



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:41 PM UTC

PDB ID : 7X11 / pdb_00007x11
Title : Crystal structure of ME1 in complex with NADPH
Authors : Amano, Y.
Deposited on : 2022-02-22
Resolution : 2.07 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

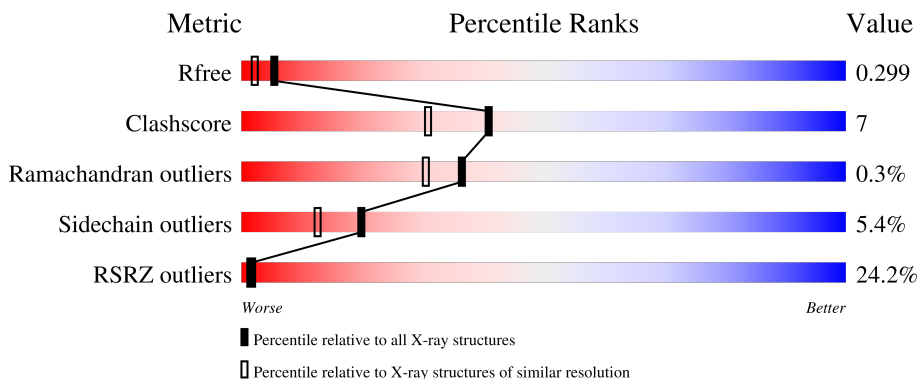
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	572	22% 81% 16% ..
1	B	572	21% 81% 17% ..
1	C	572	25% 80% 17% ..
1	D	572	28% 83% 13% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18738 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 NADP-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	B	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	C	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	D	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

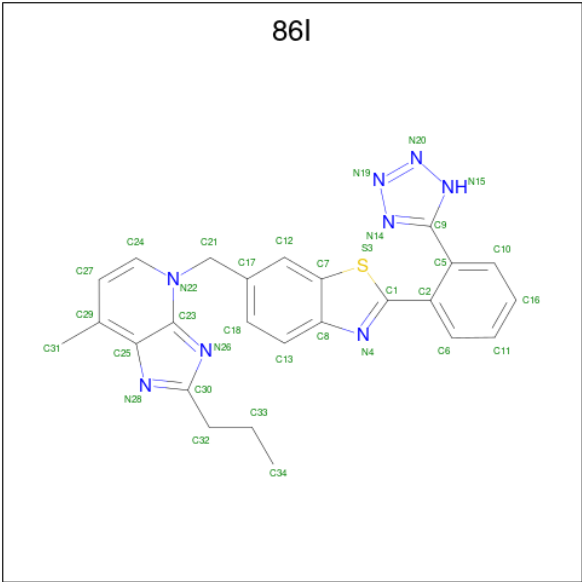
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 4 is 6-[(7-methyl-2-propyl-imidazo[4,5-b]pyridin-4-yl)methyl]-2-[2-(1H-1,2,3,4-tetrazol-5-yl)phenyl]-1,3-benzothiazole (CCD ID: 86I) (formula: C₂₅H₂₂N₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			34	25	8	1		
4	B	1	Total	C	N	S	0	0
			34	25	8	1		
4	C	1	Total	C	N	S	0	0
			34	25	8	1		
4	D	1	Total	C	N	S	0	0
			34	25	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total	O	0	0
			169	169		
5	B	200	Total	O	0	0
			200	200		
5	C	63	Total	O	0	0
			63	63		
5	D	170	Total	O	0	0
			170	170		

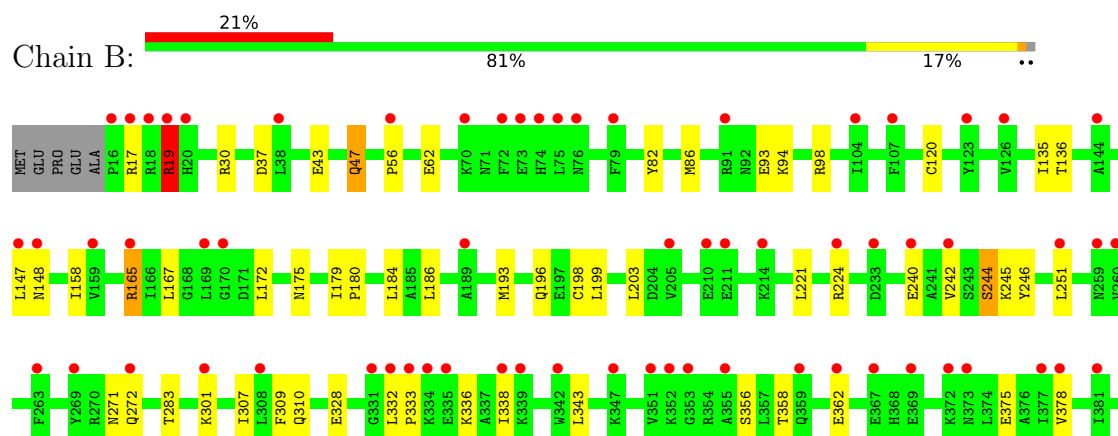
3 Residue-property plots

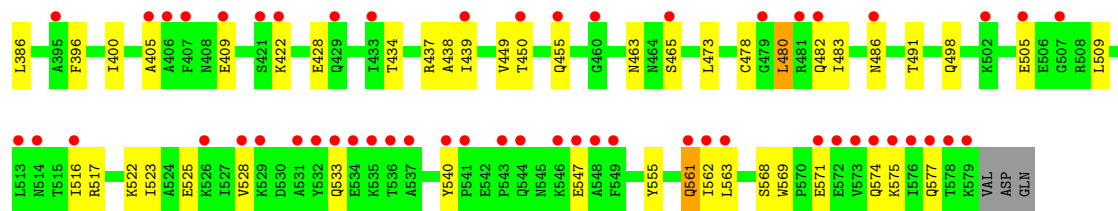
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADP-dependent malic enzyme

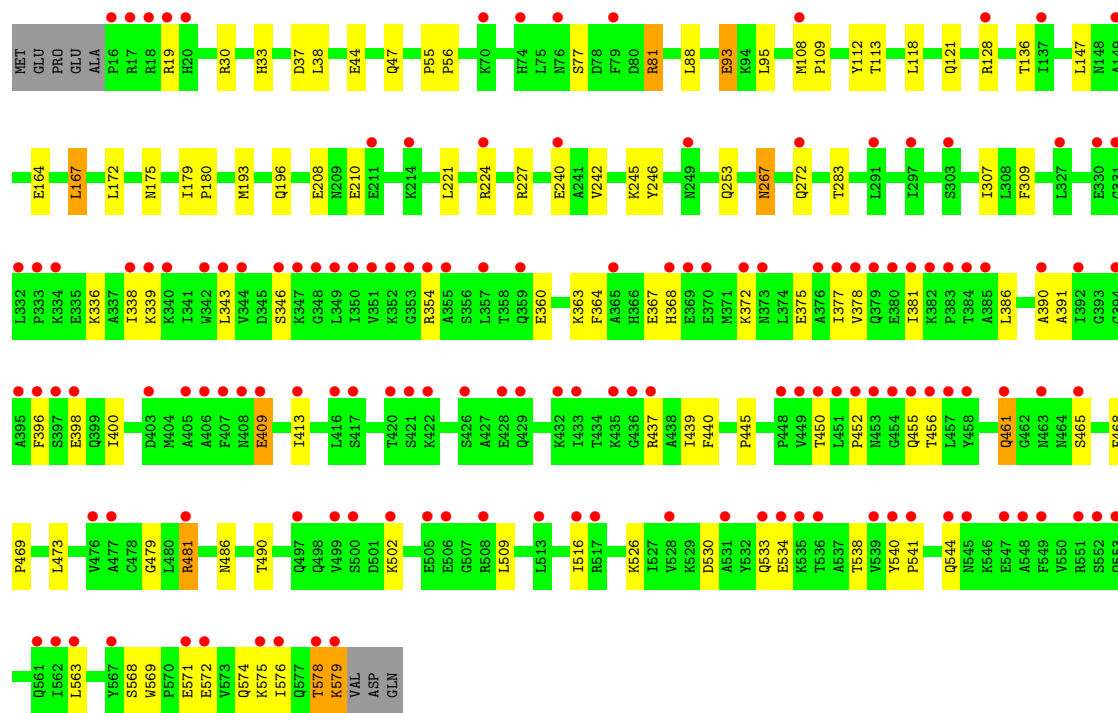
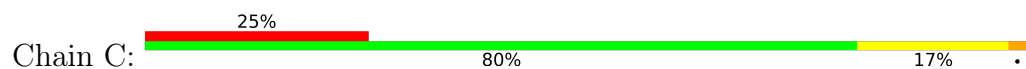


• Molecule 1: NADP-dependent malic enzyme

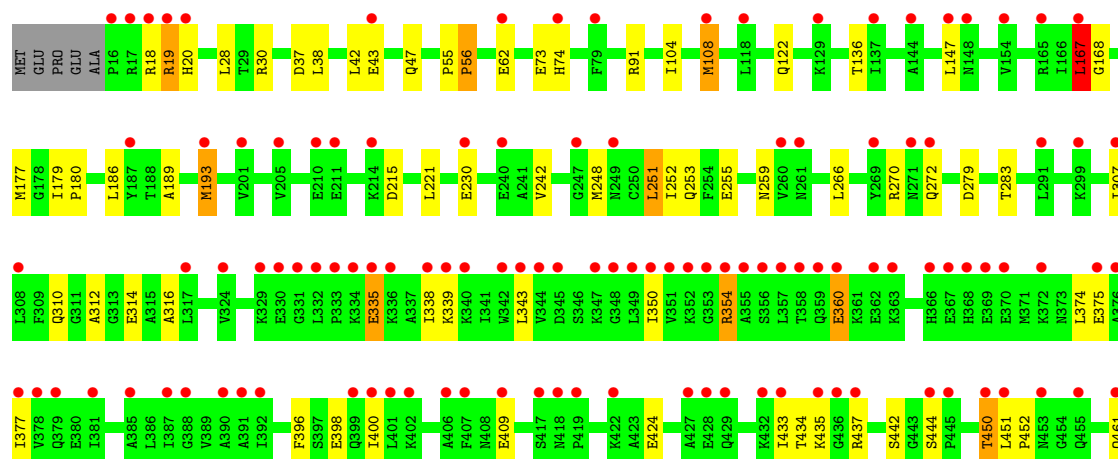
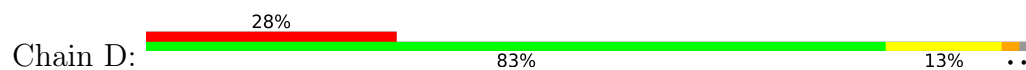


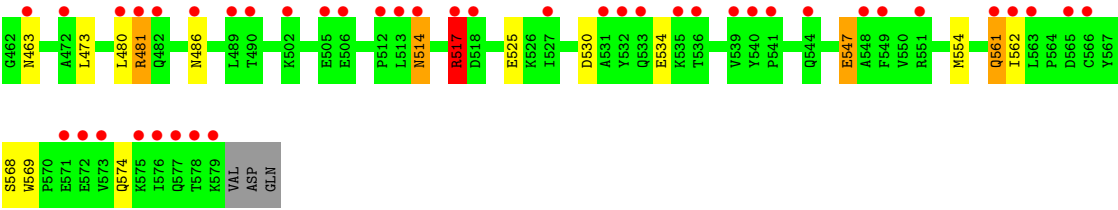


• Molecule 1: NADP-dependent malic enzyme



• Molecule 1: NADP-dependent malic enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.70Å 181.69Å 117.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.07 46.70 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.70-2.07) 93.4 (46.70-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.34 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.265 , 0.299 0.265 , 0.299	Depositor DCC
R_{free} test set	8756 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18738	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 86I, MN

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	0.53	0/4538	1.07	5/6142 (0.1%)
1	B	0.54	0/4538	1.08	5/6142 (0.1%)
1	C	0.54	0/4538	1.06	5/6142 (0.1%)
1	D	0.52	0/4538	1.08	7/6142 (0.1%)
All	All	0.53	0/18152	1.07	22/24568 (0.1%)

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	C	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ASP	CB-CA-C	-12.16	102.56	116.54
1	B	37	ASP	CB-CA-C	-11.05	102.20	117.23
1	A	129	LYS	CB-CA-C	9.32	120.47	109.85
1	A	37	ASP	CB-CA-C	-8.11	107.22	116.63
1	D	56	PRO	N-CA-CB	-7.87	97.53	102.81
1	D	450	THR	CB-CA-C	6.90	121.38	110.19
1	C	240	GLU	CB-CG-CD	6.81	124.17	112.60
1	A	450	THR	CB-CA-C	6.80	121.48	109.72
1	A	540	TYR	CB-CA-C	6.25	118.55	108.87
1	D	167	LEU	CB-CA-C	-6.16	109.45	116.54
1	B	450	THR	CB-CA-C	5.75	119.63	110.19
1	B	93	GLU	CB-CA-C	5.67	120.49	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLN	CB-CG-CD	-5.52	103.22	112.60
1	C	81	ARG	CG-CD-NE	-5.50	99.89	112.00
1	D	561	GLN	CB-CA-C	5.43	118.49	109.53
1	C	93	GLU	CB-CA-C	5.27	119.81	110.85
1	D	360	GLU	CB-CG-CD	5.20	121.43	112.60
1	B	561	GLN	CB-CA-C	5.15	118.03	109.53
1	B	540	TYR	CB-CA-C	5.04	116.88	109.22
1	C	37	ASP	CB-CA-C	-5.04	110.78	116.63
1	C	112	TYR	CB-CA-C	5.04	120.44	110.42
1	D	517	ARG	CG-CD-NE	5.03	123.06	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	578	THR	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	4451	0	4483	64	0
1	B	4451	0	4483	62	0
1	C	4451	0	4483	57	0
1	D	4451	0	4483	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	26	2	0
3	B	48	0	26	1	0
3	C	48	0	26	2	0
3	D	48	0	26	2	0
4	A	34	0	0	3	0
4	B	34	0	0	1	0
4	C	34	0	0	2	0
4	D	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	169	0	0	5	0
5	B	200	0	0	3	0
5	C	63	0	0	3	0
5	D	170	0	0	2	0
All	All	18738	0	18036	236	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 7.

