.72	102.87	108.09
3	D	402	NDP	C5A-N7A-C8A	2.69	107.67	103.45
3	E	402	NDP	C3N-C2N-N1N	-2.67	119.29	123.20
3	E	402	NDP	C6A-C5A-C4A	2.65	120.80	117.18
3	C	402	NDP	C5A-N7A-C8A	2.63	107.59	103.45
3	E	402	NDP	C5A-N7A-C8A	2.60	107.54	103.45
2	C	401	GFR	OAB-CAC-CAH	2.58	118.42	114.55
3	B	402	NDP	C5A-N7A-C8A	2.58	107.51	103.45
3	D	402	NDP	C3N-C2N-N1N	-2.57	119.43	123.20
2	B	401	GFR	CAJ-CAE-CAD	-2.56	116.03	120.43
3	B	402	NDP	C6A-C5A-C4A	2.56	120.67	117.18
2	F	401	GFR	CAS-CAR-CAN	2.55	125.39	120.62
2	A	401	GFR	OAZ-CAU-CAV	-2.52	114.22	120.13
3	A	402	NDP	C5A-N7A-C8A	2.51	107.40	103.45
2	A	401	GFR	CAK-CAO-CAN	2.51	107.21	103.05
2	F	401	GFR	CAF-CAE-CAD	2.49	121.98	118.55
3	F	402	NDP	P2B-O2B-C2B	2.48	130.07	123.43
2	F	401	GFR	OAB-CAC-CAH	2.48	118.26	114.55
3	A	402	NDP	C4B-O4B-C1B	-2.45	104.06	109.47
3	A	402	NDP	C6A-C5A-C4A	2.44	120.50	117.18
2	C	401	GFR	CAW-CAR-CAN	-2.42	114.54	119.88
2	B	401	GFR	CAY-OAX-CAV	-2.41	113.98	117.51
3	D	402	NDP	C6A-C5A-C4A	2.39	120.44	117.18
3	D	402	NDP	C5B-C4B-C3B	-2.39	106.61	115.21
3	D	402	NDP	C4A-N9A-C8A	2.34	108.19	105.74
2	E	401	GFR	CAW-CAR-CAN	-2.33	114.75	119.88
2	F	401	GFR	CAJ-CAE-CAF	2.28	125.14	120.90
3	A	402	NDP	C3N-C2N-N1N	-2.24	119.91	123.20
2	B	401	GFR	CAW-CAR-CAN	-2.23	114.96	119.88
3	D	402	NDP	C2B-C1B-N9A	2.23	117.42	113.75
2	A	401	GFR	CAT-CAS-CAR	-2.22	118.97	121.18
2	F	401	GFR	CAG-CAF-CAE	-2.21	118.09	121.00
3	F	402	NDP	C5A-N7A-C8A	2.20	106.91	103.45
2	F	401	GFR	OAZ-CAU-CAV	-2.19	114.99	120.13
3	E	402	NDP	O4B-C1B-N9A	-2.19	103.89	108.09
2	E	401	GFR	CAJ-CAE-CAF	2.18	124.96	120.90
3	E	402	NDP	O2B-C2B-C1B	-2.17	102.42	110.05
2	C	401	GFR	CAS-CAR-CAN	2.17	124.67	120.62
2	A	401	GFR	OAZ-CAU-CAT	2.16	125.17	119.36
2	E	401	GFR	OAZ-CAU-CAV	-2.11	115.19	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GFR	CAK-CAO-CAN	2.07	106.47	103.05
3	D	402	NDP	O4B-C1B-N9A	-2.05	104.15	108.09
2	E	401	GFR	OAB-CAC-CAH	2.05	117.61	114.55
2	C	401	GFR	OAX-CAV-CAU	2.03	117.60	114.55
2	A	401	GFR	CAR-CAN-CAO	-2.02	112.97	115.90

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GFR	CAE-CAJ-CAK-CAL
2	B	401	GFR	CAE-CAJ-CAK-CAL
2	C	401	GFR	CAE-CAJ-CAK-CAL
2	D	401	GFR	CAE-CAJ-CAK-CAL
2	E	401	GFR	CAE-CAJ-CAK-CAL
2	F	401	GFR	CAE-CAJ-CAK-CAL
3	D	402	NDP	C5B-O5B-PA-O1A
2	D	401	GFR	CAD-CAE-CAJ-CAK
2	F	401	GFR	CAF-CAE-CAJ-CAK
2	A	401	GFR	CAF-CAE-CAJ-CAK
2	C	401	GFR	CAF-CAE-CAJ-CAK
2	D	401	GFR	CAF-CAE-CAJ-CAK
2	F	401	GFR	CAD-CAE-CAJ-CAK
2	E	401	GFR	CAF-CAE-CAJ-CAK
2	C	401	GFR	CAD-CAE-CAJ-CAK
2	B	401	GFR	CAD-CAE-CAJ-CAK
2	B	401	GFR	CAF-CAE-CAJ-CAK
2	E	401	GFR	CAD-CAE-CAJ-CAK
2	A	401	GFR	CAD-CAE-CAJ-CAK
3	E	402	NDP	O4B-C4B-C5B-O5B
3	C	402	NDP	C1B-C2B-O2B-P2B
3	B	402	NDP	C3B-C2B-O2B-P2B
3	C	402	NDP	C3B-C2B-O2B-P2B
3	D	402	NDP	C3B-C4B-C5B-O5B
3	B	402	NDP	C1B-C2B-O2B-P2B
3	E	402	NDP	C1B-C2B-O2B-P2B
2	A	401	GFR	CAO-CAN-CAR-CAS
2	F	401	GFR	CAO-CAN-CAR-CAS
2	C	401	GFR	CAO-CAN-CAR-CAS
2	B	401	GFR	CAO-CAN-CAR-CAS
2	D	401	GFR	OAM-CAN-CAR-CAS
2	F	401	GFR	CAO-CAN-CAR-CAW

