



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 7X12 / pdb_00007x12
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

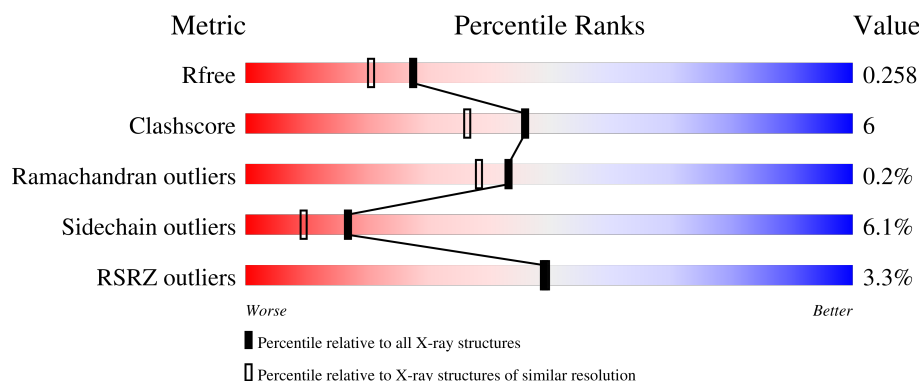
1 Overall quality at a glance

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	 10% 80% 17% ..
1	B	572	 10% 82% 14% ...
1	C	572	 10% 79% 17% ..
1	D	572	 10% 83% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18485 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 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

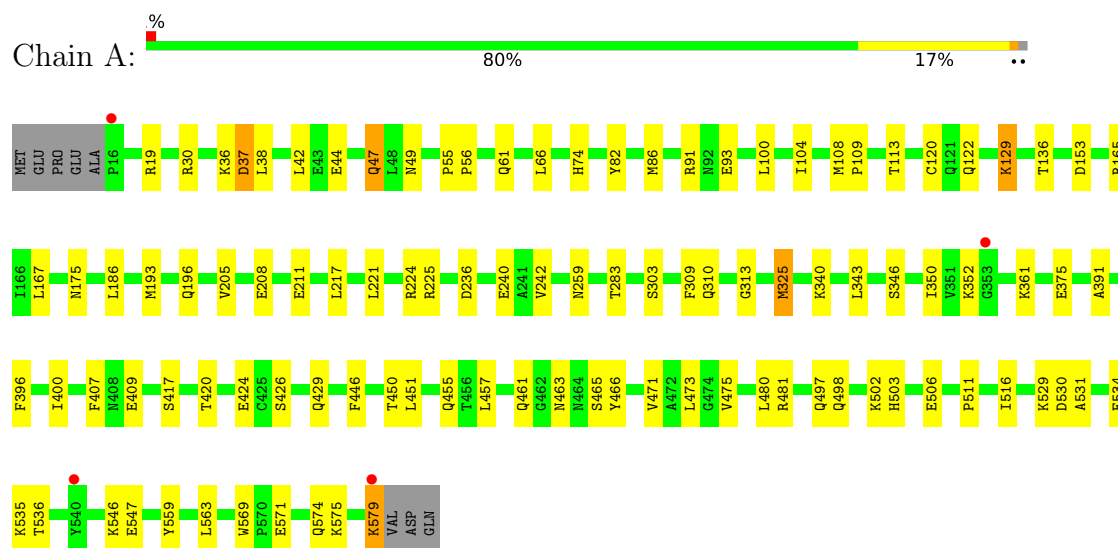
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	154	Total O 154 154	0	0
4	C	130	Total O 130 130	0	0
4	D	149	Total O 149 149	0	0