All (236) 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:148:ASN:HB2	5:B:806:HOH:O	1.32	1.26
1:A:375:GLU:HA	1:A:400:ILE:HD11	1.48	0.96
1:A:375:GLU:HA	1:A:400:ILE:CD1	1.99	0.91
1:D:251:LEU:HD12	1:D:252:ILE:N	1.88	0.88
1:B:165:ARG:HG3	1:B:165:ARG:HH11	1.43	0.83
1:D:569:TRP:H	1:D:574:GLN:NE2	1.78	0.82
1:B:569:TRP:H	1:B:574:GLN:HE21	1.24	0.80
1:A:530:ASP:O	1:A:534:GLU:HG2	1.81	0.80
1:D:19:ARG:HG2	1:D:562:ILE:HG22	1.63	0.79
1:C:530:ASP:O	1:C:534:GLU:HG2	1.84	0.76
1:B:19:ARG:HG2	1:B:562:ILE:HG22	1.68	0.76
1:C:569:TRP:H	1:C:574:GLN:NE2	1.84	0.76
1:C:579:LYS:HB2	5:C:760:HOH:O	1.86	0.74
1:A:569:TRP:H	1:A:574:GLN:NE2	1.84	0.74
1:B:569:TRP:H	1:B:574:GLN:NE2	1.87	0.71
1:B:94:LYS:HD3	1:B:555:TYR:OH	1.91	0.70
1:A:574:GLN:HE21	1:D:42:LEU:HD23	1.58	0.69
1:B:375:GLU:HA	1:B:400:ILE:CD1	2.24	0.68
1:C:343:LEU:HD12	1:C:364:PHE:HB2	1.76	0.68
1:C:569:TRP:H	1:C:574:GLN:HE21	1.41	0.66
1:C:360:GLU:HG2	4:C:603:86I:C12	2.27	0.65
1:D:251:LEU:HD12	1:D:252:ILE:H	1.61	0.64
1:A:375:GLU:CA	1:A:400:ILE:HD11	2.27	0.63
1:C:136:THR:HB	1:C:221:LEU:HD11	1.80	0.63
1:C:450:THR:HG22	1:C:456:THR:HG23	1.81	0.62
1:C:33:HIS:CE1	1:C:93:GLU:HG2	2.35	0.61
1:C:164:GLU:OE2	1:C:227:ARG:NH2	2.30	0.61
1:D:409:GLU:O	1:D:437:ARG:HD2	1.99	0.61
1:D:248:MET:HB3	1:D:481:ARG:HH12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PHE:HB2	1:C:343:LEU:HD23	1.83	0.60
1:D:375:GLU:HG2	1:D:400:ILE:HG13	1.84	0.60
1:D:108:MET:HE2	5:D:713:HOH:O	2.02	0.59
1:D:189:ALA:O	1:D:517:ARG:HD2	2.03	0.59
1:A:579:LYS:HE3	1:A:579:LYS:HA	1.84	0.59
1:A:303:SER:O	1:A:340:LYS:HE2	2.02	0.59
1:B:309:PHE:HB2	1:B:343:LEU:HD23	1.83	0.59
1:C:343:LEU:HD11	1:C:364:PHE:CD2	2.38	0.58
1:D:514:ASN:ND2	1:D:514:ASN:H	2.01	0.58
1:C:267:ASN:ND2	5:C:702:HOH:O	2.36	0.58
1:B:251:LEU:CD1	1:B:483:ILE:HD11	2.34	0.58
1:C:193:MET:HE1	1:C:473:LEU:HA	1.86	0.58
1:B:19:ARG:HH21	1:B:19:ARG:HB2	1.69	0.57
1:D:568:SER:HB2	1:D:574:GLN:HE22	1.69	0.57
1:A:529:LYS:HE3	1:A:546:LYS:HB2	1.86	0.57
1:C:439:ILE:HG22	1:C:509:LEU:HD11	1.86	0.57
1:A:481:ARG:HG2	1:A:481:ARG:HH11	1.70	0.57
1:A:498:GLN:HB2	1:A:511:PRO:HG3	1.87	0.57
1:B:465:SER:O	1:B:516:ILE:HD11	2.05	0.57
1:B:136:THR:HB	1:B:221:LEU:HD11	1.87	0.57
4:B:603:86I:C9	4:B:603:86I:S3	2.93	0.56
1:C:208:GLU:OE2	1:C:224:ARG:HD3	2.05	0.56
1:B:375:GLU:HA	1:B:400:ILE:HD11	1.86	0.56
1:D:104:ILE:O	1:D:108:MET:HB2	2.05	0.56
1:D:530:ASP:O	1:D:534:GLU:HG2	2.05	0.56
1:D:259:ASN:ND2	3:D:602:NDP:O2A	2.39	0.56
1:B:405:ALA:HB2	1:B:434:THR:HG22	1.88	0.55
1:D:525:GLU:OE2	1:D:547:GLU:HG2	2.07	0.55
1:A:571:GLU:OE2	1:A:575:LYS:HG3	2.07	0.55
1:B:120:CYS:O	1:B:175:ASN:HB3	2.07	0.55
1:C:568:SER:HB2	1:C:574:GLN:HE22	1.70	0.55
1:A:259:ASN:HB3	4:A:603:86I:C16	2.36	0.54
1:C:450:THR:HA	1:C:455:GLN:O	2.07	0.54
1:B:333:PRO:HG2	1:B:336:LYS:CG	2.37	0.54
1:A:322:LEU:HD11	1:A:489:LEU:HB2	1.89	0.54
1:D:251:LEU:HD12	1:D:251:LEU:C	2.32	0.54
1:D:19:ARG:CG	1:D:562:ILE:HG22	2.35	0.54
1:D:283:THR:HG23	3:D:602:NDP:H41N	1.89	0.53
1:A:574:GLN:NE2	1:D:42:LEU:HD23	2.24	0.53
1:B:62:GLU:HG3	1:B:98:ARG:NH2	2.24	0.53
1:B:358:THR:O	1:B:362:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:GLU:OE2	1:C:363:LYS:HE3	2.08	0.53
1:C:19:ARG:O	1:C:19:ARG:HG3	2.08	0.52
1:C:30:ARG:HB3	1:D:30:ARG:HB3	1.92	0.52
1:D:569:TRP:H	1:D:574:GLN:HE21	1.51	0.52
1:C:572:GLU:HB2	5:C:735:HOH:O	2.09	0.52
1:D:310:GLN:HG3	1:D:374:LEU:CD2	2.39	0.52
1:C:468:PHE:N	1:C:469:PRO:CD	2.73	0.52
1:D:108:MET:HE1	1:D:463:ASN:HD21	1.74	0.52
1:B:378:VAL:HG21	1:B:400:ILE:HD12	1.91	0.51
1:A:109:PRO:HA	1:A:113:THR:O	2.11	0.51
1:B:165:ARG:HH11	1:B:165:ARG:CG	2.19	0.51
1:A:259:ASN:HB3	4:A:603:86I:C11	2.40	0.51
1:A:503:HIS:O	1:A:506:GLU:HB2	2.11	0.51
1:B:439:ILE:HG22	1:B:509:LEU:HD11	1.92	0.51
1:A:208:GLU:HG2	1:A:225:ARG:HG3	1.91	0.50
1:A:56:PRO:HB3	1:B:136:THR:HG21	1.93	0.50
1:C:571:GLU:O	1:C:575:LYS:HG3	2.11	0.50
1:C:386:LEU:HG	1:C:396:PHE:CZ	2.47	0.50
1:A:86:MET:HA	1:A:86:MET:HE2	1.92	0.50
1:B:568:SER:HB2	1:B:574:GLN:HE22	1.76	0.50
1:B:193:MET:HE1	1:B:473:LEU:HA	1.94	0.50
1:C:490:THR:HG23	1:C:526:LYS:HE2	1.93	0.50
1:C:377:ILE:HG23	1:C:381:ILE:HD12	1.94	0.50
1:A:574:GLN:HE21	1:D:42:LEU:CD2	2.24	0.50
1:A:502:LYS:O	1:A:506:GLU:HG3	2.12	0.49
1:B:375:GLU:HA	1:B:400:ILE:HD13	1.94	0.49
1:C:109:PRO:HA	1:C:113:THR:O	2.12	0.49
1:B:165:ARG:HG3	1:B:165:ARG:NH1	2.19	0.49
1:C:283:THR:HG23	3:C:602:NDP:H41N	1.92	0.49
1:B:251:LEU:HD12	1:B:483:ILE:HD11	1.94	0.49
1:A:94:LYS:HD3	1:A:555:TYR:OH	2.12	0.49
1:B:386:LEU:HG	1:B:396:PHE:CZ	2.48	0.49
1:A:61:GLN:O	1:A:65:VAL:HG23	2.13	0.49
1:A:283:THR:HG23	3:A:602:NDP:H41N	1.95	0.48
1:A:532:TYR:CD1	1:A:542:GLU:HG3	2.48	0.48
1:B:478:CYS:HB3	1:B:528:VAL:HG22	1.95	0.48
1:B:517:ARG:HG2	5:B:828:HOH:O	2.12	0.48
1:B:498:GLN:OE1	1:B:522:LYS:HD2	2.12	0.48
1:A:30:ARG:HB3	1:B:30:ARG:HB3	1.95	0.48
1:A:120:CYS:O	1:A:175:ASN:HB3	2.14	0.48
1:C:481:ARG:HH11	1:C:481:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:SER:O	1:D:461:GLN:HA	2.13	0.48
1:A:118:LEU:HA	1:A:121:GLN:HE21	1.77	0.48
1:A:136:THR:HG21	1:B:56:PRO:HB3	1.96	0.48
1:C:468:PHE:N	1:C:469:PRO:HD3	2.28	0.48
1:D:248:MET:CB	1:D:481:ARG:HH12	2.26	0.48
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.79	0.47
1:A:214:LYS:HB3	5:A:770:HOH:O	2.14	0.47
1:B:333:PRO:HG2	1:B:336:LYS:HG2	1.96	0.47
1:A:451:LEU:HD11	1:A:457:LEU:HD11	1.96	0.47
1:C:346:SER:HB2	3:C:602:NDP:O2X	2.15	0.47
1:B:19:ARG:NH1	1:B:196:GLN:HE22	2.12	0.47
1:C:578:THR:O	1:C:579:LYS:HB3	2.13	0.47
1:D:136:THR:HB	1:D:221:LEU:HD11	1.96	0.47
1:D:310:GLN:HG3	1:D:374:LEU:HD22	1.97	0.46
4:D:603:86I:C9	4:D:603:86I:S3	3.04	0.46
1:B:184:LEU:HD13	1:B:198:CYS:HB3	1.98	0.46
1:C:540:TYR:HA	1:C:541:PRO:C	2.40	0.46
1:B:405:ALA:O	1:B:437:ARG:NH2	2.48	0.45
1:B:165:ARG:CG	1:B:165:ARG:NH1	2.79	0.45
1:A:42:LEU:O	1:A:46:GLN:HG3	2.17	0.45
1:C:44:GLU:HA	1:C:563:LEU:HD21	1.98	0.45
1:A:17:ARG:NH1	5:A:703:HOH:O	2.49	0.45
1:B:19:ARG:O	1:B:562:ILE:HA	2.16	0.45
1:C:172:LEU:O	1:C:175:ASN:HB2	2.17	0.45
1:D:525:GLU:CD	1:D:547:GLU:HG2	2.42	0.45
1:B:17:ARG:HE	1:B:17:ARG:HB3	1.56	0.45
1:B:375:GLU:HG3	5:B:890:HOH:O	2.17	0.45
1:D:193:MET:HE1	1:D:473:LEU:HA	1.99	0.45
1:D:434:THR:O	1:D:435:LYS:C	2.60	0.45
1:B:525:GLU:CD	1:B:547:GLU:HG2	2.42	0.45
4:A:603:86I:S3	4:A:603:86I:C9	3.04	0.44
1:A:516:ILE:O	1:A:516:ILE:HD12	2.16	0.44
1:A:137:ILE:HB	1:A:205:VAL:HG12	1.98	0.44
1:D:451:LEU:HB3	1:D:452:PRO:CD	2.48	0.44
1:A:42:LEU:HD23	1:D:574:GLN:HE21	1.82	0.44
1:A:266:LEU:O	1:A:270:ARG:HB3	2.18	0.44
1:D:177:MET:O	1:D:180:PRO:HD2	2.18	0.44
1:A:211:GLU:H	1:A:211:GLU:HG2	1.51	0.44
1:A:401:LEU:HD23	1:A:413:ILE:HD13	1.99	0.44
1:B:434:THR:HG21	1:B:438:ALA:HB2	1.99	0.44
1:D:19:ARG:NH2	1:D:19:ARG:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:GLN:HG3	1:D:463:ASN:HB2	2.00	0.44
1:B:179:ILE:HB	1:B:180:PRO:HD3	2.00	0.44
1:B:575:LYS:HE3	1:B:577:GLN:HA	2.00	0.44
1:C:367:GLU:O	1:C:368:HIS:HB2	2.18	0.44
1:A:23:GLN:NE2	5:A:705:HOH:O	2.51	0.44
1:D:167:LEU:HB3	1:D:168:GLY:H	1.53	0.44
1:B:135:ILE:O	1:B:203:LEU:HA	2.17	0.43
1:B:491:THR:HG23	1:B:523:ILE:HG12	2.00	0.43
1:D:19:ARG:HB2	1:D:19:ARG:HH21	1.82	0.43
1:A:165:ARG:NH2	3:A:602:NDP:O1A	2.51	0.43
1:A:352:LYS:HG3	5:A:706:HOH:O	2.18	0.43
1:B:82:TYR:O	1:B:86:MET:HG2	2.18	0.43
1:C:479:GLY:O	1:C:538:THR:OG1	2.36	0.43
1:D:179:ILE:HB	1:D:180:PRO:HD3	2.00	0.43
1:B:148:ASN:ND2	1:D:20:HIS:HB2	2.33	0.43
1:A:72:PHE:CE1	1:A:106:LYS:HE2	2.54	0.43
1:D:312:ALA:HA	1:D:316:ALA:HB3	2.00	0.43
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.84	0.43
1:C:38:LEU:HD21	1:C:55:PRO:HG2	2.00	0.43
1:A:167:LEU:HB3	1:A:168:GLY:H	1.56	0.43
1:D:335:GLU:H	1:D:335:GLU:CD	2.26	0.43
1:A:104:ILE:O	1:A:108:MET:HG3	2.18	0.43
1:C:108:MET:N	1:C:109:PRO:HD2	2.34	0.43
1:A:367:GLU:O	1:A:368:HIS:HB2	2.19	0.43
1:B:19:ARG:HG2	1:B:562:ILE:CG2	2.44	0.43
1:C:88:LEU:HD11	1:C:95:LEU:HD23	2.01	0.43
1:D:266:LEU:O	1:D:270:ARG:HB3	2.19	0.42
1:B:283:THR:HG23	3:B:602:NDP:H41N	2.01	0.42
1:D:253:GLN:NE2	1:D:255:GLU:OE1	2.51	0.42
1:B:328:GLU:HA	1:B:332:LEU:O	2.20	0.42
1:C:118:LEU:HA	1:C:121:GLN:HE21	1.84	0.42
1:C:534:GLU:HG2	1:C:534:GLU:H	1.74	0.42
1:C:465:SER:O	1:C:516:ILE:HD11	2.19	0.42
1:D:360:GLU:HG2	4:D:603:86I:S3	2.59	0.42
1:B:172:LEU:O	1:B:175:ASN:HB2	2.19	0.42
1:C:245:LYS:HE3	1:C:246:TYR:CE1	2.54	0.42
1:D:354:ARG:HE	1:D:354:ARG:HB3	1.60	0.42
1:B:480:LEU:HD12	1:B:480:LEU:HA	1.93	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.91	0.42
1:D:279:ASP:HB3	1:D:314:GLU:OE2	2.20	0.42
1:B:271:ASN:O	1:B:482:GLN:NE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:O	1:B:244:SER:HB3	2.19	0.42
1:C:113:THR:CG2	1:C:167:LEU:HD11	2.50	0.42
1:D:554:MET:O	5:D:701:HOH:O	2.22	0.41
1:D:19:ARG:HH21	1:D:19:ARG:CB	2.32	0.41
1:D:38:LEU:HD21	1:D:55:PRO:HG2	2.01	0.41
1:D:215:ASP:C	1:D:215:ASP:OD1	2.63	0.41
1:D:398:GLU:HG3	1:D:433:ILE:HG12	2.02	0.41
1:C:56:PRO:HB3	1:D:136:THR:HG21	2.03	0.41
1:A:343:LEU:CB	1:A:350:ILE:HD12	2.51	0.41
1:B:463:ASN:OD1	1:B:465:SER:HB2	2.20	0.41
1:C:375:GLU:HA	1:C:400:ILE:CD1	2.51	0.41
1:C:413:ILE:O	1:C:440:PHE:HA	2.20	0.41
1:A:405:ALA:O	1:A:437:ARG:NH2	2.53	0.41
1:B:428:GLU:OE2	1:B:449:VAL:HG13	2.20	0.41
1:C:576:ILE:N	1:C:576:ILE:HD12	2.36	0.41
1:C:576:ILE:HD12	1:C:576:ILE:H	1.86	0.41
4:C:603:86I:C9	4:C:603:86I:S3	3.08	0.41
1:D:374:LEU:HA	1:D:377:ILE:HD12	2.03	0.41
1:D:396:PHE:CG	1:D:424:GLU:HB3	2.55	0.41
1:A:399:GLN:NE2	5:A:709:HOH:O	2.53	0.41
1:A:19:ARG:CG	1:A:19:ARG:O	2.68	0.41
1:A:236:ASP:O	1:A:240:GLU:HG3	2.19	0.41
1:B:245:LYS:HE3	1:B:246:TYR:CE1	2.56	0.41
1:A:135:ILE:O	1:A:203:LEU:HA	2.21	0.41
1:C:390:ALA:O	1:C:391:ALA:HB3	2.20	0.41
1:C:450:THR:HG22	1:C:456:THR:CG2	2.48	0.41
1:D:343:LEU:HB2	1:D:350:ILE:HD12	2.03	0.41
1:A:113:THR:HG22	1:A:167:LEU:HD21	2.03	0.41
1:A:481:ARG:HG2	1:A:481:ARG:NH1	2.35	0.41
1:A:579:LYS:HA	1:A:579:LYS:CE	2.51	0.41
1:A:402:LYS:HE2	1:A:402:LYS:HB3	1.89	0.40
1:C:378:VAL:HG21	1:C:400:ILE:HG23	2.03	0.40
1:A:164:GLU:HG2	1:A:258:ALA:HB2	2.02	0.40
1:B:62:GLU:HG3	1:B:98:ARG:HH22	1.84	0.40
1:A:569:TRP:H	1:A:574:GLN:HE21	1.67	0.40
1:C:77:SER:O	1:C:81:ARG:HD2	2.22	0.40
1:C:179:ILE:HB	1:C:180:PRO:HD3	2.02	0.40
1:C:445:PRO:HG3	1:C:461:GLN:NE2	2.36	0.40
1:A:208:GLU:OE2	1:A:224:ARG:NH1	2.47	0.40
1:B:158:ILE:HG12	1:B:199:LEU:HB3	2.04	0.40
1:A:20:HIS:CE1	1:A:565:ASP:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLU:O	1:B:47:GLN:HB2	2.21	0.40
1:D:28:LEU:C	1:D:28:LEU:HD23	2.46	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	562/572 (98%)	546 (97%)	14 (2%)	2 (0%)	30	23
1	B	562/572 (98%)	543 (97%)	18 (3%)	1 (0%)	43	38
1	C	562/572 (98%)	544 (97%)	15 (3%)	3 (0%)	24	17
1	D	562/572 (98%)	548 (98%)	14 (2%)	0	100	100
All	All	2248/2288 (98%)	2181 (97%)	61 (3%)	6 (0%)	36	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	A	103	ASP
1	C	398	GLU
1	C	409	GLU
1	A	389	VAL
1	C	452	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	483/490 (99%)	461 (95%)	22 (5%)	24	17
1	B	483/490 (99%)	458 (95%)	25 (5%)	21	14
1	C	483/490 (99%)	458 (95%)	25 (5%)	21	14
1	D	483/490 (99%)	451 (93%)	32 (7%)	15	8
All	All	1932/1960 (99%)	1828 (95%)	104 (5%)	20	12