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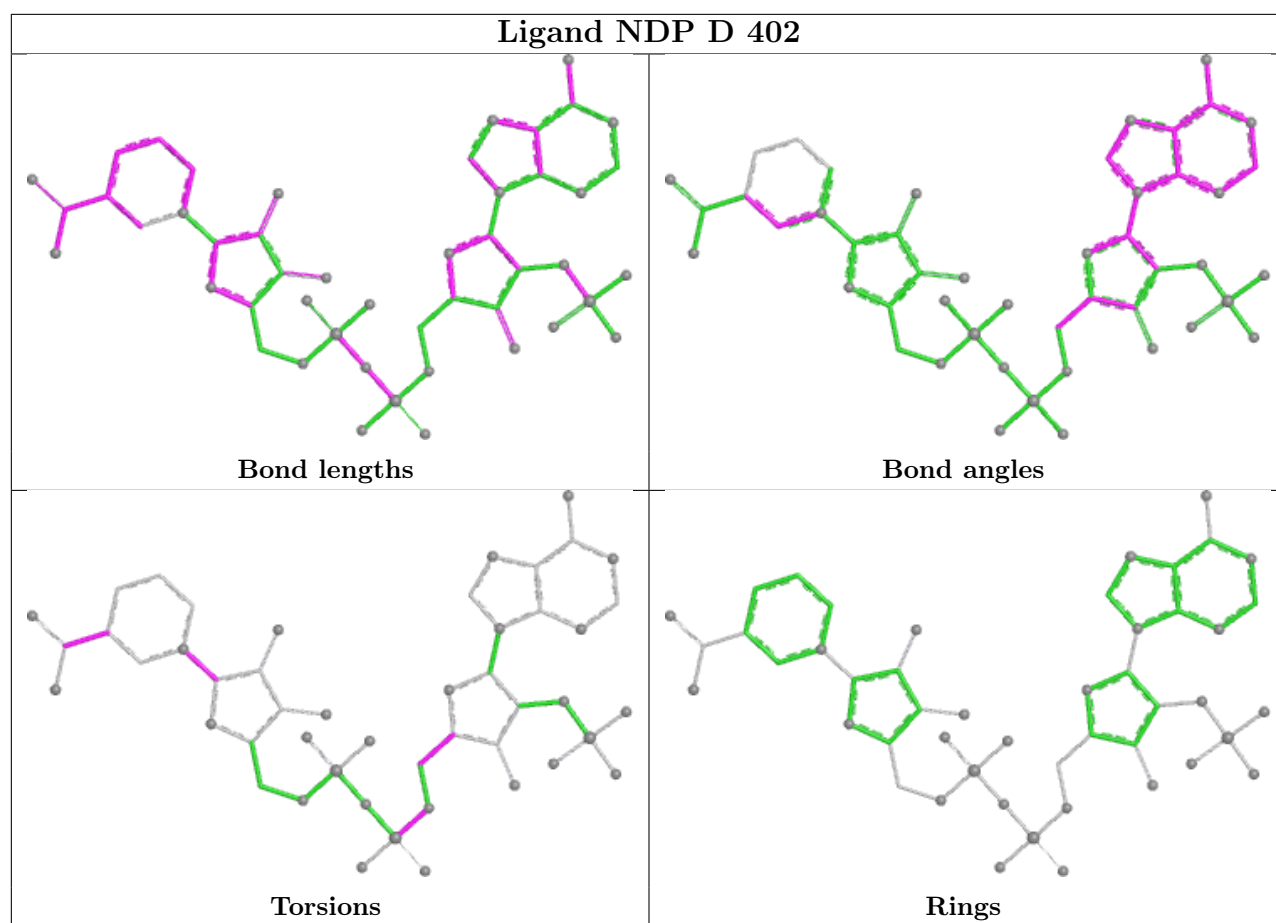
Mol	Chain	Res	Type	Atoms
2	E	401	GFR	OAM-CAN-CAR-CAS
2	B	401	GFR	CAO-CAN-CAR-CAW
2	C	401	GFR	CAO-CAN-CAR-CAW
2	E	401	GFR	CAO-CAN-CAR-CAW
2	F	401	GFR	OAM-CAN-CAR-CAS
2	A	401	GFR	CAO-CAN-CAR-CAW
2	D	401	GFR	CAO-CAN-CAR-CAW
3	C	402	NDP	C2N-C3N-C7N-N7N
2	D	401	GFR	CAO-CAN-CAR-CAS
2	E	401	GFR	CAO-CAN-CAR-CAS
2	A	401	GFR	OAM-CAN-CAR-CAS
3	E	402	NDP	C3B-C2B-O2B-P2B
2	D	401	GFR	OAM-CAN-CAR-CAW
3	D	402	NDP	O4D-C1D-N1N-C2N
3	C	402	NDP	C2N-C3N-C7N-O7N
3	C	402	NDP	O4D-C1D-N1N-C2N
2	B	401	GFR	OAM-CAN-CAR-CAS
2	C	401	GFR	OAM-CAN-CAR-CAS
2	E	401	GFR	OAM-CAN-CAR-CAW
3	C	402	NDP	PN-O3-PA-O2A
2	A	401	GFR	OAM-CAN-CAR-CAW
3	E	402	NDP	O4D-C1D-N1N-C2N
3	A	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	O4D-C1D-N1N-C2N
2	C	401	GFR	OAM-CAN-CAR-CAW
3	D	402	NDP	O4B-C4B-C5B-O5B
3	D	402	NDP	C2N-C3N-C7N-N7N
3	F	402	NDP	O4D-C1D-N1N-C2N
3	C	402	NDP	C2B-O2B-P2B-O1X
3	F	402	NDP	C1B-C2B-O2B-P2B
2	B	401	GFR	OAM-CAN-CAR-CAW
2	F	401	GFR	OAM-CAN-CAR-CAW
3	B	402	NDP	C2D-C1D-N1N-C2N
3	F	402	NDP	C2D-C1D-N1N-C2N
3	B	402	NDP	PN-O3-PA-O2A
3	A	402	NDP	C2D-C1D-N1N-C2N
3	E	402	NDP	C2B-O2B-P2B-O1X
3	F	402	NDP	C2B-O2B-P2B-O1X
3	D	402	NDP	C2N-C3N-C7N-O7N
3	B	402	NDP	PN-O3-PA-O1A

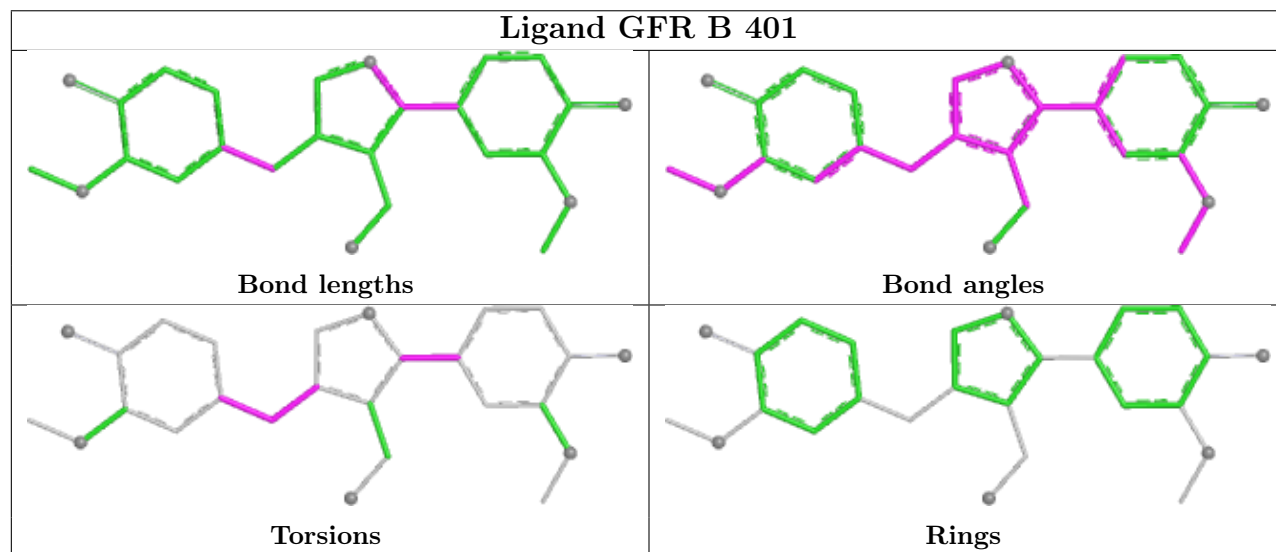
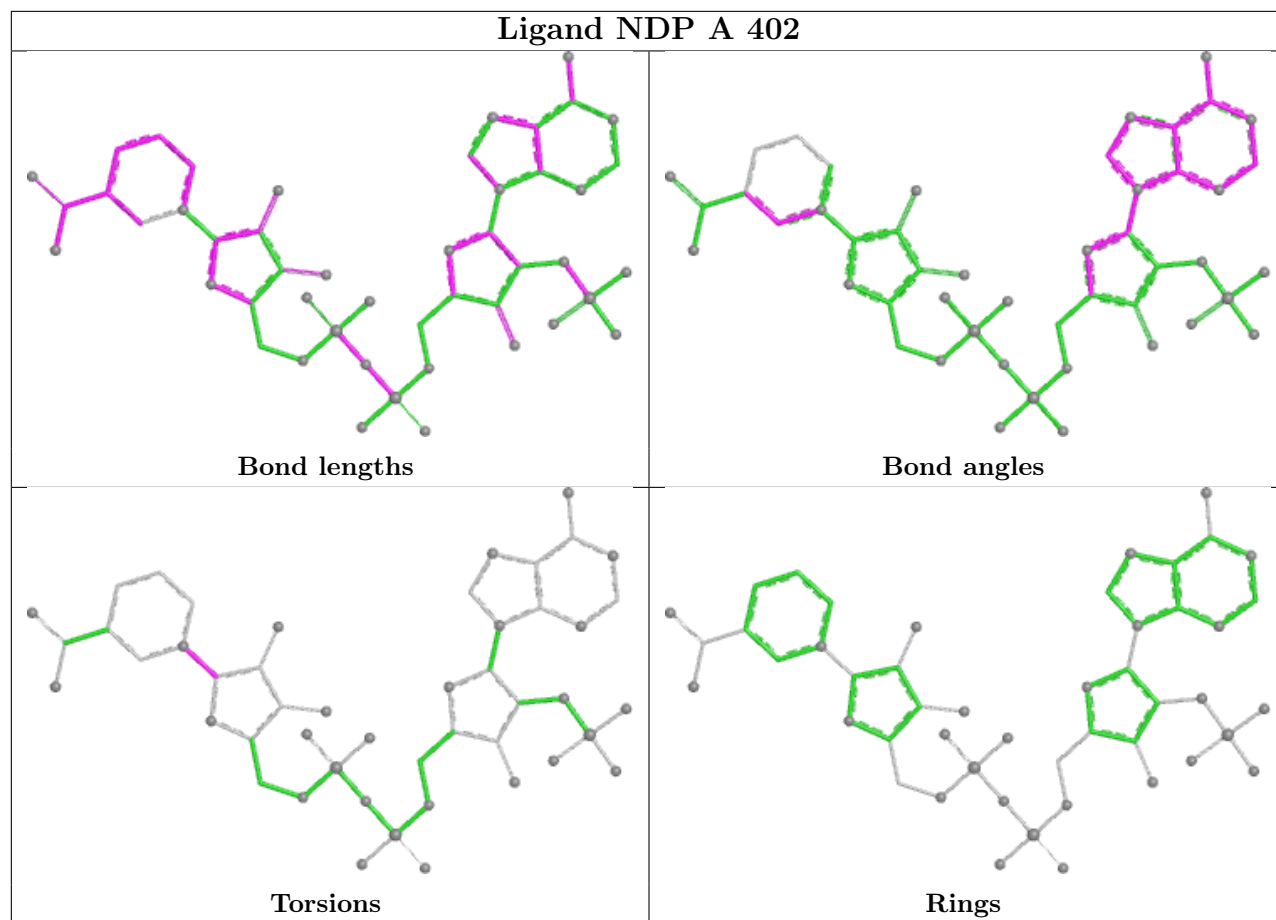
There are no ring outliers.