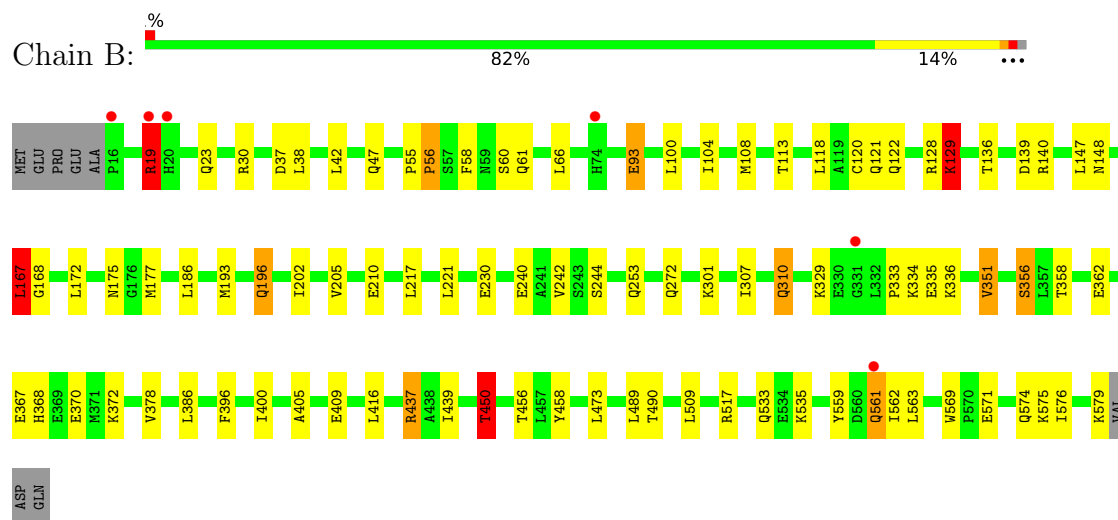
3 Residue-property plots

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

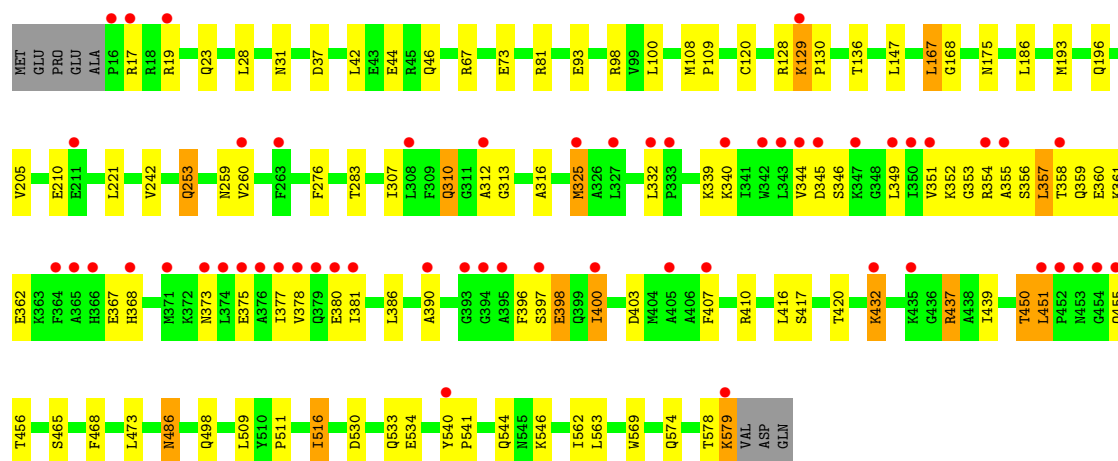


• Molecule 1: NADP-dependent malic enzyme

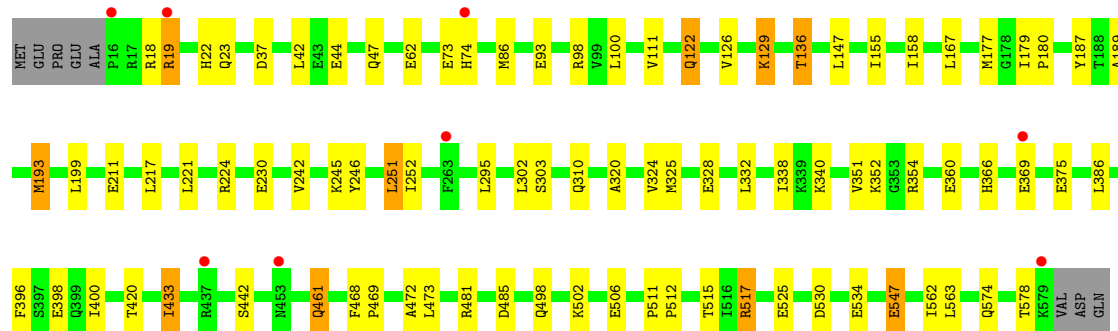
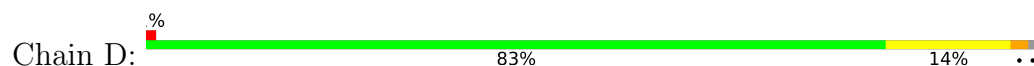