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	47	GLN
1	A	84	LEU
1	A	93	GLU
1	A	100	LEU
1	A	122	GLN
1	A	129	LYS
1	A	147	LEU
1	A	167	LEU
1	A	186	LEU
1	A	211	GLU
1	A	242	VAL
1	A	352	LYS
1	A	363	LYS
1	A	420	THR
1	A	461	GLN
1	A	480	LEU
1	A	516	ILE
1	A	547	GLU
1	A	571	GLU
1	A	575	LYS
1	A	579	LYS
1	B	19	ARG
1	B	47	GLN
1	B	147	LEU
1	B	165	ARG
1	B	167	LEU
1	B	186	LEU
1	B	224	ARG
1	B	242	VAL

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Mol	Chain	Res	Type
1	B	244	SER
1	B	272	GLN
1	B	301	LYS
1	B	307	ILE
1	B	310	GLN
1	B	338	ILE
1	B	356	SER
1	B	409	GLU
1	B	422	LYS
1	B	455	GLN
1	B	480	LEU
1	B	486	ASN
1	B	505	GLU
1	B	533	GLN
1	B	561	GLN
1	B	563	LEU
1	B	571	GLU
1	C	47	GLN
1	C	128	ARG
1	C	147	LEU
1	C	167	LEU
1	C	196	GLN
1	C	210	GLU
1	C	242	VAL
1	C	253	GLN
1	C	267	ASN
1	C	272	GLN
1	C	307	ILE
1	C	336	LYS
1	C	338	ILE
1	C	339	LYS
1	C	354	ARG
1	C	372	LYS
1	C	409	GLU
1	C	437	ARG
1	C	461	GLN
1	C	481	ARG
1	C	486	ASN
1	C	502	LYS
1	C	533	GLN
1	C	544	GLN
1	C	579	LYS

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Mol	Chain	Res	Type
1	D	18	ARG
1	D	19	ARG
1	D	43	GLU
1	D	47	GLN
1	D	56	PRO
1	D	62	GLU
1	D	73	GLU
1	D	74	HIS
1	D	108	MET
1	D	122	GLN
1	D	147	LEU
1	D	167	LEU
1	D	186	LEU
1	D	193	MET
1	D	230	GLU
1	D	242	VAL
1	D	251	LEU
1	D	272	GLN
1	D	307	ILE
1	D	335	GLU
1	D	338	ILE
1	D	339	LYS
1	D	354	ARG
1	D	444	SER
1	D	450	THR
1	D	480	LEU
1	D	481	ARG
1	D	486	ASN
1	D	514	ASN
1	D	517	ARG
1	D	547	GLU
1	D	561	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	23	GLN
1	A	49	ASN
1	A	76	ASN
1	A	121	GLN
1	A	455	GLN

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	561	GLN
1	A	574	GLN
1	B	22	HIS
1	B	47	GLN
1	B	71	ASN
1	B	76	ASN
1	B	121	GLN
1	B	196	GLN
1	B	259	ASN
1	B	310	GLN
1	B	399	GLN
1	B	461	GLN
1	B	574	GLN
1	C	22	HIS
1	C	33	HIS
1	C	47	GLN
1	C	49	ASN
1	C	121	GLN
1	C	122	GLN
1	C	196	GLN
1	C	267	ASN
1	C	321	HIS
1	C	455	GLN
1	C	461	GLN
1	C	533	GLN
1	C	574	GLN
1	D	47	GLN
1	D	49	ASN
1	D	74	HIS
1	D	76	ASN
1	D	249	ASN
1	D	321	HIS
1	D	514	ASN
1	D	561	GLN
1	D	574	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NDP	A	602	-	51,52,52	1.40	5 (9%)	71,80,80	1.32	12 (16%)
3	NDP	C	602	-	51,52,52	1.44	6 (11%)	71,80,80	1.58	16 (22%)
4	86I	D	603	-	38,39,39	1.08	2 (5%)	45,56,56	2.15	15 (33%)
4	86I	B	603	-	38,39,39	1.07	5 (13%)	45,56,56	1.87	11 (24%)
3	NDP	D	602	-	51,52,52	1.49	5 (9%)	71,80,80	1.38	12 (16%)
4	86I	A	603	-	38,39,39	1.02	2 (5%)	45,56,56	1.99	16 (35%)
4	86I	C	603	-	38,39,39	1.11	3 (7%)	45,56,56	1.88	10 (22%)
3	NDP	B	602	-	51,52,52	1.51	5 (9%)	71,80,80	1.32	6 (8%)

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	A	602	-	-	3/34/77/77	0/5/5/5
3	NDP	C	602	-	-	8/34/77/77	0/5/5/5
4	86I	D	603	-	-	6/15/15/15	0/6/6/6
4	86I	B	603	-	-	6/15/15/15	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	602	-	-	6/34/77/77	0/5/5/5
4	86I	A	603	-	-	6/15/15/15	0/6/6/6
4	86I	C	603	-	-	3/15/15/15	0/6/6/6
3	NDP	B	602	-	-	3/34/77/77	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NDP	C4N-C3N	-6.20	1.38	1.50
3	A	602	NDP	C4N-C3N	-6.00	1.38	1.50
3	C	602	NDP	C4N-C3N	-5.64	1.39	1.50
3	B	602	NDP	C4N-C3N	-5.55	1.39	1.50
3	B	602	NDP	PA-O3	5.16	1.65	1.59
3	B	602	NDP	C4N-C5N	-4.14	1.38	1.49
3	A	602	NDP	C4N-C5N	-4.06	1.38	1.49
3	D	602	NDP	C4N-C5N	-4.02	1.38	1.49
3	C	602	NDP	C4N-C5N	-3.92	1.38	1.49
3	D	602	NDP	PA-O3	3.70	1.63	1.59
3	B	602	NDP	PN-O3	3.20	1.62	1.59
3	C	602	NDP	C6A-N6A	3.19	1.42	1.34
3	A	602	NDP	PA-O3	3.14	1.62	1.59
3	C	602	NDP	P2B-O2B	3.12	1.65	1.59
3	A	602	NDP	PN-O3	3.07	1.62	1.59
3	D	602	NDP	PN-O3	3.06	1.62	1.59
3	C	602	NDP	PN-O3	2.83	1.62	1.59
4	C	603	86I	C32-C30	2.61	1.52	1.49
3	D	602	NDP	P2B-O2B	2.61	1.64	1.59
4	B	603	86I	C9-N14	2.61	1.38	1.32
3	B	602	NDP	P2B-O2B	2.58	1.64	1.59
4	D	603	86I	C5-C9	-2.58	1.42	1.47
4	A	603	86I	C32-C30	2.23	1.52	1.49
4	C	603	86I	C9-N14	2.23	1.37	1.32
4	A	603	86I	C9-N14	2.15	1.37	1.32
4	C	603	86I	C5-C9	-2.14	1.43	1.47
4	B	603	86I	N20-N19	2.13	1.34	1.30
4	B	603	86I	C23-N26	-2.12	1.28	1.33
4	B	603	86I	C24-N22	2.06	1.40	1.37
3	A	602	NDP	C7N-N7N	2.05	1.39	1.33
3	C	602	NDP	PA-O3	2.05	1.61	1.59
4	B	603	86I	N15-N20	2.04	1.37	1.35
4	D	603	86I	C9-N14	2.03	1.36	1.32