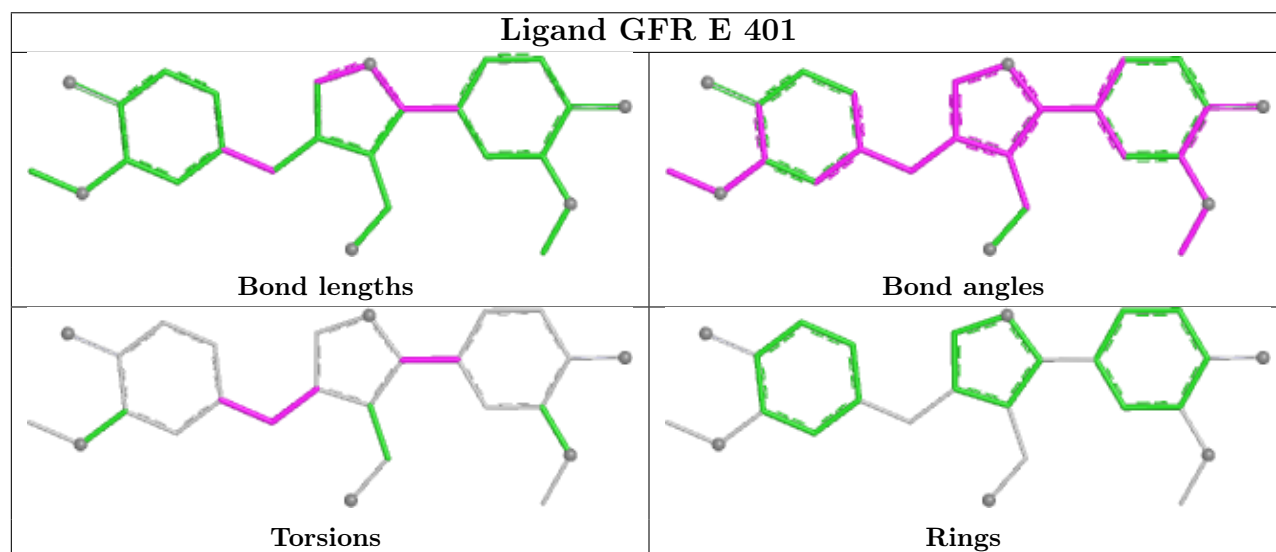
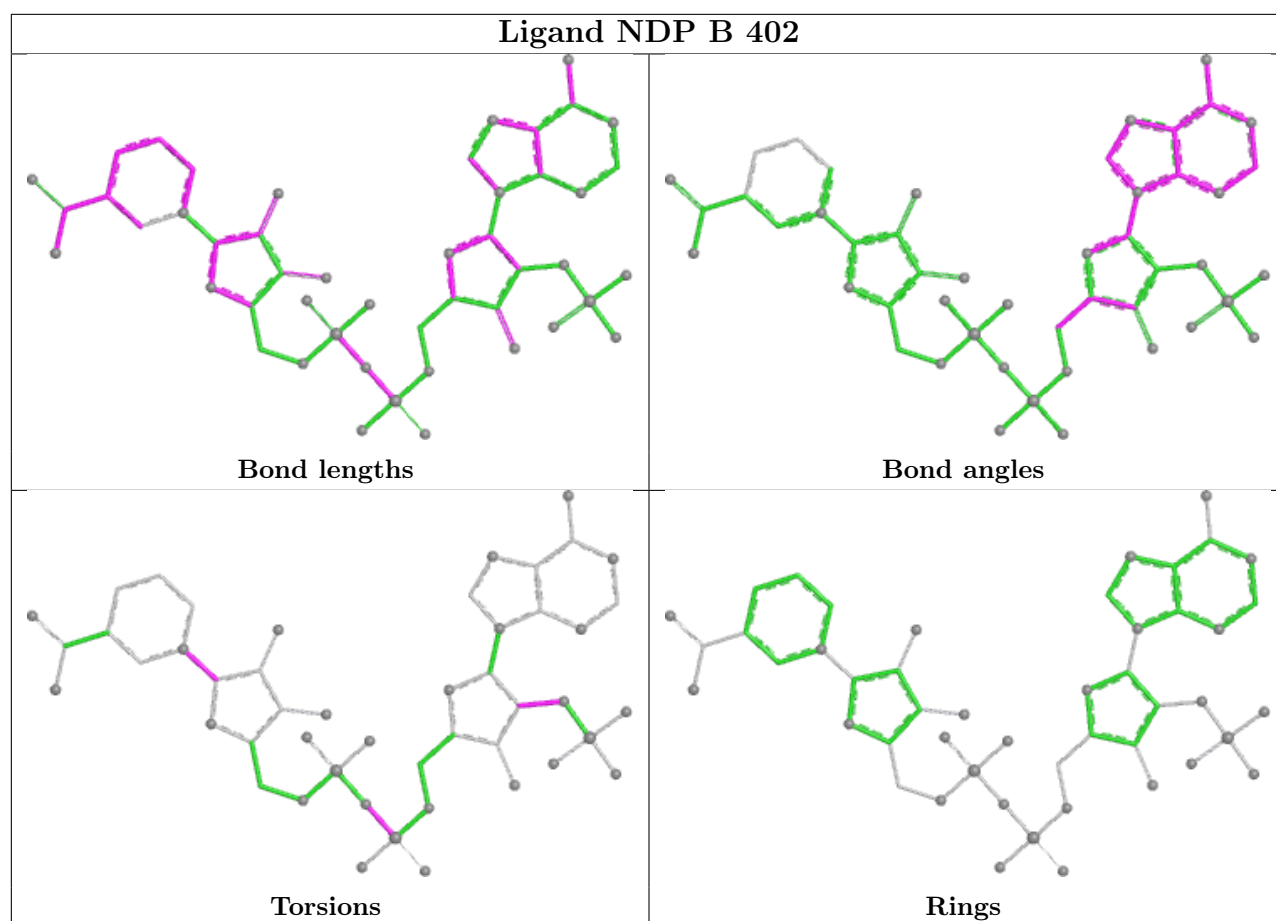
8 monomers are involved in 35 short contacts:

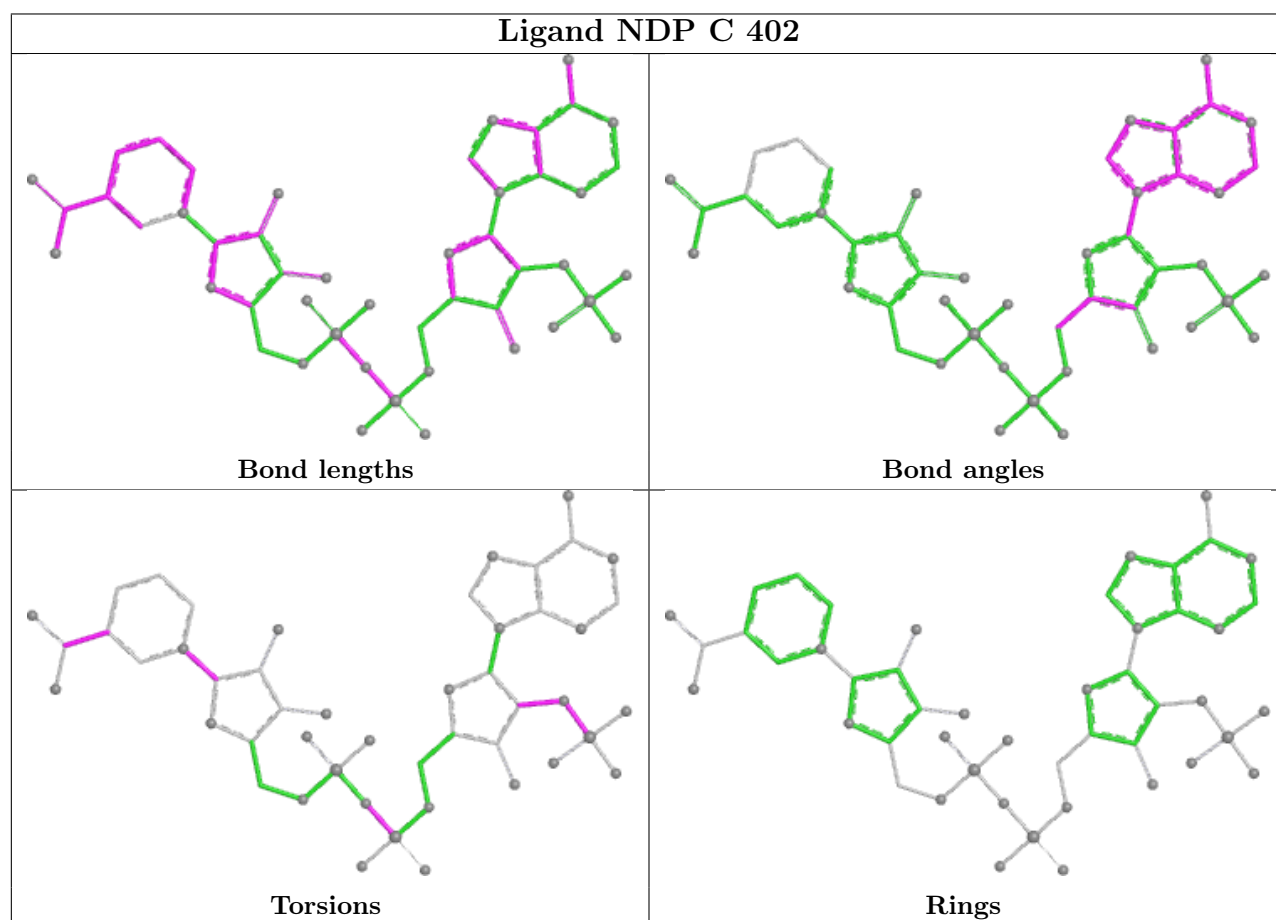
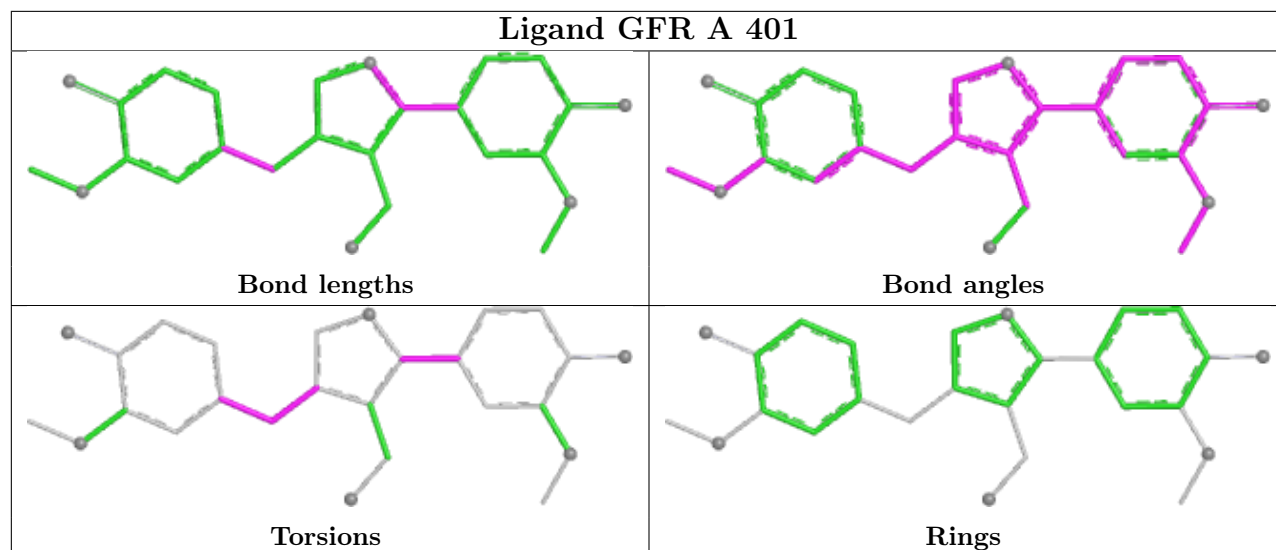
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	NDP	5	0
3	A	402	NDP	6	0
3	B	402	NDP	5	0
3	C	402	NDP	3	0
3	E	402	NDP	9	0
2	C	401	GFR	1	0
2	D	401	GFR	1	0
3	F	402	NDP	5	0

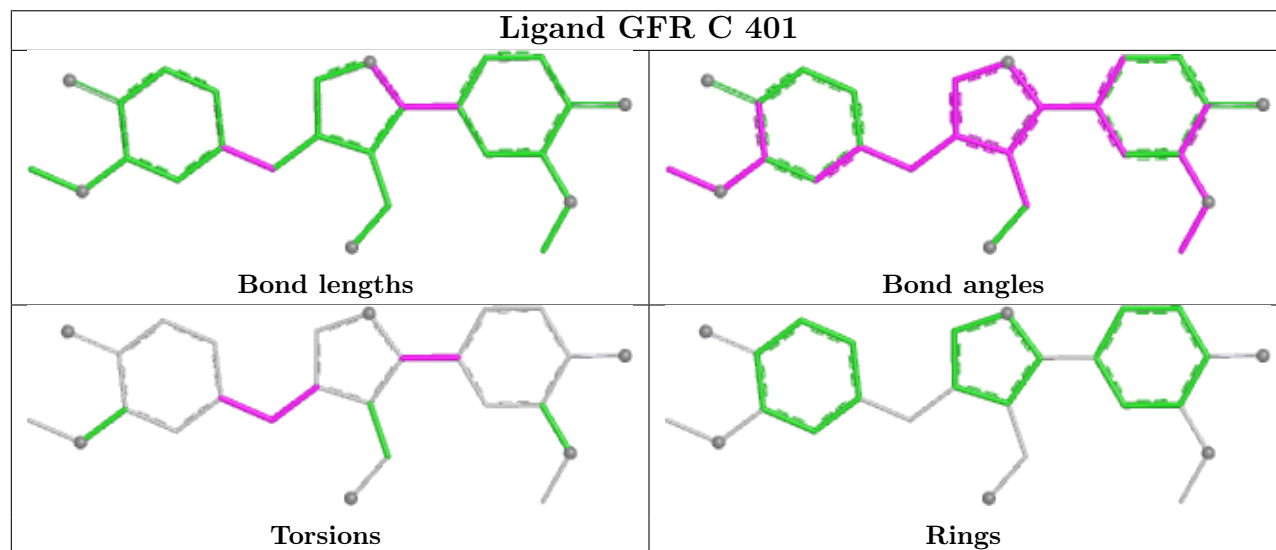
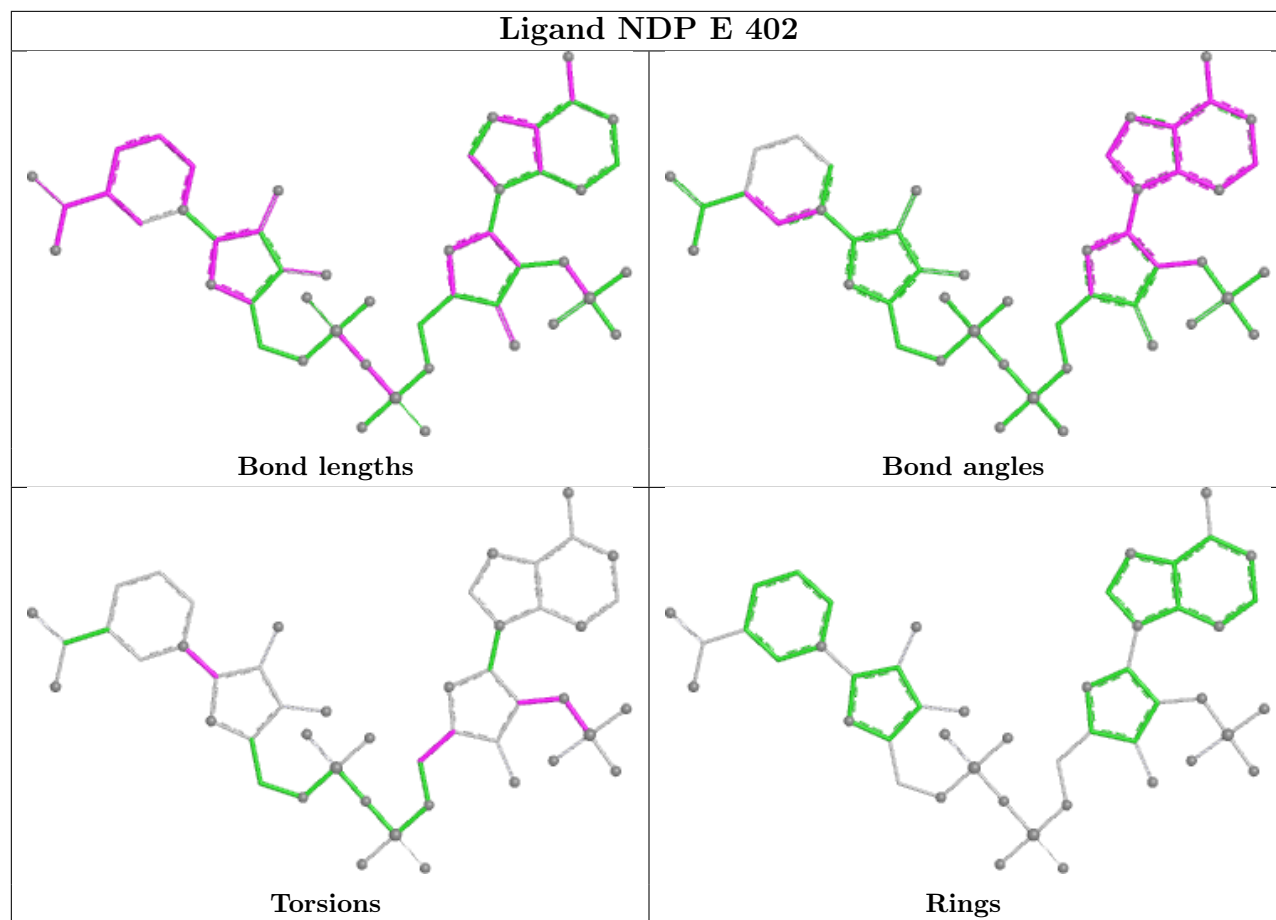
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