• Molecule 1: NADP-dependent malic enzyme





• 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	142.28Å 181.59Å 116.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 2.07 45.18 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.2 (45.18-2.07) 95.2 (45.18-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.216 , 0.258 0.216 , 0.258	Depositor DCC
R_{free} test set	8760 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18485	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.55	0/4538	1.09	6/6142 (0.1%)
1	B	0.55	0/4538	1.09	10/6142 (0.2%)
1	C	0.53	0/4538	1.10	6/6142 (0.1%)
1	D	0.53	0/4538	1.08	2/6142 (0.0%)
All	All	0.54	0/18152	1.09	24/24568 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ASP	CB-CA-C	-13.62	100.88	116.54
1	A	37	ASP	CB-CA-C	-9.55	105.55	116.63
1	A	129	LYS	CB-CA-C	9.47	120.65	109.85
1	C	37	ASP	CB-CA-C	-9.08	106.09	116.54
1	C	129	LYS	CB-CA-C	8.35	121.31	110.13
1	C	205	VAL	N-CA-C	-6.26	106.22	112.17
1	A	450	THR	CB-CA-C	6.25	120.32	110.19
1	C	98	ARG	CG-CD-NE	-5.97	98.86	112.00
1	B	93	GLU	CB-CG-CD	5.95	122.72	112.60
1	B	56	PRO	N-CA-CB	-5.87	98.88	102.81
1	C	81	ARG	CG-CD-NE	-5.78	99.28	112.00
1	C	93	GLU	CB-CG-CD	5.78	122.42	112.60
1	B	450	THR	CB-CA-C	5.73	119.21	109.75
1	B	490	THR	CA-CB-OG1	-5.54	101.28	109.60
1	B	58	PHE	CB-CA-C	5.52	119.32	110.16
1	B	167	LEU	CB-CA-C	-5.51	110.20	116.54
1	B	561	GLN	CB-CA-C	5.51	118.62	109.53
1	B	437	ARG	CB-CG-CD	5.44	123.82	111.30
1	B	205	VAL	N-CA-C	-5.35	107.09	112.17
1	B	129	LYS	CB-CA-C	5.34	115.94	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	ARG	CG-CD-NE	-5.20	100.56	112.00
1	A	205	VAL	N-CA-C	-5.18	107.25	112.17
1	A	153	ASP	CB-CA-C	-5.09	102.20	110.85
1	A	407	PHE	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	56	0
1	B	4451	0	4483	53	0
1	C	4451	0	4483	69	0
1	D	4451	0	4483	44	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	4	0
3	B	48	0	26	1	0
3	C	48	0	26	6	0
3	D	48	0	26	0	0
4	A	52	0	0	0	0
4	B	154	0	0	8	0
4	C	130	0	0	4	0
4	D	149	0	0	3	0
All	All	18485	0	18036	208	0