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	86I	C17-C21-N22	7.26	124.11	112.84
4	D	603	86I	C17-C21-N22	6.41	122.78	112.84
4	B	603	86I	C17-C21-N22	6.28	122.58	112.84
4	C	603	86I	C17-C21-N22	5.68	121.66	112.84
4	C	603	86I	N22-C23-N26	5.38	132.75	127.61
4	D	603	86I	N22-C23-N26	5.02	132.41	127.61
4	B	603	86I	N22-C23-N26	4.13	131.55	127.61
3	C	602	NDP	C4A-N9A-C8A	4.09	110.04	105.74
4	A	603	86I	N14-N19-N20	-3.93	105.81	110.50
4	D	603	86I	N14-N19-N20	-3.88	105.87	110.50
3	B	602	NDP	C3N-C2N-N1N	-3.85	117.55	123.20
3	B	602	NDP	C6N-N1N-C2N	3.77	123.35	119.32
3	C	602	NDP	N9A-C8A-N7A	-3.76	108.61	113.94
3	C	602	NDP	O4D-C1D-N1N	3.74	115.22	108.08
4	C	603	86I	N14-N19-N20	-3.72	106.06	110.50
4	D	603	86I	N15-N20-N19	3.69	111.92	106.68
3	A	602	NDP	O3-PA-O1A	-3.53	100.10	110.70
4	C	603	86I	C25-C23-N22	-3.53	118.52	121.89
4	B	603	86I	N14-N19-N20	-3.47	106.35	110.50
4	D	603	86I	C2-C1-S3	-3.35	117.08	122.01
3	A	602	NDP	O4D-C1D-N1N	3.33	114.43	108.08
3	A	602	NDP	C6N-N1N-C2N	3.24	122.79	119.32
3	B	602	NDP	O4B-C1B-N9A	3.23	114.30	108.09
4	D	603	86I	C5-C9-N14	-3.16	121.28	126.39
4	B	603	86I	C25-C23-N26	-3.12	108.22	111.06
4	D	603	86I	C25-C23-N22	-3.06	118.96	121.89
4	A	603	86I	N22-C23-N26	3.06	130.53	127.61
3	D	602	NDP	O4D-C1D-N1N	3.04	113.89	108.08
4	B	603	86I	N15-N20-N19	3.04	111.00	106.68
3	C	602	NDP	C3N-C2N-N1N	-3.02	118.77	123.20
3	D	602	NDP	N9A-C8A-N7A	-2.98	109.70	113.94
3	C	602	NDP	O3X-P2B-O2X	2.97	118.95	107.80
3	B	602	NDP	O4D-C1D-N1N	2.92	113.65	108.08
3	C	602	NDP	P2B-O2B-C2B	-2.91	115.67	123.43
4	D	603	86I	C2-C5-C9	-2.90	118.34	124.36
4	D	603	86I	C5-C2-C1	2.89	127.56	123.14
3	C	602	NDP	O2A-PA-O1A	2.88	125.84	112.44
3	D	602	NDP	O4B-C1B-N9A	2.84	113.54	108.09
4	B	603	86I	C2-C5-C9	-2.83	118.49	124.36
4	D	603	86I	C9-N15-N20	-2.80	104.17	108.56
4	A	603	86I	N15-N20-N19	2.76	110.60	106.68
3	D	602	NDP	O3X-P2B-O2X	2.74	118.06	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	NDP	C1D-N1N-C2N	-2.73	116.64	121.14
4	A	603	86I	C23-C25-N28	-2.72	105.29	110.31
3	D	602	NDP	C3B-C2B-C1B	-2.72	97.60	102.81
4	C	603	86I	N15-N20-N19	2.70	110.52	106.68
3	C	602	NDP	C4A-N9A-C1B	-2.70	120.33	126.63
3	A	602	NDP	C3N-C2N-N1N	-2.69	119.25	123.20
3	A	602	NDP	C2D-C1D-N1N	-2.67	106.73	113.31
4	D	603	86I	C25-C23-N26	-2.67	108.64	111.06
4	A	603	86I	C6-C2-C1	-2.64	114.40	119.26
3	D	602	NDP	C4A-N9A-C8A	2.63	108.50	105.74
4	D	603	86I	C10-C5-C2	2.62	122.20	119.26
3	D	602	NDP	C3N-C2N-N1N	-2.60	119.39	123.20
4	C	603	86I	C2-C5-C9	-2.58	119.01	124.36
3	A	602	NDP	C1D-N1N-C2N	-2.57	116.90	121.14
4	C	603	86I	C25-C23-N26	-2.56	108.73	111.06
3	A	602	NDP	O4B-C1B-C2B	-2.51	102.28	106.59
3	C	602	NDP	O3-PA-O1A	-2.49	103.22	110.70
4	A	603	86I	C9-N14-N19	2.48	108.74	106.10
3	A	602	NDP	C2B-C1B-N9A	2.47	117.81	113.75
4	A	603	86I	C25-C23-N26	-2.46	108.82	111.06
4	D	603	86I	C2-C1-N4	2.45	126.78	122.91
4	A	603	86I	C21-N22-C24	2.45	123.58	119.28
4	A	603	86I	C5-C9-N14	-2.45	122.43	126.39
4	B	603	86I	C5-C9-N14	-2.41	122.48	126.39
4	C	603	86I	C23-C25-N28	-2.40	105.89	110.31
4	D	603	86I	C6-C2-C1	-2.38	114.88	119.26
3	D	602	NDP	O2A-PA-O1A	2.38	123.50	112.44
3	C	602	NDP	O2N-PN-O1N	2.36	123.44	112.44
3	C	602	NDP	C5A-N7A-C8A	2.34	107.13	103.45
4	A	603	86I	C32-C30-N28	2.33	127.49	123.99
3	D	602	NDP	O7N-C7N-C3N	-2.32	116.52	120.90
4	A	603	86I	C5-C2-C1	2.32	126.69	123.14
3	C	602	NDP	O4B-C1B-N9A	2.31	112.53	108.09
4	A	603	86I	C12-C7-C8	2.29	123.69	121.99
4	A	603	86I	C2-C1-S3	-2.28	118.65	122.01
4	C	603	86I	C5-C2-C1	2.25	126.58	123.14
4	B	603	86I	C6-C2-C1	-2.25	115.13	119.26
3	C	602	NDP	C6N-N1N-C2N	2.24	121.72	119.32
3	A	602	NDP	O2B-C2B-C1B	-2.23	102.20	110.05
4	B	603	86I	C9-N15-N20	-2.22	105.09	108.56
3	C	602	NDP	C3B-C2B-C1B	-2.22	98.57	102.81
4	A	603	86I	C5-C9-N15	2.21	128.85	125.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NDP	C2D-C1D-N1N	-2.19	107.93	113.31
4	C	603	86I	C9-N14-N19	2.15	108.39	106.10
3	D	602	NDP	C5A-N7A-C8A	2.15	106.83	103.45
3	D	602	NDP	C6N-N1N-C2N	2.13	121.60	119.32
3	B	602	NDP	C1D-N1N-C2N	-2.10	117.67	121.14
3	B	602	NDP	O2A-PA-O1A	2.09	122.17	112.44
4	B	603	86I	C5-C2-C1	2.08	126.33	123.14
4	D	603	86I	C23-C25-N28	-2.07	106.49	110.31
3	A	602	NDP	O2A-PA-O1A	2.07	122.07	112.44
3	A	602	NDP	O2X-P2B-O2B	-2.06	97.82	105.85
3	A	602	NDP	O2A-PA-O3	2.05	112.81	107.27
4	B	603	86I	C21-N22-C24	2.04	122.88	119.28
4	A	603	86I	C32-C30-N26	-2.04	115.66	120.27
3	C	602	NDP	O5D-PN-O1N	-2.02	100.95	108.94

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	NDP	C5B-O5B-PA-O1A
4	A	603	86I	C30-C32-C33-C34
3	A	602	NDP	C3B-C2B-O2B-P2B
3	B	602	NDP	C1B-C2B-O2B-P2B
3	B	602	NDP	C3B-C2B-O2B-P2B
3	C	602	NDP	C3B-C2B-O2B-P2B
3	D	602	NDP	C3B-C2B-O2B-P2B
3	A	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	C1B-C2B-O2B-P2B
3	D	602	NDP	C1B-C2B-O2B-P2B
4	A	603	86I	S3-C1-C2-C6
4	D	603	86I	S3-C1-C2-C6
4	B	603	86I	N26-C30-C32-C33
4	A	603	86I	N4-C1-C2-C6
4	D	603	86I	N4-C1-C2-C6
3	D	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	O4B-C4B-C5B-O5B
4	D	603	86I	C10-C5-C9-N14
4	B	603	86I	S3-C1-C2-C6
4	C	603	86I	S3-C1-C2-C6
4	A	603	86I	C2-C5-C9-N14
4	D	603	86I	C2-C5-C9-N15
4	D	603	86I	C2-C5-C9-N14

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Mol	Chain	Res	Type	Atoms
3	C	602	NDP	O4D-C1D-N1N-C2N
4	C	603	86I	N4-C1-C2-C6
3	B	602	NDP	O4D-C1D-N1N-C2N
3	D	602	NDP	C2B-O2B-P2B-O1X
3	C	602	NDP	C3B-C4B-C5B-O5B
4	D	603	86I	C10-C5-C9-N15
4	B	603	86I	N4-C1-C2-C6
4	A	603	86I	C10-C5-C9-N14
4	B	603	86I	C10-C5-C9-N14
4	C	603	86I	C10-C5-C9-N14
3	D	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C2B-O2B-P2B-O1X
4	A	603	86I	C2-C5-C9-N15
4	B	603	86I	C2-C5-C9-N15
4	B	603	86I	C2-C5-C9-N14
3	A	602	NDP	C1B-C2B-O2B-P2B
3	D	602	NDP	C3B-C4B-C5B-O5B
3	C	602	NDP	C2B-O2B-P2B-O2X

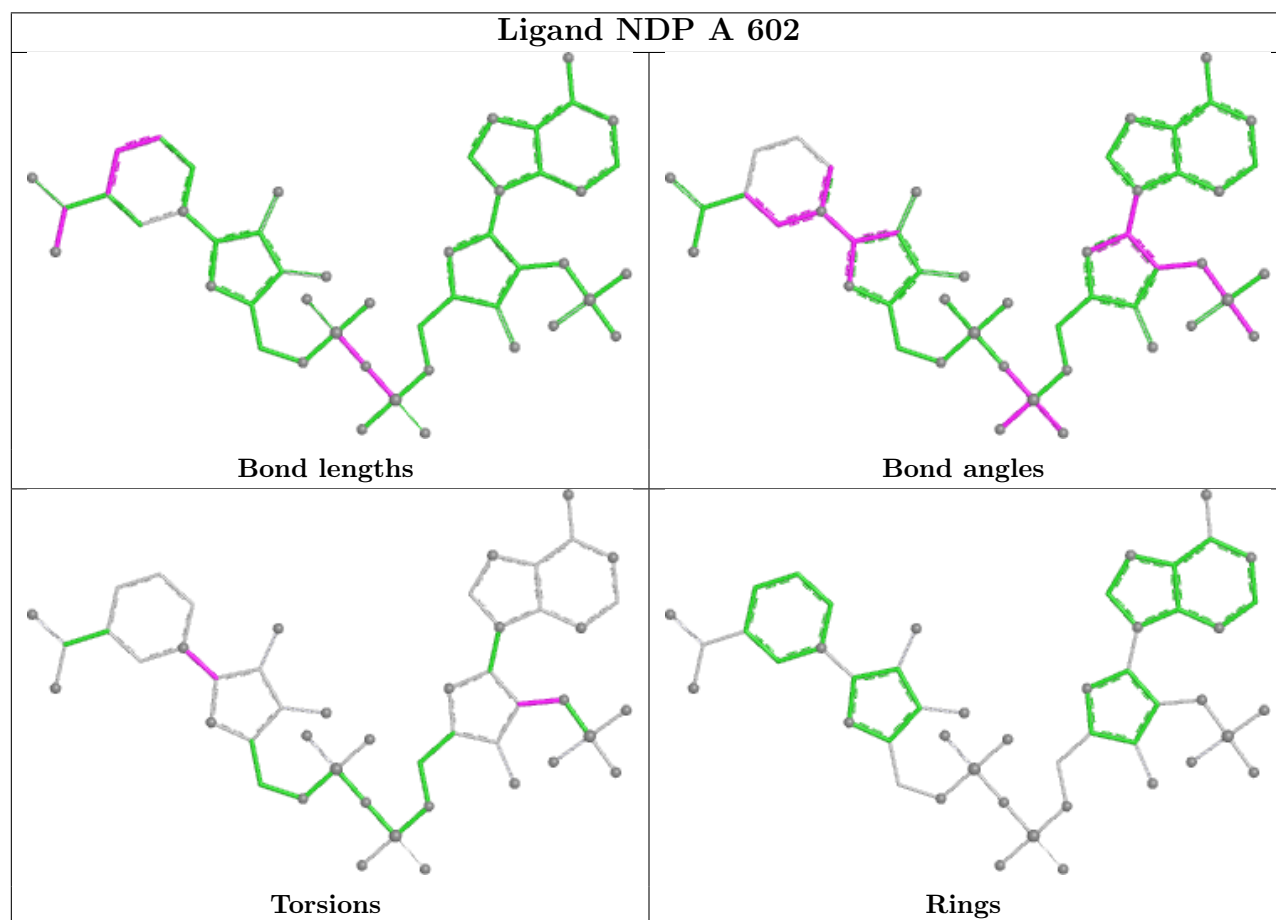
There are no ring outliers.