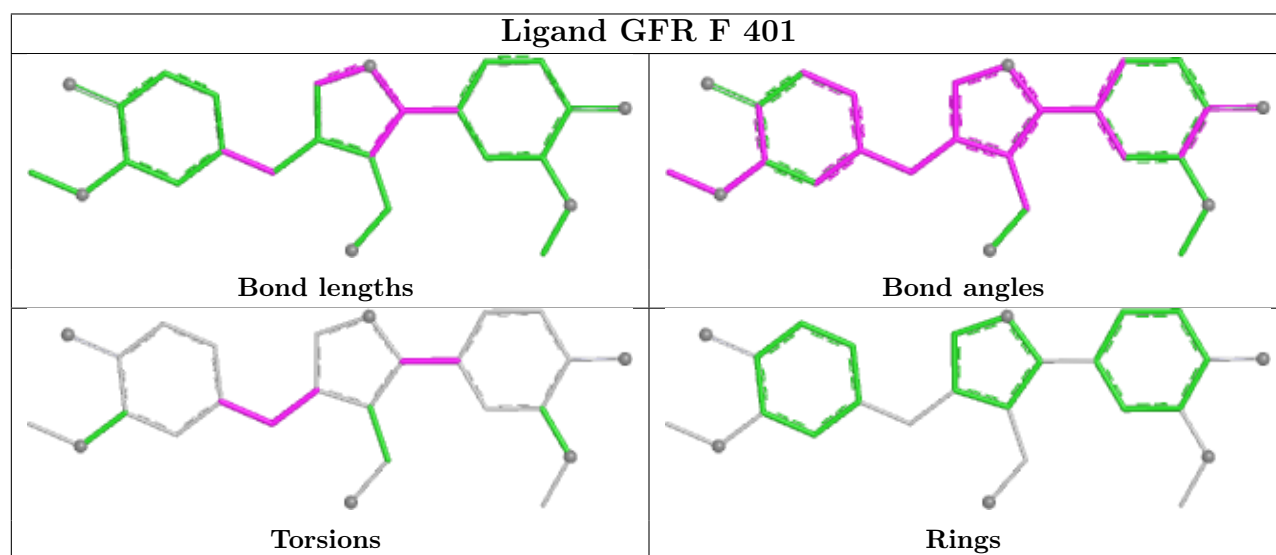
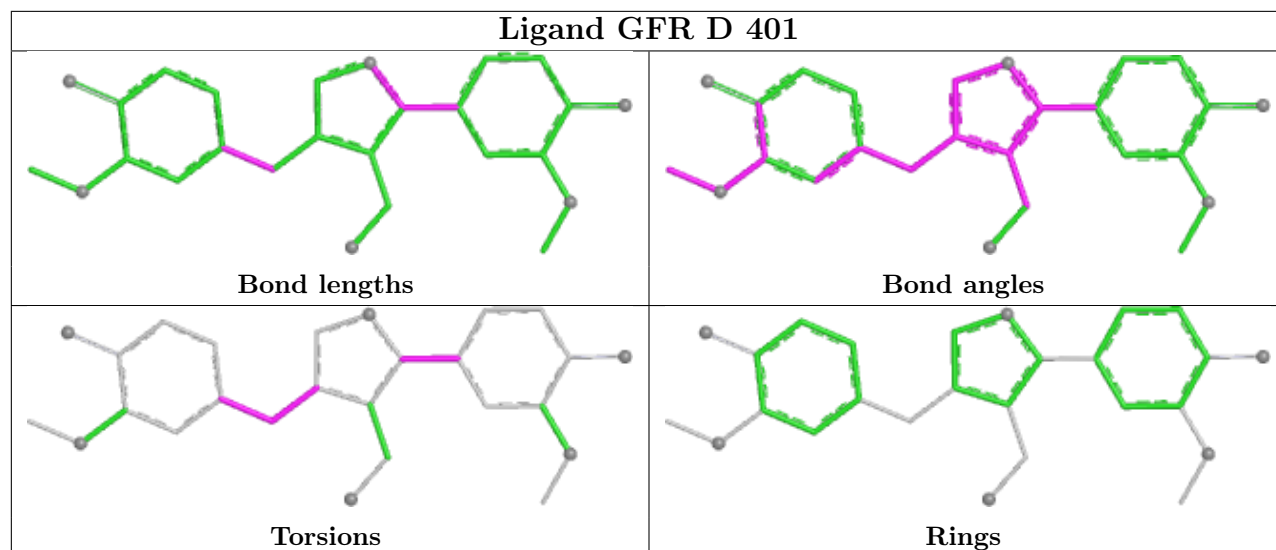