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

All (208) 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	4:B:834:HOH:O	1.48	1.13
1:C:129:LYS:HB2	4:C:798:HOH:O	1.51	1.09
1:B:37:ASP:HB2	4:B:764:HOH:O	1.58	1.02
1:A:375:GLU:HA	1:A:400:ILE:HD11	1.43	1.00
1:A:375:GLU:HA	1:A:400:ILE:CD1	2.02	0.89
1:A:42:LEU:HD23	1:D:574:GLN:HE21	1.38	0.88
1:C:310:GLN:O	1:C:390:ALA:HB2	1.75	0.85
1:C:310:GLN:O	1:C:310:GLN:HG3	1.77	0.85
1:D:19:ARG:HG2	1:D:562:ILE:HG22	1.55	0.85
1:B:19:ARG:HH21	1:B:19:ARG:HB2	1.47	0.79
1:B:333:PRO:HG2	1:B:336:LYS:HG3	1.66	0.78
1:D:19:ARG:HB2	1:D:19:ARG:HH21	1.49	0.77
1:B:19:ARG:HG2	1:B:562:ILE:HG22	1.69	0.74
1:C:378:VAL:HG21	1:C:400:ILE:HG23	1.68	0.74
1:D:129:LYS:HB2	4:D:738:HOH:O	1.86	0.74
1:B:19:ARG:NH1	1:B:196:GLN:HE22	1.87	0.73
1:C:193:MET:HE1	1:C:473:LEU:HA	1.70	0.72
1:A:569:TRP:H	1:A:574:GLN:NE2	1.89	0.70
1:C:313:GLY:HA3	3:C:602:NDP:O5B	1.91	0.69
1:C:451:LEU:HD12	1:C:455:GLN:HB2	1.76	0.68
1:A:574:GLN:HE21	1:D:42:LEU:HD23	1.59	0.68
1:B:37:ASP:CB	4:B:764:HOH:O	2.31	0.65
1:D:44:GLU:HA	1:D:563:LEU:HD21	1.77	0.65
1:D:193:MET:HE1	1:D:473:LEU:HA	1.78	0.65
1:C:19:ARG:NH2	1:C:196:GLN:HE22	1.97	0.62
1:A:375:GLU:CA	1:A:400:ILE:HD11	2.25	0.62
1:D:502:LYS:NZ	1:D:506:GLU:OE2	2.33	0.62
1:C:373:ASN:O	1:C:377:ILE:HG13	2.00	0.61
1:C:546:LYS:HE2	4:C:823:HOH:O	1.99	0.61
1:B:129:LYS:HB2	4:B:840:HOH:O	2.01	0.61
1:A:193:MET:HE1	1:A:473:LEU:HA	1.83	0.61
1:D:19:ARG:HB2	1:D:19:ARG:NH2	2.14	0.60
1:B:136:THR:HB	1:B:221:LEU:HD11	1.82	0.60
1:D:187:TYR:HE2	1:D:472:ALA:HB2	1.67	0.60
1:B:333:PRO:HG2	1:B:336:LYS:CG	2.30	0.60
1:A:120:CYS:O	1:A:175:ASN:HB3	2.02	0.59
1:C:359:GLN:HA	1:C:362:GLU:HG2	1.83	0.59
1:C:349:LEU:O	1:C:354:ARG:NH1	2.36	0.58
1:C:569:TRP:H	1:C:574:GLN:NE2	2.02	0.58
1:A:530:ASP:O	1:A:534:GLU:HG2	2.03	0.58
1:A:498:GLN:HB2	1:A:511:PRO:HG3	1.86	0.57
1:C:44:GLU:HA	1:C:563:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ALA:O	1:B:437:ARG:NH2	2.39	0.56
1:B:38:LEU:HD21	1:B:55:PRO:HG2	1.86	0.56
1:C:375:GLU:HA	1:C:400:ILE:HD13	1.87	0.56
1:C:310:GLN:O	1:C:390:ALA:CB	2.52	0.56
1:B:42:LEU:HD23	1:C:574:GLN:HE21	1.71	0.56
1:B:193:MET:HE1	1:B:473:LEU:HA	1.87	0.56
1:C:344:VAL:HG12	3:C:602:NDP:H2A	1.86	0.55
1:C:28:LEU:C	1:C:28:LEU:HD23	2.31	0.55
1:C:530:ASP:O	1:C:534:GLU:HG2	2.07	0.55
1:C:345:ASP:HB2	3:C:602:NDP:O2X	2.07	0.55
1:C:386:LEU:HG	1:C:396:PHE:CZ	2.41	0.55
1:B:19:ARG:O	1:B:562:ILE:HA	2.06	0.55
1:A:303:SER:O	1:A:340:LYS:HE2	2.07	0.54
1:A:38:LEU:HD21	1:A:55:PRO:HG2	1.89	0.54
1:C:310:GLN:O	1:C:310:GLN:CG	2.54	0.54
1:A:208:GLU:OE2	1:A:224:ARG:HD3	2.08	0.54
1:B:333:PRO:CG	1:B:336:LYS:HG3	2.37	0.54
1:B:386:LEU:HG	1:B:396:PHE:CZ	2.44	0.53
1:D:251:LEU:HD12	1:D:252:ILE:N	2.24	0.53
1:B:517:ARG:HG2	4:B:816:HOH:O	2.09	0.53
1:D:136:THR:HB	1:D:221:LEU:HD11	1.91	0.52
1:B:569:TRP:H	1:B:574:GLN:NE2	2.06	0.52
1:A:529:LYS:HE3	1:A:546:LYS:HB2	1.91	0.52
1:C:367:GLU:O	1:C:368:HIS:HB2	2.09	0.52
1:C:439:ILE:HG22	1:C:509:LEU:HD11	1.92	0.52
1:D:530:ASP:O	1:D:534:GLU:HG2	2.10	0.52
1:C:23:GLN:NE2	4:C:703:HOH:O	2.42	0.52
1:A:208:GLU:HG2	1:A:225:ARG:HG3	1.91	0.51
1:A:104:ILE:O	1:A:108:MET:HG3	2.11	0.51