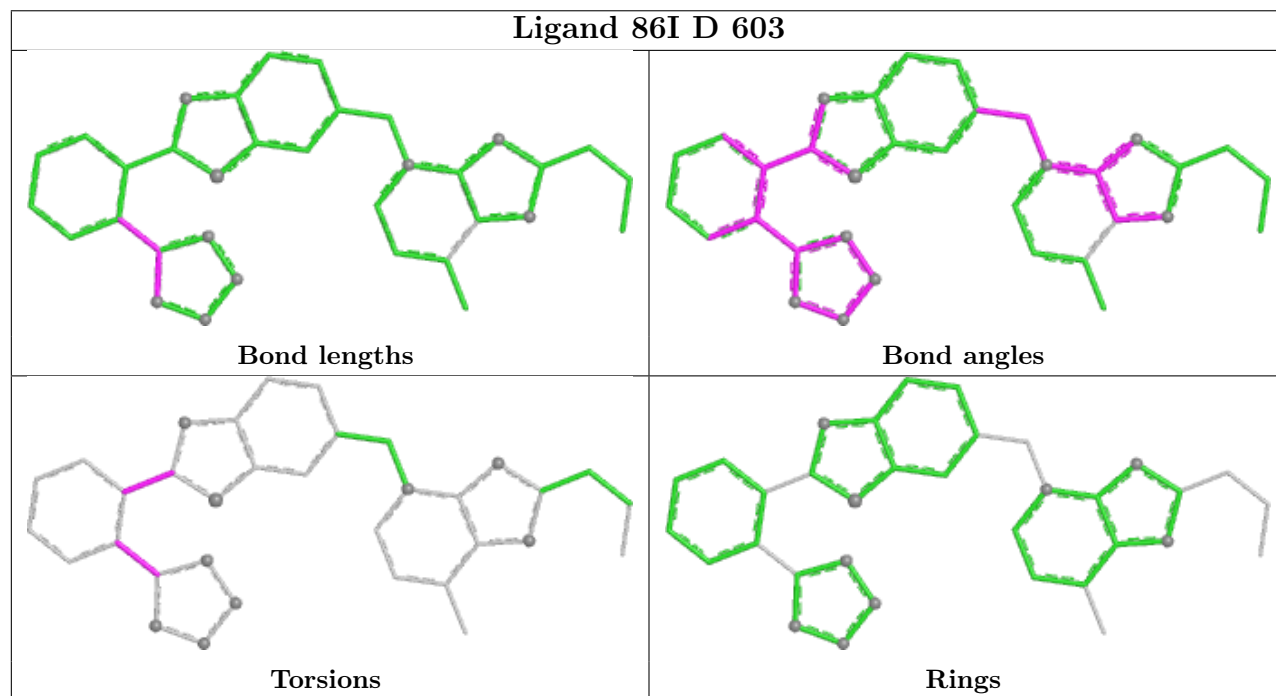
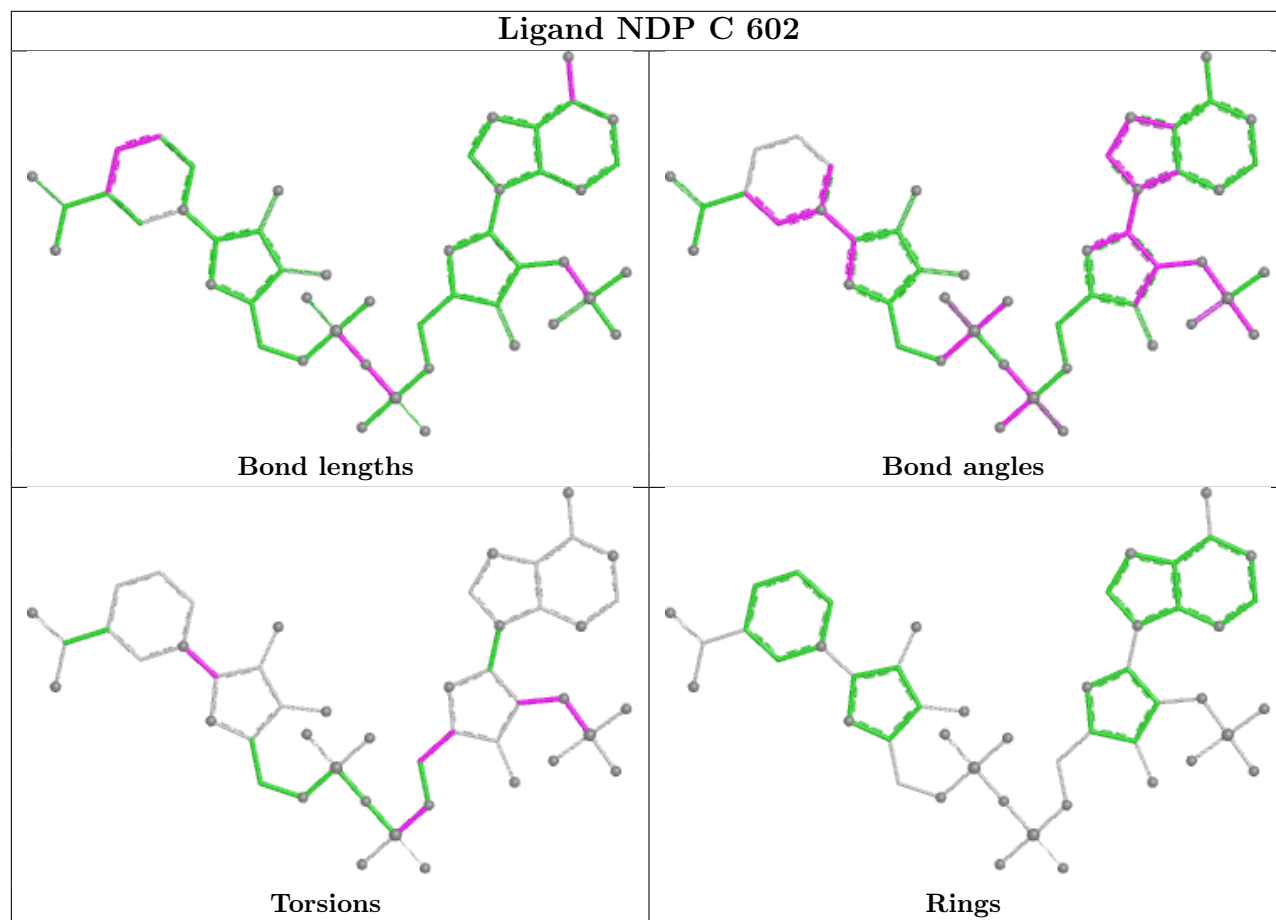
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NDP	2	0
3	C	602	NDP	2	0
4	D	603	86I	2	0
4	B	603	86I	1	0
3	D	602	NDP	2	0
4	A	603	86I	3	0
4	C	603	86I	2	0
3	B	602	NDP	1	0

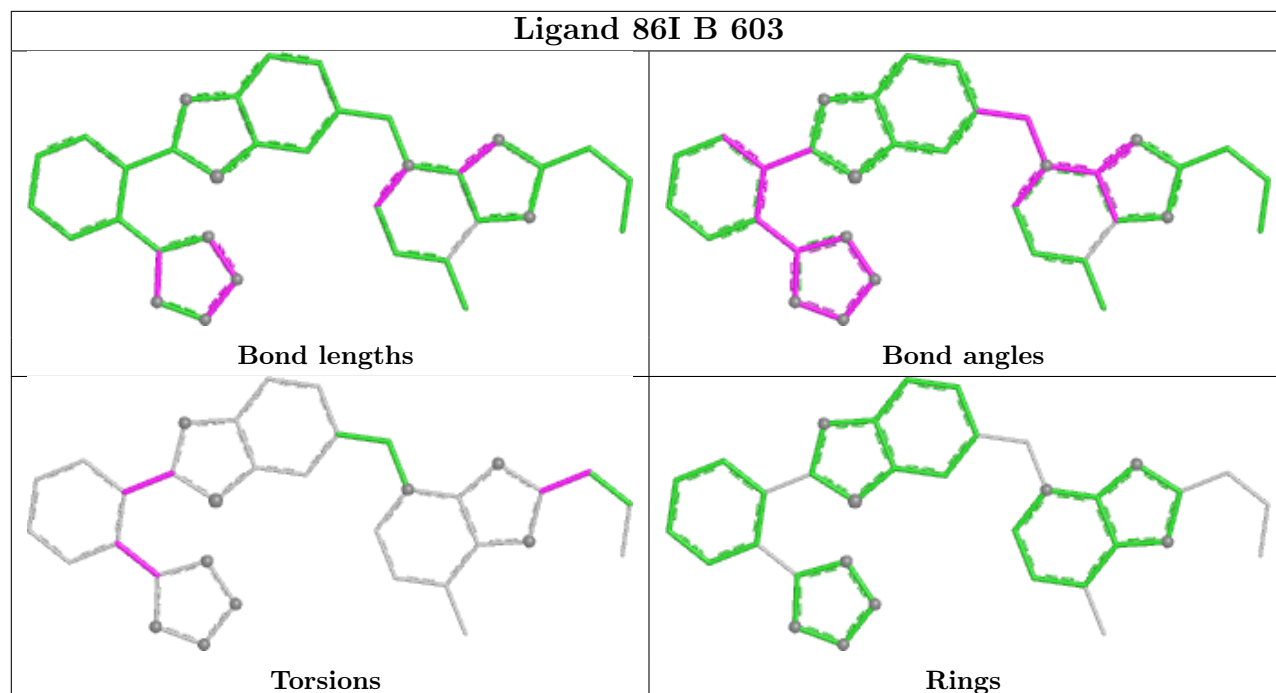
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