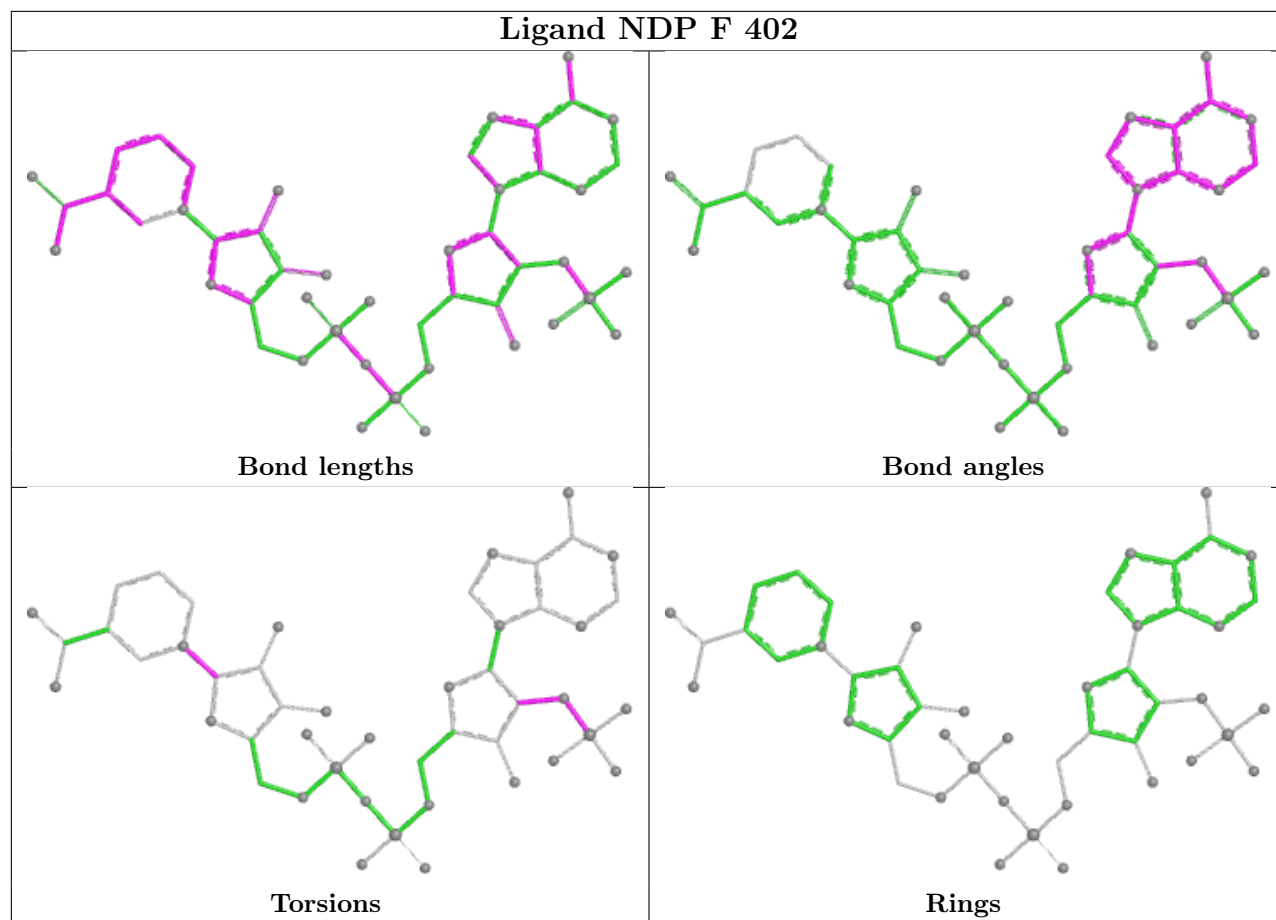












5.7 Other polymers [i](#)

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	286/317 (90%)	-0.14	8 (2%) 55 52	25, 35, 56, 85	0
1	B	289/317 (91%)	0.21	22 (7%) 20 17	22, 35, 69, 83	0
1	C	287/317 (90%)	0.22	13 (4%) 38 35	26, 41, 67, 92	0
1	D	289/317 (91%)	-0.00	6 (2%) 63 60	27, 39, 56, 84	0
1	E	287/317 (90%)	-0.11	10 (3%) 47 44	26, 34, 57, 82	0
1	F	300/317 (94%)	-0.27	6 (2%) 65 62	21, 30, 53, 77	0
All	All	1738/1902 (91%)	-0.02	65 (3%) 45 42	21, 36, 63, 92	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	ILE	7.2
1	D	263	ILE	6.2
1	B	7	GLY	5.8
1	D	7	GLY	5.8
1	E	263	ILE	5.6
1	D	131	GLY	5.4
1	D	261	ALA	5.1
1	C	91	GLY	4.9
1	B	94	PHE	4.8
1	E	7	GLY	4.7
1	C	272	ALA	4.6
1	B	92	VAL	4.5
1	A	272	ALA	4.2
1	F	130	MET	4.2
1	C	97	HIS	4.0
1	B	254	ILE	4.0
1	B	261	ALA	3.9
1	B	273	GLY	3.8
1	E	272	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	130	MET	3.8
1	B	260	LEU	3.7
1	B	272	ALA	3.6
1	B	189	ILE	3.5
1	E	44	THR	3.5
1	C	261	ALA	3.4
1	A	97	HIS	3.4
1	A	261	ALA	3.1
1	B	256	ALA	3.1
1	B	249	LEU	3.1
1	C	271	GLN	2.9
1	C	262	ASP	2.9
1	F	263	ILE	2.8
1	B	192	ASP	2.8
1	E	261	ALA	2.8
1	B	93	HIS	2.8
1	C	7	GLY	2.8
1	A	130	MET	2.7
1	E	45	ARG	2.7
1	E	46	VAL	2.7
1	C	273	GLY	2.7
1	D	97	HIS	2.6
1	B	187	VAL	2.6
1	C	98	SER	2.6
1	B	97	HIS	2.6
1	B	252	THR	2.6
1	F	7	GLY	2.6
1	B	129	ARG	2.5
1	C	49	GLU	2.4
1	B	190	TYR	2.4
1	A	44	THR	2.4
1	B	278	TYR	2.3
1	B	259	PHE	2.2
1	F	92	VAL	2.2
1	A	91	GLY	2.2
1	B	282	TYR	2.2
1	A	260	LEU	2.2
1	B	289	HIS	2.2
1	E	91	GLY	2.2
1	C	191	GLY	2.1
1	C	260	LEU	2.1
1	C	252	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	266	LYS	2.0
1	F	264	GLU	2.0
1	E	262	ASP	2.0
1	D	116	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

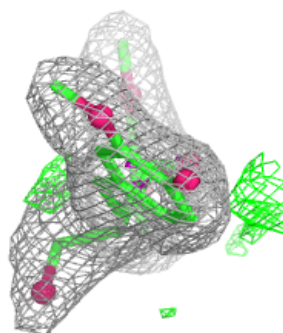
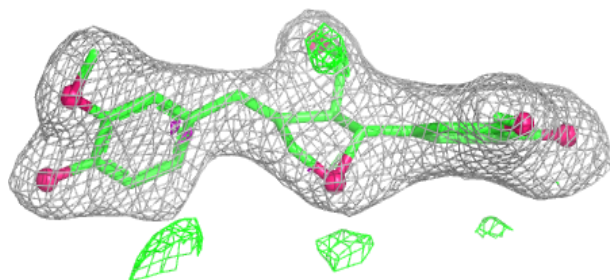
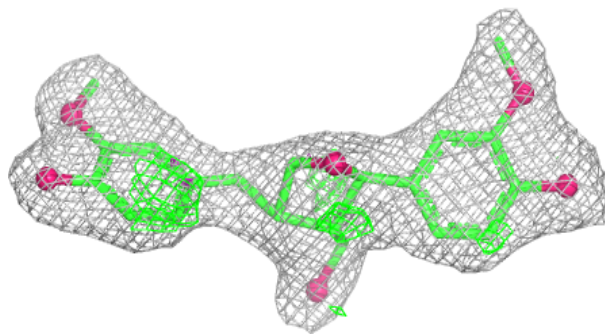
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GFR	D	401	26/26	0.89	0.12	39,48,54,54	0
2	GFR	B	401	26/26	0.90	0.11	38,46,52,54	0
2	GFR	E	401	26/26	0.90	0.10	33,40,46,47	0
2	GFR	A	401	26/26	0.91	0.10	34,45,51,54	0
2	GFR	C	401	26/26	0.91	0.10	41,51,56,58	0
2	GFR	F	401	26/26	0.94	0.07	20,26,31,33	0
3	NDP	A	402	48/48	0.96	0.06	30,43,58,70	0
3	NDP	C	402	48/48	0.96	0.06	34,45,59,71	0
3	NDP	D	402	48/48	0.96	0.06	33,45,58,68	0
3	NDP	E	402	48/48	0.96	0.06	27,39,51,56	0
3	NDP	B	402	48/48	0.97	0.05	25,33,43,47	0
3	NDP	F	402	48/48	0.97	0.06	20,29,41,44	0