1:D:193:MET:HE1	1:D:473:LEU:CA	2.40	0.51
1:B:23:GLN:NE2	4:B:707:HOH:O	2.44	0.51
1:A:283:THR:HG23	3:A:602:NDP:H41N	1.93	0.51
1:B:517:ARG:CG	4:B:816:HOH:O	2.59	0.51
1:A:86:MET:HA	1:A:86:MET:HE2	1.93	0.50
1:B:113:THR:CG2	1:B:167:LEU:HD11	2.41	0.50
1:B:329:LYS:HD2	1:B:489:LEU:HD21	1.92	0.50
1:D:398:GLU:HG3	1:D:433:ILE:HG12	1.93	0.50
1:D:338:ILE:HG22	1:D:366:HIS:HE1	1.75	0.50
1:B:439:ILE:HG22	1:B:509:LEU:HD11	1.92	0.50
1:D:158:ILE:HG12	1:D:199:LEU:HB3	1.93	0.49
1:D:375:GLU:HG3	1:D:400:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ASP:HB3	1:C:407:PHE:CE2	2.48	0.49
1:C:17:ARG:HH21	1:C:19:ARG:HB3	1.77	0.49
1:C:360:GLU:C	1:C:362:GLU:H	2.19	0.49
1:C:403:ASP:HB3	1:C:407:PHE:HE2	1.78	0.49
1:D:442:SER:O	1:D:461:GLN:HA	2.13	0.48
1:A:61:GLN:HG3	1:A:559:TYR:CE2	2.47	0.48
1:C:450:THR:HG22	1:C:456:THR:HG23	1.94	0.48
1:B:118:LEU:HA	1:B:121:GLN:HE21	1.77	0.48
1:A:136:THR:HG21	1:B:56:PRO:HB3	1.95	0.48
1:A:391:ALA:HA	1:A:417:SER:HB3	1.96	0.48
1:A:451:LEU:HD11	1:A:457:LEU:HD11	1.95	0.48
1:B:61:GLN:HG3	1:B:559:TYR:CE2	2.48	0.48
1:A:19:ARG:O	1:A:19:ARG:HG3	2.14	0.48
1:B:19:ARG:NH1	1:B:196:GLN:NE2	2.61	0.48
1:A:217:LEU:HD21	1:B:66:LEU:HD23	1.96	0.47
1:B:42:LEU:CD2	1:C:574:GLN:HE21	2.27	0.47
1:C:380:GLU:HG3	1:C:381:ILE:HG13	1.97	0.47
1:D:512:PRO:HG2	1:D:515:THR:HG23	1.97	0.47
1:A:49:ASN:HB3	1:D:22:HIS:CE1	2.49	0.47
1:B:167:LEU:HB3	1:B:168:GLY:H	1.58	0.47
1:C:283:THR:HG23	3:C:602:NDP:H41N	1.96	0.47
1:D:498:GLN:HB2	1:D:511:PRO:HG3	1.97	0.47
1:A:136:THR:HB	1:A:221:LEU:HD11	1.97	0.47
1:A:30:ARG:HB3	1:B:30:ARG:HB3	1.97	0.46
1:A:165:ARG:NH2	3:A:602:NDP:O1A	2.48	0.46
1:B:351:VAL:HG21	1:B:370:GLU:HG2	1.96	0.46
1:D:122:GLN:O	1:D:126:VAL:HG22	2.15	0.46
1:C:253:GLN:HG3	1:C:276:PHE:CZ	2.50	0.46
1:C:498:GLN:HB2	1:C:511:PRO:HG3	1.98	0.46
1:D:187:TYR:HE2	1:D:472:ALA:CB	2.27	0.46
1:A:66:LEU:HD23	1:B:217:LEU:HD21	1.98	0.46
1:D:23:GLN:NE2	4:D:707:HOH:O	2.48	0.46
1:D:189:ALA:O	1:D:517:ARG:HD2	2.16	0.46
1:A:579:LYS:HA	1:A:579:LYS:HE3	1.98	0.46
1:C:19:ARG:O	1:C:562:ILE:HA	2.16	0.45
1:C:129:LYS:HA	1:C:130:PRO:HD2	1.67	0.45
1:C:397:SER:H	1:C:400:ILE:HG13	1.81	0.45
1:D:468:PHE:N	1:D:469:PRO:CD	2.79	0.45
1:A:236:ASP:O	1:A:240:GLU:HG3	2.17	0.45
1:B:128:ARG:HD3	4:B:763:HOH:O	2.16	0.45
1:B:120:CYS:O	1:B:175:ASN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.98	0.45
1:B:450:THR:HB	1:B:456:THR:OG1	2.16	0.45
1:A:346:SER:OG	3:A:602:NDP:O2X	2.35	0.45
1:C:432:LYS:HA	1:C:432:LYS:HE3	1.98	0.45
1:B:240:GLU:O	1:B:244:SER:HB3	2.17	0.45
1:C:67:ARG:HB2	1:D:217:LEU:HD22	1.99	0.45
1:D:295:LEU:HD11	1:D:302:LEU:HD13	1.98	0.45
1:A:313:GLY:HA3	3:A:602:NDP:O5B	2.17	0.45
1:C:400:ILE:H	1:C:400:ILE:HG12	1.64	0.44
1:C:417:SER:HA	3:C:602:NDP:H1D	1.99	0.44
1:D:62:GLU:HG3	1:D:98:ARG:NH2	2.32	0.44
1:D:328:GLU:HA	1:D:332:LEU:O	2.17	0.44
1:B:60:SER:HB3	1:C:578:THR:HG22	1.99	0.44
1:A:481:ARG:HG2	1:A:481:ARG:HH11	1.82	0.44
1:C:465:SER:O	1:C:516:ILE:HD11	2.17	0.44
1:A:481:ARG:HG2	1:A:481:ARG:NH1	2.32	0.44
1:D:351:VAL:O	1:D:354:ARG:HB2	2.18	0.44
1:B:456:THR:HG22	1:B:458:TYR:CE1	2.52	0.44
1:C:31:ASN:OD1	1:C:31:ASN:C	2.61	0.44
1:D:86:MET:HE3	1:D:111:VAL:HG12	2.00	0.44