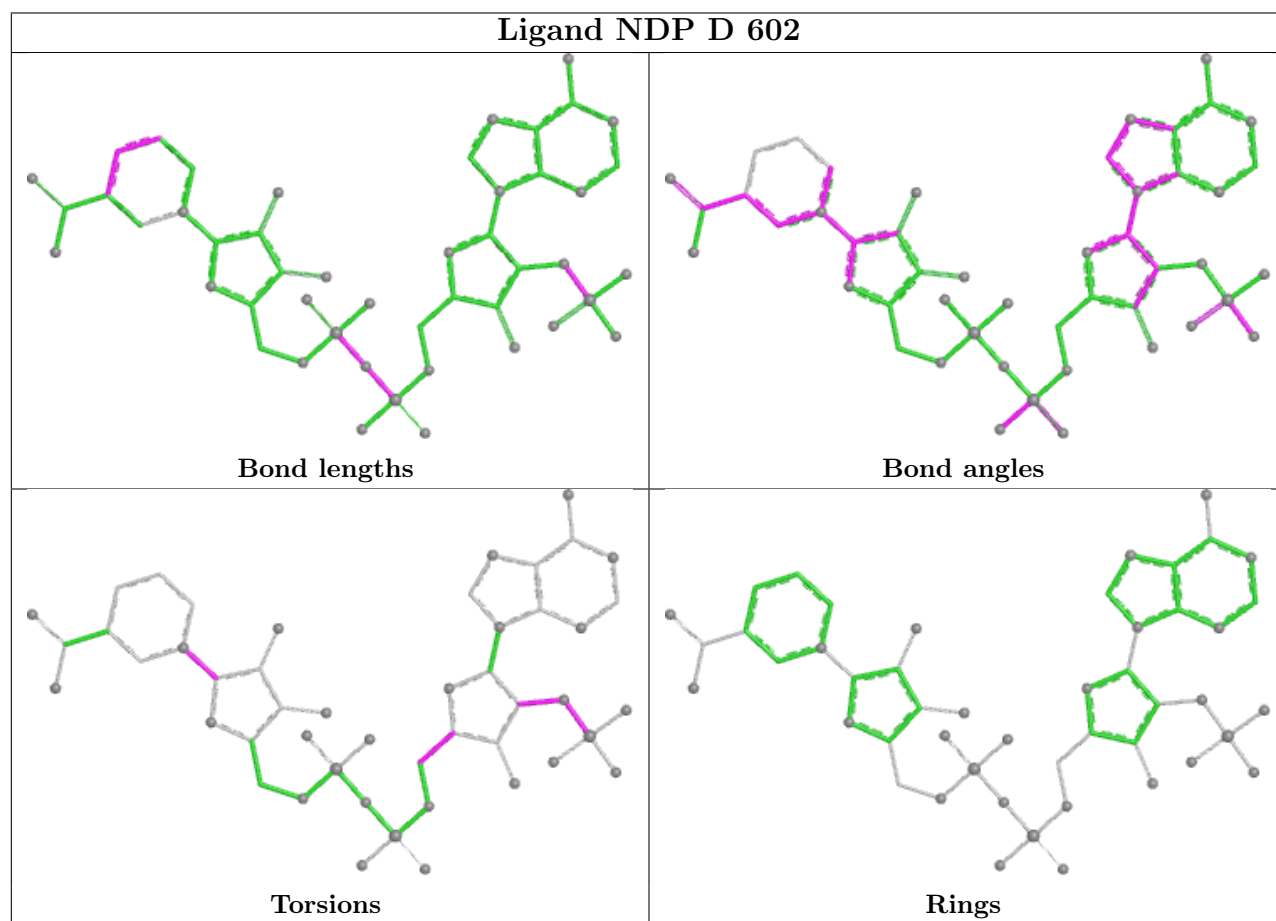




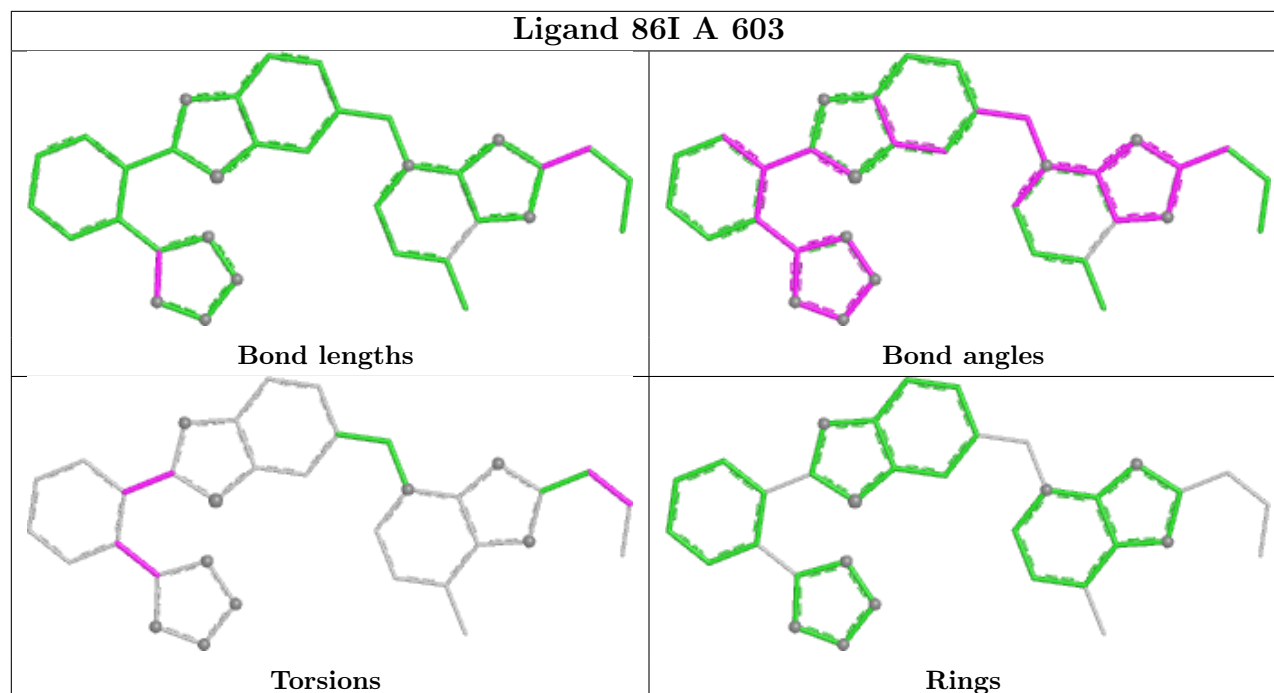
Ligand 86I B 603



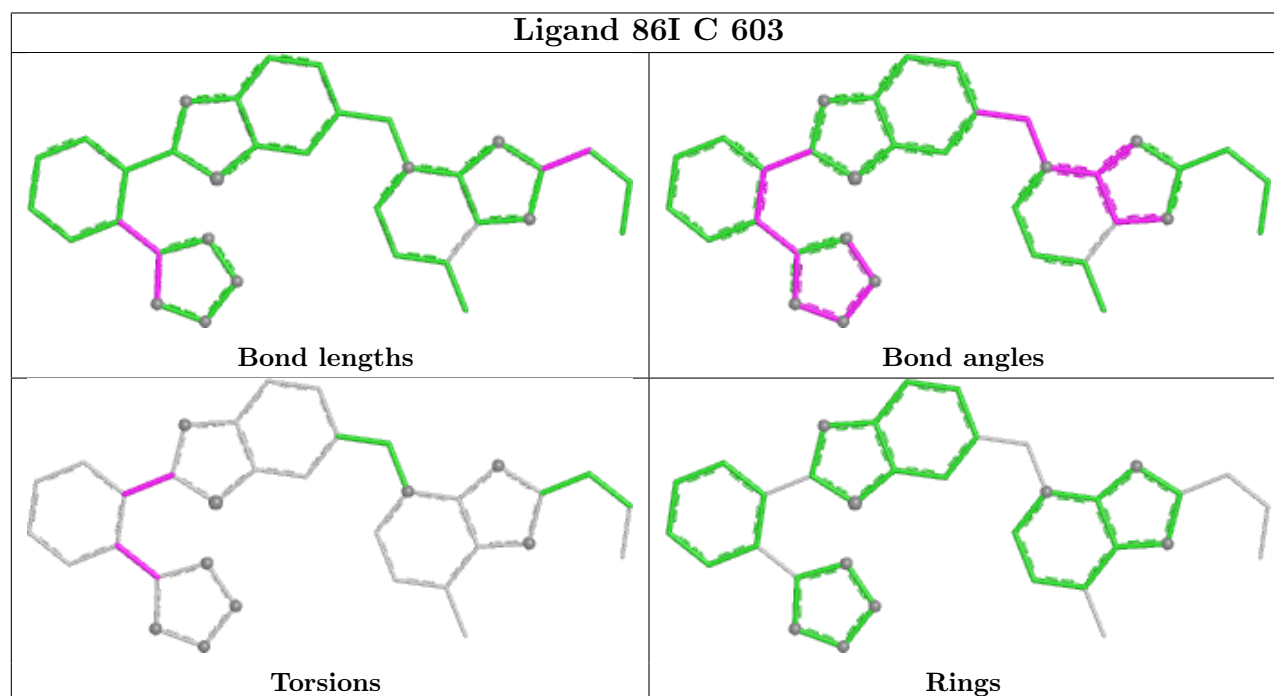
Ligand NDP D 602

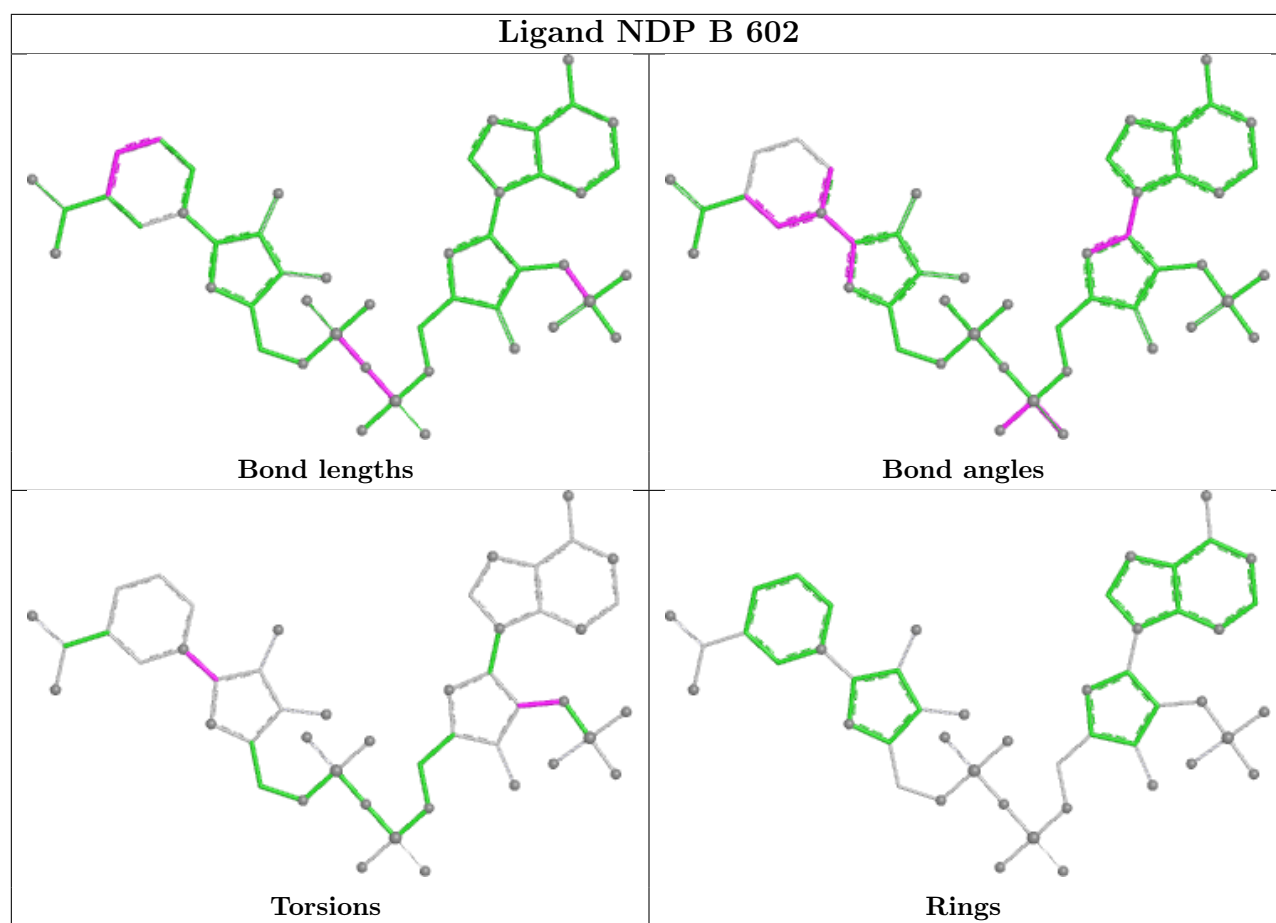


Ligand 86I A 603



Ligand 86I C 603





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	564/572 (98%)	1.43	125 (22%) 2 2	20, 32, 51, 88	0
1	B	564/572 (98%)	1.38	119 (21%) 2 2	19, 31, 53, 81	0
1	C	564/572 (98%)	1.47	143 (25%) 1 1	19, 32, 57, 99	0
1	D	564/572 (98%)	1.51	158 (28%) 1 1	20, 32, 57, 94	0
All	All	2256/2288 (98%)	1.45	545 (24%) 2 1	19, 32, 56, 99	0