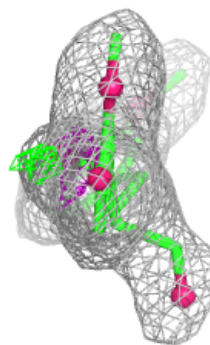
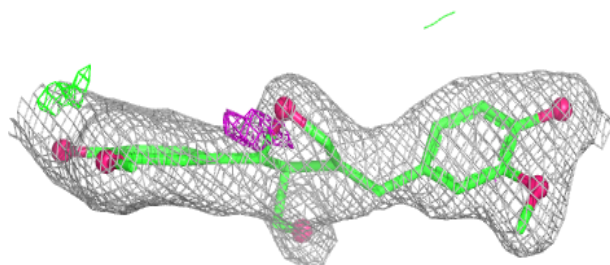
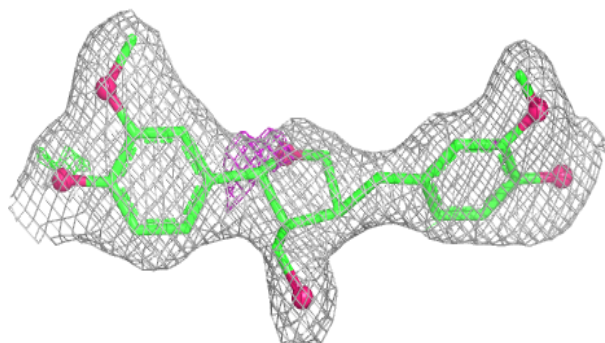
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GFR D 401:

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

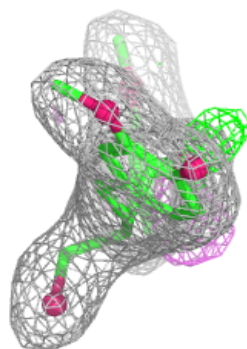
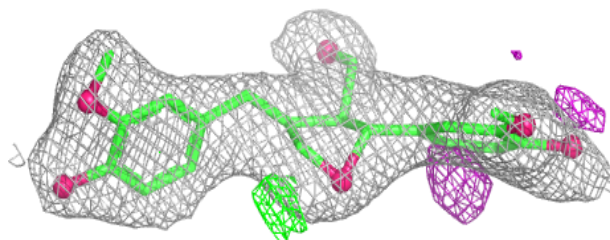
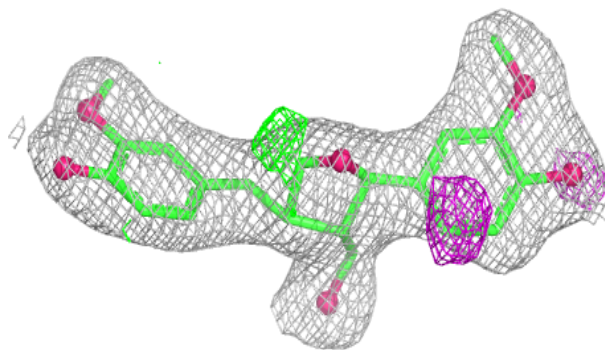
**Electron density around GFR B 401:**

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

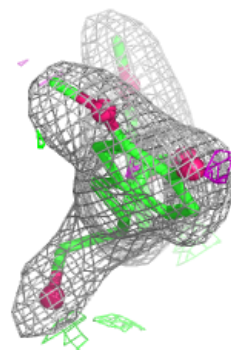
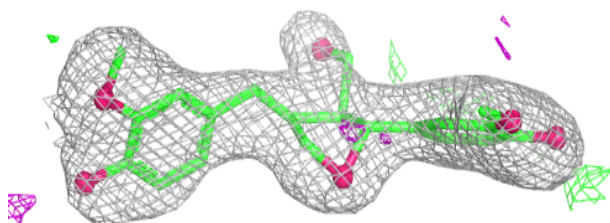
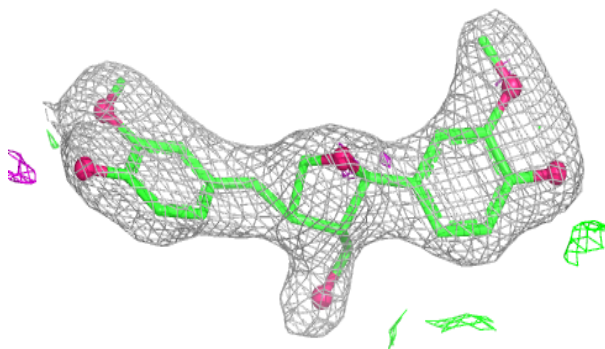


Electron density around GFR E 401:

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

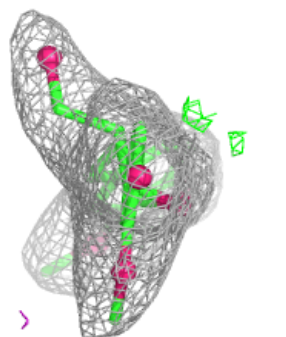
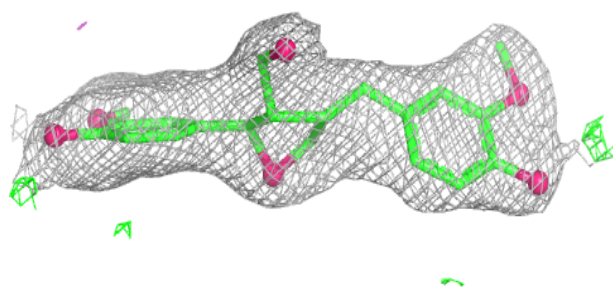
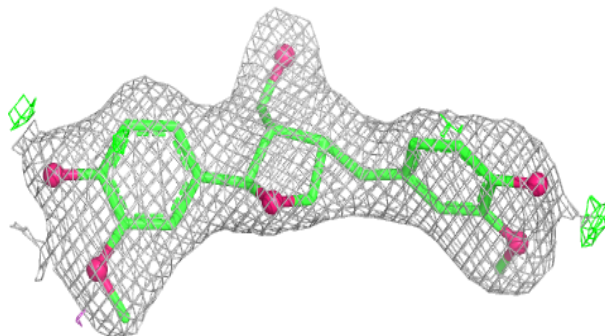
**Electron density around GFR A 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

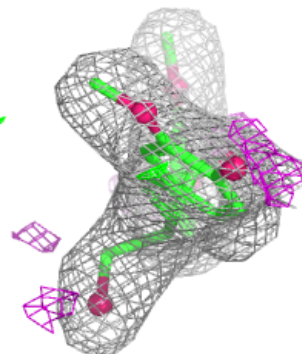
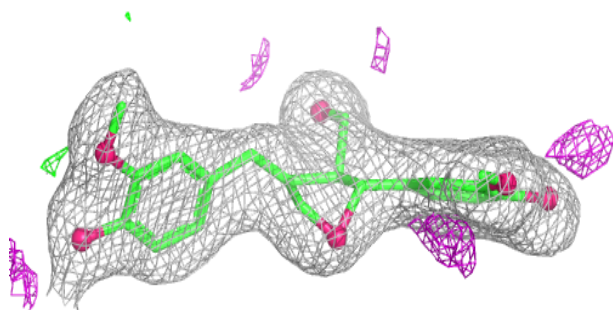
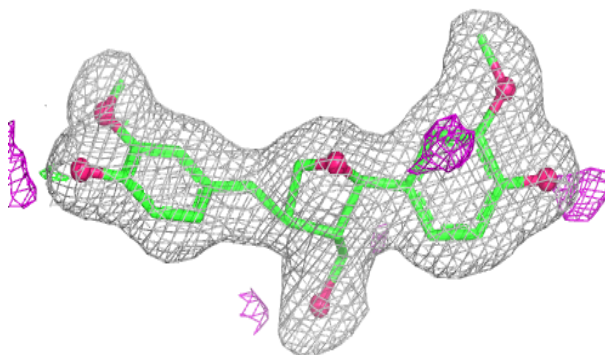


Electron density around GFR C 401:

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

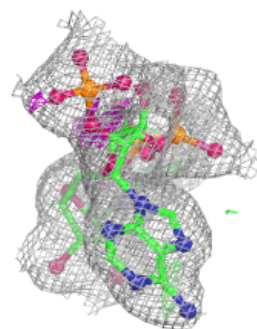
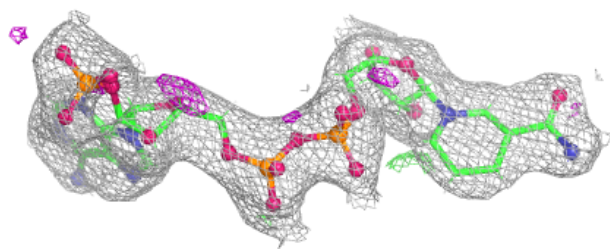
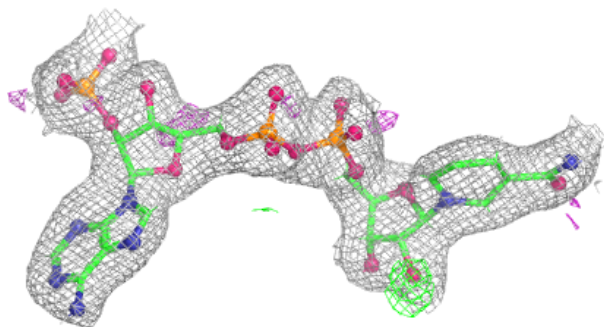
**Electron density around GFR F 401:**

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

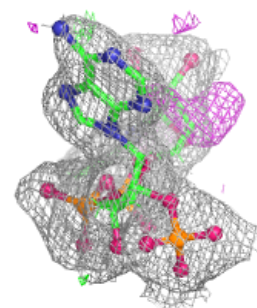
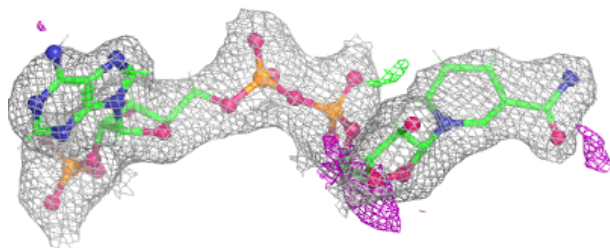
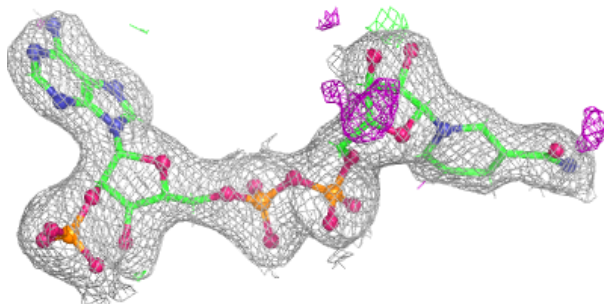


Electron density around NDP A 402:

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

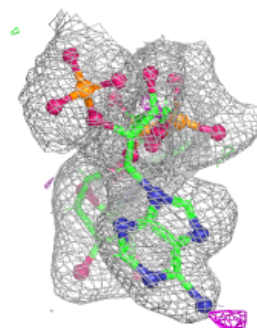
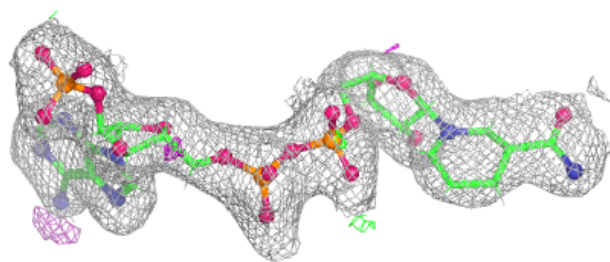
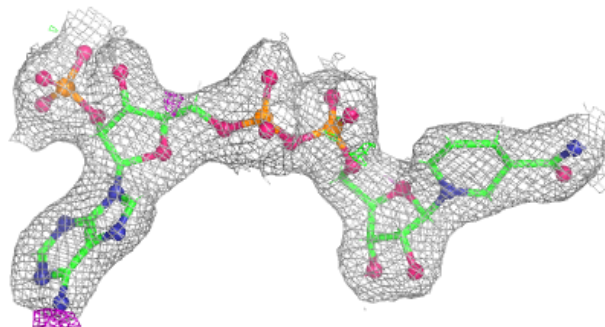
**Electron density around NDP C 402:**

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

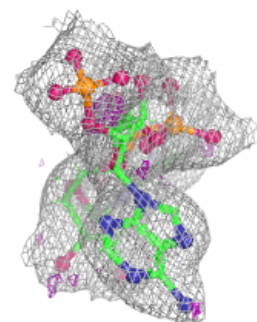
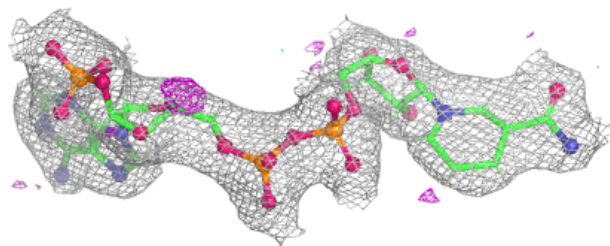
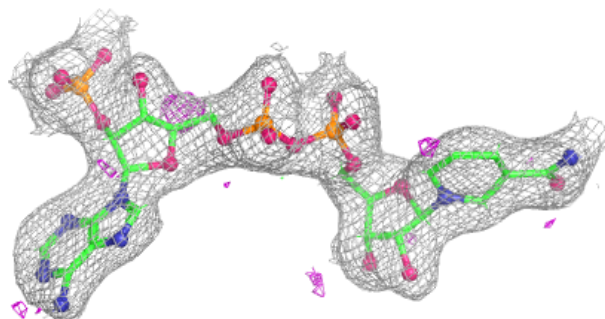


Electron density around NDP D 402:

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

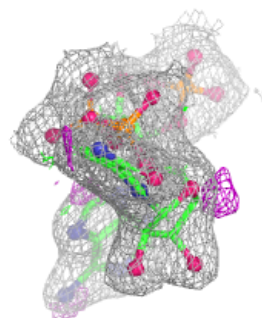
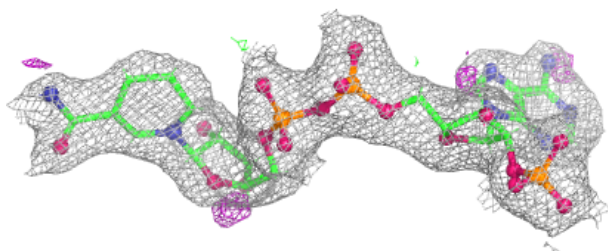
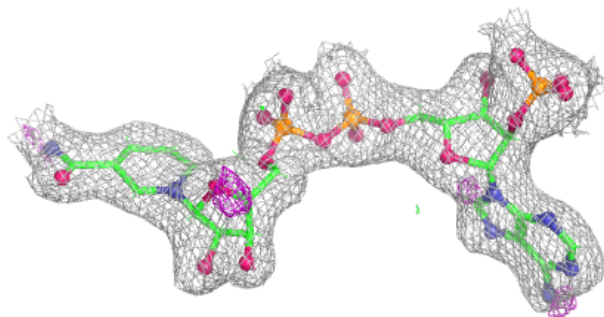
**Electron density around NDP E 402:**

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

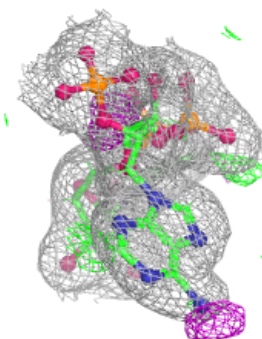
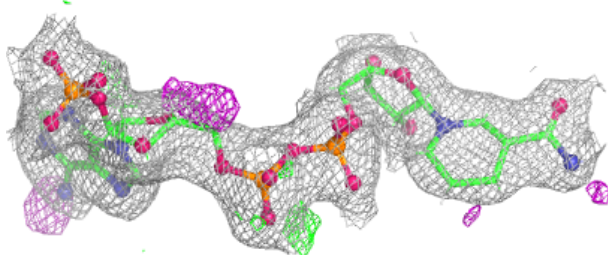
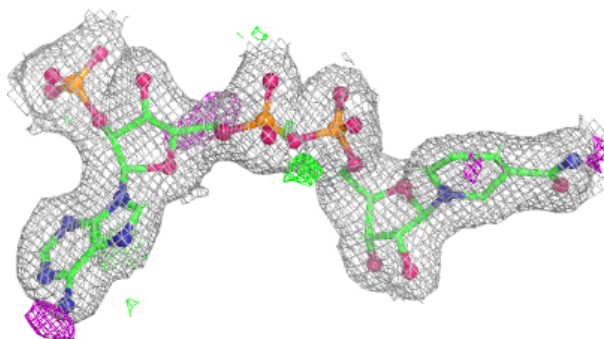


Electron density around NDP B 402:

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

**Electron density around NDP F 402:**

$2mF_o-DF_c$ (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.