1:A:466:TYR:HA	1:A:516:ILE:HD11	2.00	0.43
1:B:367:GLU:O	1:B:368:HIS:HB2	2.17	0.43
1:A:471:VAL:O	1:A:475:VAL:HG23	2.18	0.43
1:B:416:LEU:O	3:B:602:NDP:H2N	2.19	0.43
1:A:44:GLU:HA	1:A:563:LEU:HD21	1.99	0.43
1:C:358:THR:OG1	1:C:361:LYS:HG3	2.18	0.43
1:A:574:GLN:HE21	1:D:42:LEU:CD2	2.30	0.43
1:A:91:ARG:HG3	1:B:129:LYS:HD3	2.00	0.43
1:B:310:GLN:HE21	1:B:310:GLN:HA	1.83	0.43
1:D:325:MET:SD	1:D:485:ASP:HB3	2.58	0.43
1:D:177:MET:O	1:D:180:PRO:HD2	2.18	0.43
1:C:19:ARG:HG3	1:C:562:ILE:HG22	2.00	0.43
1:C:540:TYR:HA	1:C:541:PRO:C	2.44	0.43
1:C:450:THR:HA	1:C:455:GLN:O	2.18	0.43
1:C:310:GLN:NE2	4:C:702:HOH:O	2.26	0.43
1:C:416:LEU:O	3:C:602:NDP:H2N	2.19	0.43
1:C:310:GLN:HA	1:C:310:GLN:HE21	1.84	0.42
1:A:108:MET:HE2	1:A:108:MET:HB3	1.87	0.42
1:D:320:ALA:O	1:D:324:VAL:HG23	2.19	0.42
1:C:354:ARG:HG2	1:C:355:ALA:N	2.34	0.42
1:D:525:GLU:OE2	1:D:547:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:O	1:B:175:ASN:HB2	2.19	0.42
1:C:120:CYS:O	1:C:175:ASN:HB3	2.20	0.42
1:C:397:SER:O	1:C:398:GLU:C	2.62	0.42
1:D:325:MET:HE2	1:D:325:MET:HB3	1.83	0.42
1:A:82:TYR:O	1:A:86:MET:HG2	2.20	0.42
1:C:578:THR:OG1	1:C:579:LYS:N	2.50	0.42
1:A:47:GLN:HG2	1:A:563:LEU:HD22	2.02	0.42
1:A:375:GLU:HA	1:A:400:ILE:HD13	1.97	0.42
1:B:358:THR:O	1:B:362:GLU:HG2	2.20	0.42
1:C:312:ALA:HA	1:C:316:ALA:HB3	2.02	0.42
1:C:354:ARG:O	1:C:357:LEU:HB2	2.19	0.42
1:A:396:PHE:CG	1:A:424:GLU:HB3	2.54	0.42
1:A:463:ASN:OD1	1:A:465:SER:HB2	2.20	0.41
1:B:104:ILE:HG13	1:B:108:MET:HG3	2.01	0.41
1:C:42:LEU:O	1:C:46:GLN:HG3	2.20	0.41
1:A:56:PRO:HB3	1:B:136:THR:HG21	2.03	0.41
1:A:531:ALA:HA	1:A:536:THR:OG1	2.20	0.41
1:A:36:LYS:O	1:A:37:ASP:HB2	2.21	0.41
1:B:563:LEU:HD23	1:B:563:LEU:HA	1.84	0.41
1:C:354:ARG:HG2	1:C:355:ALA:H	1.85	0.41
1:D:303:SER:O	1:D:340:LYS:NZ	2.53	0.41
1:A:426:SER:HA	1:A:446:PHE:CZ	2.55	0.41
1:B:575:LYS:HG2	1:B:576:ILE:N	2.35	0.41
1:D:245:LYS:HE3	4:D:718:HOH:O	2.19	0.41
1:D:386:LEU:HG	1:D:396:PHE:CZ	2.56	0.41
1:B:139:ASP:O	1:B:140:ARG:C	2.64	0.41
1:A:503:HIS:O	1:A:506:GLU:HB2	2.20	0.41
1:C:167:LEU:HB3	1:C:168:GLY:H	1.61	0.41
1:C:360:GLU:C	1:C:362:GLU:N	2.78	0.41
1:A:309:PHE:HB2	1:A:343:LEU:HD23	2.03	0.41
1:B:177:MET:HE2	1:B:202:ILE:HG22	2.02	0.40
1:C:325:MET:HE1	1:C:486:ASN:ND2	2.35	0.40
1:C:359:GLN:O	1:C:362:GLU:HB2	2.21	0.40
1:C:410:ARG:HA	1:C:437:ARG:O	2.21	0.40
1:A:350:ILE:HD13	1:A:361:LYS:HB3	2.03	0.40
1:C:465:SER:HA	1:C:468:PHE:CE2	2.55	0.40
1:A:109:PRO:HA	1:A:113:THR:O	2.21	0.40
1:C:108:MET:N	1:C:109:PRO:CD	2.85	0.40
1:A:19:ARG:CZ	1:A:196:GLN:HE22	2.34	0.40
1:A:325:MET:HE3	1:A:325:MET:HB3	1.71	0.40
1:B:378:VAL:HG21	1:B:400:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:HB	1:C:221:LEU:HD11	2.02	0.40
1:D:155:ILE:HB	1:D:246:TYR:CD1	2.56	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%)	542 (96%)	20 (4%)	0	100	100
1	B	562/572 (98%)	547 (97%)	13 (2%)	2 (0%)	30	23
1	C	562/572 (98%)	529 (94%)	30 (5%)	3 (0%)	24	17
1	D	562/572 (98%)	546 (97%)	16 (3%)	0	100	100
All	All	2248/2288 (98%)	2164 (96%)	79 (4%)	5 (0%)	43	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	C	353	GLY
1	C	398	GLU
1	C	332	LEU
1	B	356	SER