All (545) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	GLY	8.6
1	C	452	PRO	8.3
1	A	454	GLY	7.5
1	A	579	LYS	6.7
1	C	355	ALA	6.7
1	D	16	PRO	6.4
1	C	579	LYS	6.0
1	A	453	ASN	5.8
1	B	579	LYS	5.7
1	A	452	PRO	5.7
1	A	540	TYR	5.5
1	B	260	VAL	5.5
1	D	20	HIS	5.5
1	C	450	THR	5.3
1	B	406	ALA	5.3
1	C	420	THR	5.2
1	C	333	PRO	5.1
1	A	575	LYS	5.1
1	C	451	LEU	5.0
1	D	17	ARG	4.9
1	C	16	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	19	ARG	4.9
1	D	358	THR	4.8
1	D	433	ILE	4.8
1	B	481	ARG	4.8
1	C	17	ARG	4.8
1	D	579	LYS	4.8
1	D	359	GLN	4.8
1	B	74	HIS	4.7
1	B	16	PRO	4.7
1	D	18	ARG	4.7
1	A	16	PRO	4.7
1	B	573	VAL	4.6
1	D	369	GLU	4.6
1	D	353	GLY	4.5
1	B	18	ARG	4.5
1	C	575	LYS	4.5
1	D	578	THR	4.5
1	A	450	THR	4.5
1	A	451	LEU	4.4
1	A	455	GLN	4.4
1	A	481	ARG	4.4
1	D	372	LYS	4.4
1	A	74	HIS	4.3
1	A	18	ARG	4.3
1	A	19	ARG	4.3
1	D	573	VAL	4.3
1	D	575	LYS	4.3
1	C	407	PHE	4.3
1	A	17	ARG	4.2
1	C	563	LEU	4.2
1	C	18	ARG	4.2
1	A	260	VAL	4.2
1	B	17	ARG	4.1
1	D	407	PHE	4.1
1	C	576	ILE	4.1
1	D	350	ILE	4.1
1	D	540	TYR	4.1
1	D	344	VAL	4.1
1	B	571	GLU	4.1
1	C	429	GLN	4.0
1	D	453	ASN	4.0
1	A	548	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLY	4.0
1	C	540	TYR	3.9
1	D	338	ILE	3.9
1	A	169	LEU	3.9
1	B	73	GLU	3.9
1	D	74	HIS	3.8
1	C	455	GLN	3.8
1	D	576	ILE	3.8
1	C	435	LYS	3.8
1	D	260	VAL	3.8
1	C	456	THR	3.8
1	C	351	VAL	3.8
1	C	433	ILE	3.7
1	D	332	LEU	3.7
1	D	406	ALA	3.7
1	D	422	LYS	3.7
1	B	19	ARG	3.7
1	C	378	VAL	3.7
1	A	214	LYS	3.7
1	B	333	PRO	3.7
1	B	378	VAL	3.7
1	D	356	SER	3.6
1	A	576	ILE	3.6
1	B	536	THR	3.6
1	B	332	LEU	3.6
1	D	333	PRO	3.6
1	B	572	GLU	3.6
1	C	432	LYS	3.6
1	D	351	VAL	3.6
1	D	577	GLN	3.6
1	C	453	ASN	3.6
1	C	552	SER	3.6
1	B	433	ILE	3.6
1	C	405	ALA	3.6
1	C	369	GLU	3.6
1	C	476	VAL	3.5
1	A	578	THR	3.5
1	C	562	ILE	3.5
1	D	377	ILE	3.5
1	B	76	ASN	3.5
1	B	372	LYS	3.5
1	C	214	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	3.5
1	C	224	ARG	3.5
1	D	342	TRP	3.5
1	D	352	LYS	3.5
1	D	400	ILE	3.5
1	D	437	ARG	3.5
1	A	272	GLN	3.5
1	D	409	GLU	3.4
1	D	429	GLN	3.4
1	A	456	THR	3.4
1	A	240	GLU	3.4
1	D	362	GLU	3.4
1	A	330	GLU	3.4
1	A	572	GLU	3.4
1	D	571	GLU	3.4
1	D	455	GLN	3.4
1	B	540	TYR	3.4
1	C	421	SER	3.4
1	B	422	LYS	3.4
1	C	332	LEU	3.4
1	D	272	GLN	3.4
1	D	513	LEU	3.4
1	B	575	LYS	3.3
1	C	394	GLY	3.3
1	A	409	GLU	3.3
1	C	339	LYS	3.3
1	D	331	GLY	3.3
1	D	348	GLY	3.3
1	B	531	ALA	3.3
1	B	211	GLU	3.3
1	D	450	THR	3.3
1	D	19	ARG	3.3
1	D	214	LYS	3.3
1	A	505	GLU	3.2
1	B	429	GLN	3.2
1	B	578	THR	3.2
1	C	409	GLU	3.2
1	C	571	GLU	3.2
1	C	376	ALA	3.2
1	D	355	ALA	3.2
1	D	544	GLN	3.2
1	C	437	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	372	LYS	3.2
1	D	514	ASN	3.2
1	B	359	GLN	3.2
1	D	531	ALA	3.1
1	C	297	ILE	3.1
1	A	73	GLU	3.1
1	B	20	HIS	3.1
1	C	240	GLU	3.1
1	A	339	LYS	3.1
1	C	108	MET	3.1
1	C	544	GLN	3.1
1	A	224	ARG	3.1
1	A	449	VAL	3.1
1	C	377	ILE	3.1
1	A	135	ILE	3.1
1	A	129	LYS	3.1
1	D	481	ARG	3.1
1	B	352	LYS	3.1
1	D	205	VAL	3.1
1	B	147	LEU	3.1
1	C	349	LEU	3.1
1	C	381	ILE	3.1
1	A	458	TYR	3.0
1	A	113	THR	3.0
1	B	148	ASN	3.0
1	C	211	GLU	3.0
1	C	352	LYS	3.0
1	D	363	LYS	3.0
1	D	390	ALA	3.0
1	B	104	ILE	3.0
1	B	395	ALA	3.0
1	C	461	GLN	3.0
1	D	399	GLN	3.0
1	B	91	ARG	3.0
1	D	330	GLU	3.0
1	C	383	PRO	3.0
1	A	372	LYS	3.0
1	B	342	TRP	3.0
1	C	70	LYS	3.0
1	C	76	ASN	3.0
1	B	214	LYS	3.0
1	A	212	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	259	ASN	2.9
1	C	331	GLY	2.9
1	C	353	GLY	2.9
1	A	400	ILE	2.9
1	A	433	ILE	2.9
1	A	561	GLN	2.9
1	D	108	MET	2.9
1	B	362	GLU	2.9
1	C	390	ALA	2.9
1	C	395	ALA	2.9
1	B	460	GLY	2.9
1	C	502	LYS	2.9
1	B	562	ILE	2.9
1	D	307	ILE	2.9
1	D	536	THR	2.9
1	C	497	GLN	2.9
1	D	240	GLU	2.9
1	B	70	LYS	2.9
1	B	373	ASN	2.9
1	D	339	LYS	2.9
1	C	365	ALA	2.9
1	A	147	LEU	2.8
1	D	533	GLN	2.8
1	B	450	THR	2.8
1	D	432	LYS	2.8
1	C	346	SER	2.8
1	A	549	PHE	2.8
1	D	561	GLN	2.8
1	B	353	GLY	2.8
1	B	513	LEU	2.8
1	C	342	TRP	2.8
1	C	506	GLU	2.8
1	D	539	VAL	2.8
1	A	429	GLN	2.8
1	D	375	GLU	2.8
1	D	308	LEU	2.8
1	B	240	GLU	2.8
1	D	211	GLU	2.8
1	B	479	GLY	2.8
1	D	532	TYR	2.8
1	B	38	LEU	2.8
1	D	317	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	378	VAL	2.8
1	B	381	ILE	2.8
1	D	392	ILE	2.8
1	A	421	SER	2.7
1	B	407	PHE	2.7
1	A	390	ALA	2.7
1	A	513	LEU	2.7
1	C	578	THR	2.7
1	A	47	GLN	2.7
1	A	573	VAL	2.7
1	B	272	GLN	2.7
1	B	544	GLN	2.7
1	D	527	ILE	2.7
1	D	562	ILE	2.7
1	C	505	GLU	2.7
1	D	417	SER	2.7
1	B	339	LYS	2.7
1	C	334	LYS	2.7
1	C	359	GLN	2.7
1	C	249	ASN	2.7
1	A	552	SER	2.7
1	A	117	GLY	2.7
1	C	406	ALA	2.7
1	B	577	GLN	2.7
1	C	561	GLN	2.7
1	C	357	LEU	2.7
1	A	448	PRO	2.7
1	D	572	GLU	2.7
1	D	444	SER	2.7
1	A	447	ASP	2.7
1	A	435	LYS	2.7
1	B	224	ARG	2.7
1	D	354	ARG	2.7
1	A	211	GLU	2.6
1	D	427	ALA	2.6
1	A	418	ASN	2.6
1	A	417	SER	2.6
1	D	535	LYS	2.6
1	C	379	GLN	2.6
1	B	335	GLU	2.6
1	B	189	ALA	2.6
1	D	366	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	333	PRO	2.6
1	D	147	LEU	2.6
1	D	402	LYS	2.6
1	D	435	LYS	2.6
1	B	369	GLU	2.6
1	D	549	PHE	2.6
1	B	126	VAL	2.6
1	D	379	GLN	2.6
1	A	362	GLU	2.6
1	D	428	GLU	2.6
1	A	331	GLY	2.6
1	C	517	ARG	2.6
1	D	391	ALA	2.6
1	A	419	PRO	2.6
1	C	465	SER	2.6
1	A	359	GLN	2.5
1	C	370	GLU	2.5
1	D	62	GLU	2.5
1	C	338	ILE	2.5
1	B	532	TYR	2.5
1	A	422	LYS	2.5
1	B	535	LYS	2.5
1	C	408	ASN	2.5
1	C	422	LYS	2.5
1	A	128	ARG	2.5
1	C	354	ARG	2.5
1	C	384	THR	2.5
1	D	541	PRO	2.5
1	A	213	LEU	2.5
1	A	553	GLN	2.5
1	B	482	GLN	2.5
1	A	380	GLU	2.5
1	B	547	GLU	2.5
1	A	407	PHE	2.5
1	A	414	PHE	2.5
1	B	263	PHE	2.5
1	D	247	GLY	2.5
1	D	368	HIS	2.5
1	A	352	LYS	2.5
1	A	502	LYS	2.5
1	C	458	TYR	2.5
1	A	62	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	376	ALA	2.5
1	D	512	PRO	2.5
1	D	167	LEU	2.5
1	C	74	HIS	2.5
1	D	347	LYS	2.5
1	D	502	LYS	2.5
1	B	528	VAL	2.5
1	D	486	ASN	2.5
1	C	303	SER	2.5
1	B	301	LYS	2.5
1	C	382	LYS	2.5
1	A	437	ARG	2.5
1	A	486	ASN	2.5
1	C	350	ILE	2.5
1	D	187	TYR	2.4
1	D	490	THR	2.4
1	A	441	ALA	2.4
1	B	169	LEU	2.4
1	D	329	LYS	2.4
1	A	544	GLN	2.4
1	B	534	GLU	2.4
1	D	565	ASP	2.4
1	C	397	SER	2.4
1	B	56	PRO	2.4
1	D	144	ALA	2.4
1	A	401	LEU	2.4
1	A	457	LEU	2.4
1	B	75	LEU	2.4
1	C	513	LEU	2.4
1	D	401	LEU	2.4
1	D	451	LEU	2.4
1	D	563	LEU	2.4
1	A	353	GLY	2.4
1	D	436	GLY	2.4
1	C	463	ASN	2.4
1	D	463	ASN	2.4
1	B	533	GLN	2.4
1	B	561	GLN	2.4
1	D	210	GLU	2.4
1	D	506	GLU	2.4
1	A	301	LYS	2.4
1	A	334	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	336	LYS	2.4
1	B	543	PRO	2.4
1	C	548	ALA	2.4
1	A	75	LEU	2.4
1	A	118	LEU	2.4
1	D	370	GLU	2.4
1	D	249	ASN	2.4
1	D	388	GLY	2.4
1	B	502	LYS	2.4
1	A	298	THR	2.4
1	A	420	THR	2.4
1	C	567	TYR	2.3
1	B	355	ALA	2.3
1	B	405	ALA	2.3
1	B	537	ALA	2.3
1	C	572	GLU	2.3
1	D	367	GLU	2.3
1	A	480	LEU	2.3
1	B	259	ASN	2.3
1	C	545	ASN	2.3
1	D	343	LEU	2.3
1	D	357	LEU	2.3
1	C	348	GLY	2.3
1	D	518	ASP	2.3
1	D	165	ARG	2.3
1	D	193	MET	2.3
1	C	330	GLU	2.3
1	C	534	GLU	2.3
1	B	107	PHE	2.3
1	D	137	ILE	2.3
1	D	419	PRO	2.3
1	A	37	ASP	2.3
1	A	571	GLU	2.3
1	C	20	HIS	2.3
1	C	426	SER	2.3
1	B	79	PHE	2.3
1	C	549	PHE	2.3
1	D	230	GLU	2.3
1	A	379	GLN	2.3
1	B	455	GLN	2.3
1	C	272	GLN	2.3
1	D	461	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	551	ARG	2.3
1	B	526	LYS	2.3
1	B	548	ALA	2.3
1	C	385	ALA	2.3
1	D	472	ALA	2.3
1	C	436	GLY	2.3
1	C	416	LEU	2.3
1	A	230	GLU	2.2
1	B	367	GLU	2.2
1	D	335	GLU	2.2
1	B	72	PHE	2.2
1	B	576	ILE	2.2
1	C	539	VAL	2.2
1	D	148	ASN	2.2
1	D	271	ASN	2.2
1	A	87	ASP	2.2
1	A	403	ASP	2.2
1	A	415	ALA	2.2
1	B	251	LEU	2.2
1	B	269	TYR	2.2
1	C	547	GLU	2.2
1	D	269	TYR	2.2
1	D	505	GLU	2.2
1	A	533	GLN	2.2
1	A	397	SER	2.2
1	C	500	SER	2.2
1	A	76	ASN	2.2
1	B	377	ILE	2.2
1	C	373	ASN	2.2
1	B	205	VAL	2.2
1	C	541	PRO	2.2
1	D	154	VAL	2.2
1	A	391	ALA	2.2
1	A	566	CYS	2.2
1	D	566	CYS	2.2
1	C	533	GLN	2.2
1	C	417	SER	2.2
1	B	546	LYS	2.2
1	C	340	LYS	2.2
1	D	340	LYS	2.2
1	A	545	ASN	2.2
1	C	392	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	476	VAL	2.2
1	B	507	GLY	2.2
1	D	43	GLU	2.2
1	A	357	LEU	2.2
1	B	563	LEU	2.2
1	D	291	LEU	2.2
1	C	128	ARG	2.2
1	A	70	LYS	2.2
1	B	529	LYS	2.2
1	D	129	LYS	2.2
1	C	536	THR	2.2
1	D	345	ASP	2.2
1	D	445	PRO	2.1
1	B	210	GLU	2.1
1	C	380	GLU	2.1
1	C	396	PHE	2.1
1	C	516	ILE	2.1
1	B	170	GLY	2.1
1	C	477	ALA	2.1
1	D	385	ALA	2.1
1	C	291	LEU	2.1
1	C	343	LEU	2.1
1	C	508	ARG	2.1
1	D	517	ARG	2.1
1	B	465	SER	2.1
1	B	347	LYS	2.1
1	D	334	LYS	2.1
1	A	532	TYR	2.1
1	B	123	TYR	2.1
1	C	398	GLU	2.1
1	C	428	GLU	2.1
1	A	434	THR	2.1
1	A	515	THR	2.1
1	A	536	THR	2.1
1	A	543	PRO	2.1
1	A	263	PHE	2.1
1	B	338	ILE	2.1
1	C	137	ILE	2.1
1	D	381	ILE	2.1
1	C	449	VAL	2.1
1	C	528	VAL	2.1
1	D	324	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	326	ALA	2.1
1	C	149	ALA	2.1
1	B	334	LYS	2.1
1	C	535	LYS	2.1
1	D	480	LEU	2.1
1	A	335	GLU	2.1
1	D	261	ASN	2.1
1	B	541	PRO	2.1
1	D	482	GLN	2.1
1	C	368	HIS	2.1
1	A	516	ILE	2.1
1	C	413	ILE	2.1
1	D	387	ILE	2.1
1	B	159	VAL	2.1
1	C	347	LYS	2.1
1	B	144	ALA	2.1
1	B	308	LEU	2.1
1	B	421	SER	2.1
1	C	457	LEU	2.1
1	D	349	LEU	2.1
1	B	505	GLU	2.1
1	D	360	GLU	2.1
1	A	514	ASN	2.1
1	B	574	GLN	2.1
1	A	114	PRO	2.1
1	A	366	HIS	2.1
1	C	448	PRO	2.1
1	A	168	GLY	2.1
1	A	276	PHE	2.1
1	A	519	VAL	2.1
1	B	242	VAL	2.1
1	B	351	VAL	2.1
1	C	344	VAL	2.1
1	C	499	VAL	2.1
1	C	531	ALA	2.1
1	D	118	LEU	2.0
1	D	489	LEU	2.0
1	B	486	ASN	2.0
1	B	514	ASN	2.0
1	D	418	ASN	2.0
1	B	233	ASP	2.0
1	A	459	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	510	TYR	2.0
1	B	439	ILE	2.0
1	B	516	ILE	2.0
1	A	550	VAL	2.0
1	B	409	GLU	2.0
1	B	549	PHE	2.0
1	C	79	PHE	2.0
1	D	79	PHE	2.0
1	D	201	VAL	2.0
1	D	548	ALA	2.0
1	A	308	LEU	2.0
1	A	343	LEU	2.0
1	C	327	LEU	2.0
1	C	553	GLN	2.0
1	C	403	ASP	2.0
1	B	165	ARG	2.0
1	C	481	ARG	2.0
1	C	551	ARG	2.0
1	A	20	HIS	2.0
1	D	299	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(Å ²)	Q<0.9
4	86I	A	603	34/34	0.83	0.14	31,35,42,44	0
4	86I	D	603	34/34	0.86	0.14	26,37,46,48	0
4	86I	B	603	34/34	0.87	0.12	26,33,42,44	0

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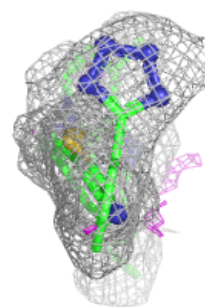
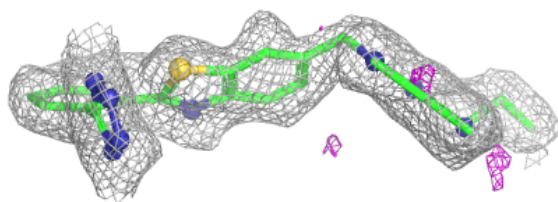
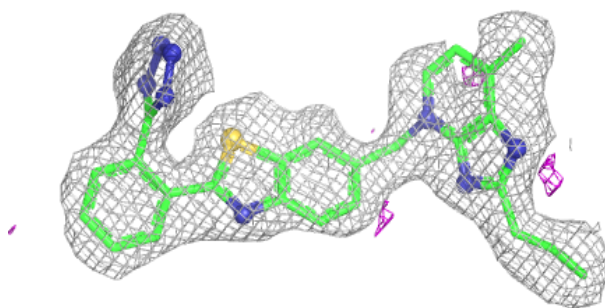
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	86I	C	603	34/34	0.89	0.12	26,32,39,42	0
3	NDP	D	602	48/48	0.90	0.11	28,36,43,46	0
3	NDP	C	602	48/48	0.93	0.09	30,35,39,42	0
3	NDP	A	602	48/48	0.94	0.09	27,31,35,38	0
3	NDP	B	602	48/48	0.95	0.08	25,29,32,34	0
2	MN	C	601	1/1	0.98	0.04	35,35,35,35	0
2	MN	A	601	1/1	0.98	0.05	37,37,37,37	0
2	MN	B	601	1/1	0.98	0.06	38,38,38,38	0
2	MN	D	601	1/1	0.99	0.04	34,34,34,34	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.