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%)	456 (94%)	27 (6%)	19	12
1	B	483/490 (99%)	453 (94%)	30 (6%)	16	9
1	C	483/490 (99%)	451 (93%)	32 (7%)	15	8
1	D	483/490 (99%)	455 (94%)	28 (6%)	18	11
All	All	1932/1960 (99%)	1815 (94%)	117 (6%)	17	9

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	74	HIS
1	A	93	GLU
1	A	100	LEU
1	A	122	GLN
1	A	129	LYS
1	A	167	LEU
1	A	186	LEU
1	A	211	GLU
1	A	242	VAL
1	A	259	ASN
1	A	310	GLN
1	A	325	MET
1	A	352	LYS
1	A	409	GLU
1	A	420	THR
1	A	429	GLN
1	A	455	GLN
1	A	461	GLN
1	A	480	LEU
1	A	497	GLN
1	A	502	LYS
1	A	535	LYS
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	93	GLU
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	122	GLN
1	B	129	LYS
1	B	147	LEU
1	B	167	LEU
1	B	186	LEU
1	B	196	GLN
1	B	210	GLU
1	B	230	GLU
1	B	242	VAL
1	B	253	GLN
1	B	272	GLN
1	B	301	LYS
1	B	307	ILE
1	B	310	GLN
1	B	334	LYS
1	B	335	GLU
1	B	351	VAL
1	B	356	SER
1	B	372	LYS
1	B	409	GLU
1	B	450	THR
1	B	533	GLN
1	B	535	LYS
1	B	561	GLN
1	B	571	GLU
1	B	579	LYS
1	C	73	GLU
1	C	100	LEU
1	C	128	ARG
1	C	147	LEU
1	C	167	LEU
1	C	186	LEU
1	C	210	GLU
1	C	242	VAL
1	C	253	GLN
1	C	259	ASN
1	C	260	VAL
1	C	307	ILE
1	C	310	GLN
1	C	325	MET
1	C	339	LYS
1	C	340	LYS

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Mol	Chain	Res	Type
1	C	346	SER
1	C	351	VAL
1	C	352	LYS
1	C	356	SER
1	C	357	LEU
1	C	400	ILE
1	C	420	THR
1	C	432	LYS
1	C	437	ARG
1	C	450	THR
1	C	451	LEU
1	C	486	ASN
1	C	516	ILE
1	C	533	GLN
1	C	544	GLN
1	C	579	LYS
1	D	18	ARG
1	D	19	ARG
1	D	47	GLN
1	D	73	GLU
1	D	74	HIS
1	D	93	GLU
1	D	100	LEU
1	D	122	GLN
1	D	129	LYS
1	D	136	THR
1	D	147	LEU
1	D	167	LEU
1	D	193	MET
1	D	211	GLU
1	D	230	GLU
1	D	242	VAL
1	D	251	LEU
1	D	310	GLN
1	D	352	LYS
1	D	360	GLU
1	D	369	GLU
1	D	420	THR
1	D	433	ILE
1	D	461	GLN
1	D	481	ARG
1	D	517	ARG