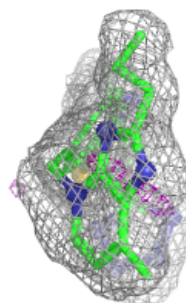
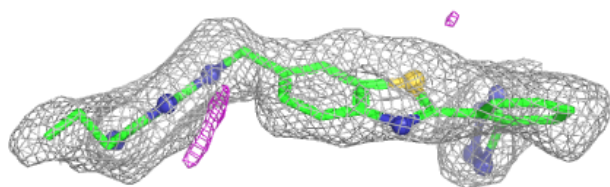
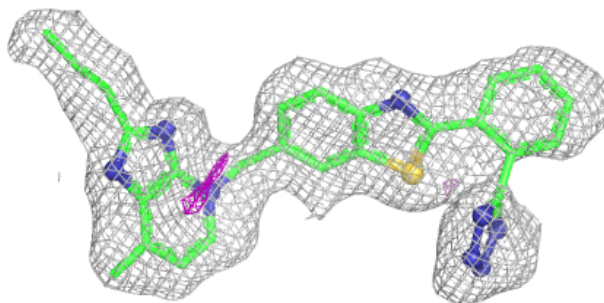
Electron density around 86I A 603:

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

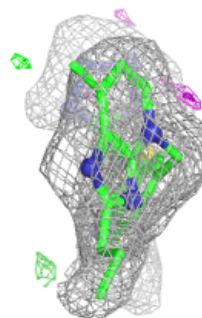
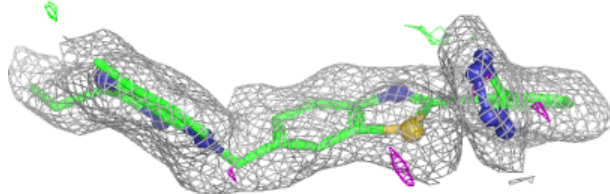
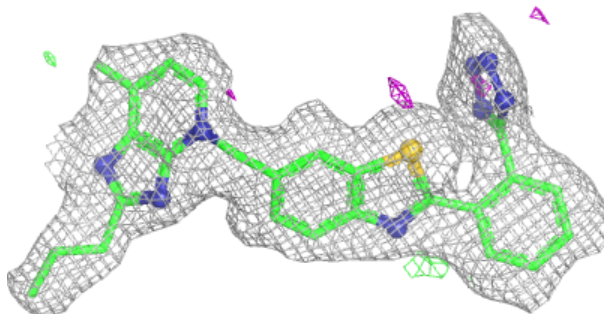


Electron density around 86I D 603:

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

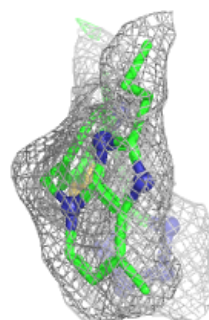
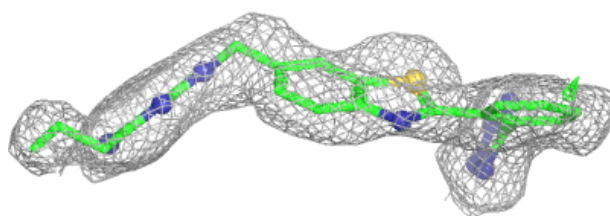
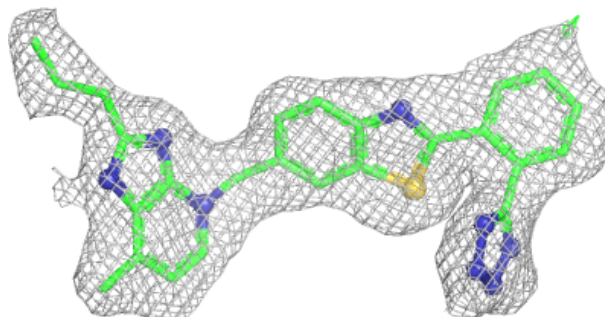
**Electron density around 86I B 603:**

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

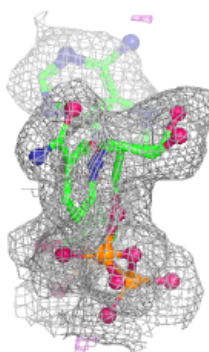
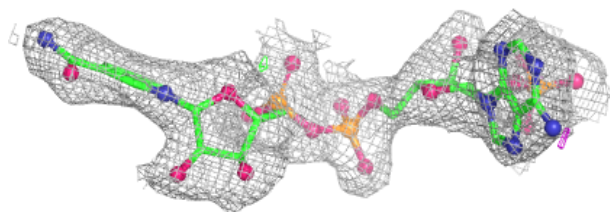
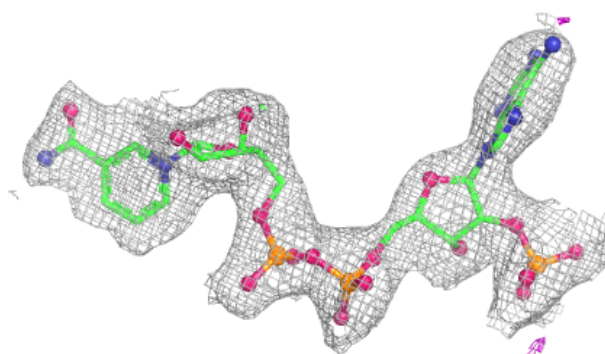


Electron density around 86I C 603:

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

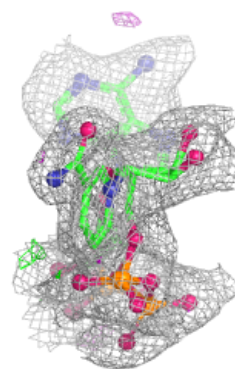
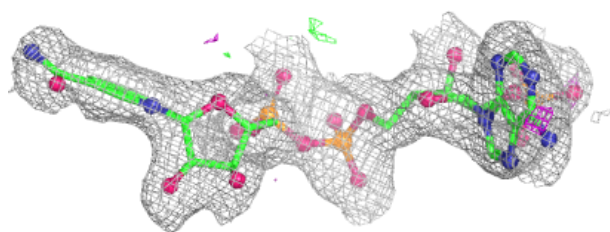
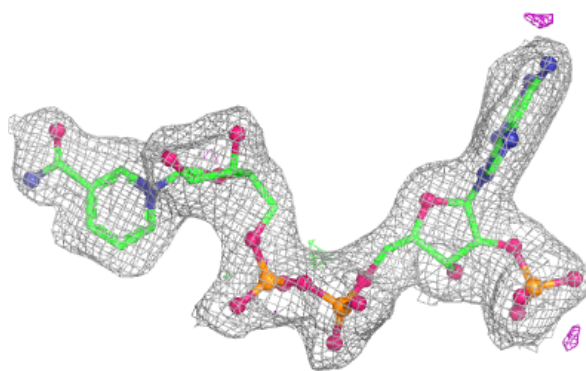
**Electron density around NDP D 602:**

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

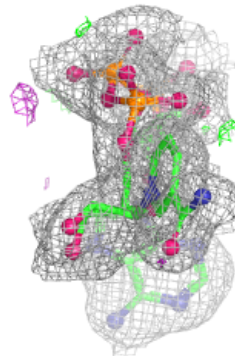
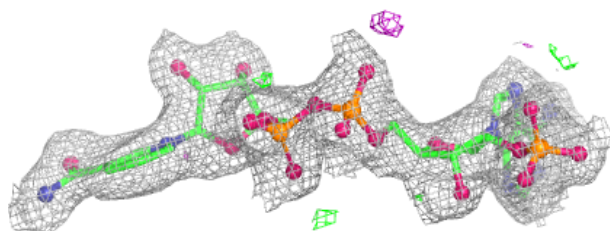
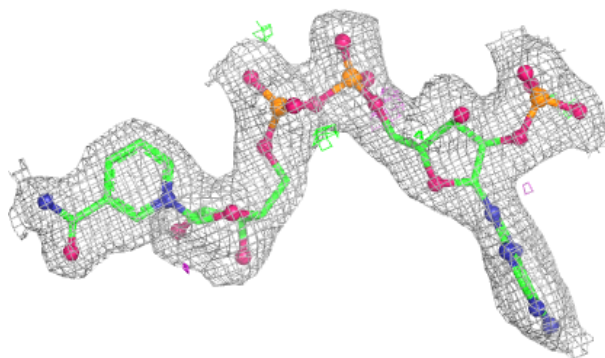


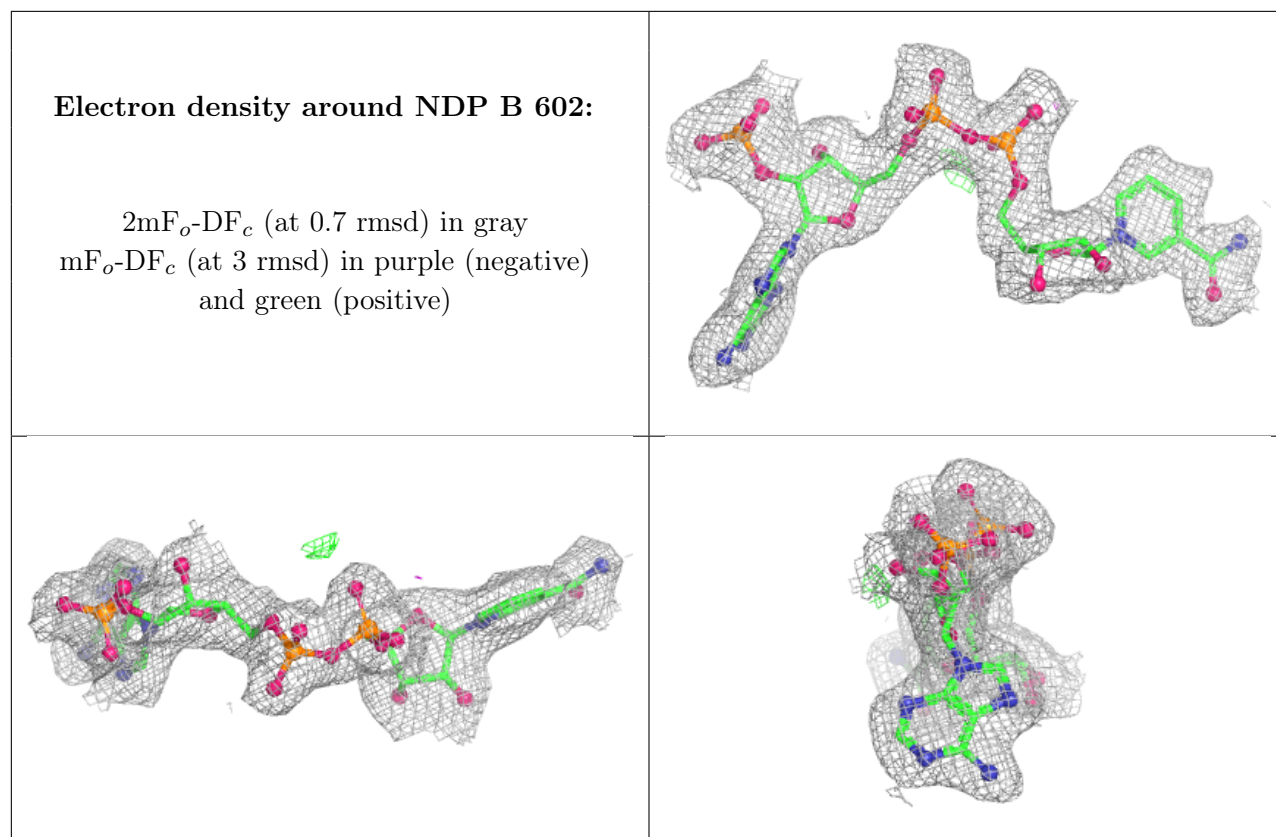
Electron density around NDP C 602:

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

**Electron density around NDP A 602:**

$2mF_o-DF_c$ (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.