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Mol	Chain	Res	Type
1	D	547	GLU
1	D	578	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	49	ASN
1	A	76	ASN
1	A	121	GLN
1	A	196	GLN
1	A	249	ASN
1	A	310	GLN
1	A	455	GLN
1	A	574	GLN
1	B	23	GLN
1	B	35	ASN
1	B	49	ASN
1	B	76	ASN
1	B	121	GLN
1	B	148	ASN
1	B	196	GLN
1	B	249	ASN
1	B	310	GLN
1	B	399	GLN
1	B	574	GLN
1	C	22	HIS
1	C	23	GLN
1	C	49	ASN
1	C	89	GLN
1	C	121	GLN
1	C	196	GLN
1	C	249	ASN
1	C	310	GLN
1	C	366	HIS
1	C	368	HIS
1	C	373	ASN
1	C	455	GLN
1	C	486	ASN
1	C	497	GLN
1	C	533	GLN
1	C	544	GLN

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Mol	Chain	Res	Type
1	C	561	GLN
1	C	574	GLN
1	D	20	HIS
1	D	22	HIS
1	D	23	GLN
1	D	47	GLN
1	D	74	HIS
1	D	122	GLN
1	D	148	ASN
1	D	249	ASN
1	D	310	GLN
1	D	321	HIS
1	D	498	GLN
1	D	514	ASN
1	D	561	GLN
1	D	574	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	D	602	-	51,52,52	1.39	5 (9%)	71,80,80	1.40	10 (14%)
3	NDP	C	602	-	51,52,52	1.47	5 (9%)	71,80,80	1.59	17 (23%)
3	NDP	B	602	-	51,52,52	1.51	6 (11%)	71,80,80	1.47	10 (14%)
3	NDP	A	602	-	51,52,52	1.47	5 (9%)	71,80,80	1.44	10 (14%)

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	602	-	-	3/34/77/77	0/5/5/5
3	NDP	C	602	-	-	5/34/77/77	0/5/5/5
3	NDP	B	602	-	-	5/34/77/77	0/5/5/5
3	NDP	A	602	-	-	3/34/77/77	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NDP	C4N-C3N	-6.40	1.37	1.50
3	D	602	NDP	C4N-C3N	-6.11	1.38	1.50
3	C	602	NDP	C4N-C3N	-5.96	1.38	1.50
3	B	602	NDP	C4N-C3N	-5.29	1.40	1.50
3	C	602	NDP	PA-O3	4.89	1.64	1.59
3	B	602	NDP	PA-O3	4.65	1.64	1.59
3	B	602	NDP	C4N-C5N	-4.03	1.38	1.49
3	D	602	NDP	PA-O3	3.92	1.63	1.59
3	A	602	NDP	C4N-C5N	-3.91	1.38	1.49
3	D	602	NDP	C4N-C5N	-3.71	1.39	1.49
3	C	602	NDP	C4N-C5N	-3.67	1.39	1.49
3	A	602	NDP	P2B-O2B	3.62	1.65	1.59
3	B	602	NDP	PN-O3	3.31	1.63	1.59
3	A	602	NDP	PA-O3	3.00	1.62	1.59
3	C	602	NDP	P2B-O2B	2.77	1.64	1.59
3	B	602	NDP	P2B-O2B	2.54	1.64	1.59
3	B	602	NDP	C6A-N6A	2.18	1.39	1.34
3	D	602	NDP	PN-O3	2.12	1.61	1.59
3	D	602	NDP	C6N-C5N	2.05	1.39	1.33
3	A	602	NDP	C7N-N7N	2.04	1.39	1.33
3	C	602	NDP	C6A-N6A	2.02	1.39	1.34

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NDP	O4D-C1D-N1N	4.10	115.90	108.08
3	D	602	NDP	O3X-P2B-O2X	4.06	123.01	107.80
3	C	602	NDP	C6N-N1N-C2N	3.90	123.49	119.32
3	A	602	NDP	O4D-C1D-N1N	3.71	115.17	108.08
3	D	602	NDP	O4B-C1B-N9A	3.68	115.16	108.09
3	A	602	NDP	O4B-C1B-N9A	3.66	115.12	108.09
3	B	602	NDP	O4B-C1B-N9A	3.55	114.90	108.09
3	D	602	NDP	O4B-C1B-C2B	-3.53	100.52	106.59
3	B	602	NDP	C3N-C2N-N1N	-3.50	118.07	123.20
3	A	602	NDP	C1D-N1N-C2N	-3.41	115.52	121.14
3	B	602	NDP	C6N-N1N-C2N	3.37	122.93	119.32
3	C	602	NDP	C1D-N1N-C2N	-3.21	115.85	121.14
3	A	602	NDP	O3-PA-O1A	-3.07	101.46	110.70
3	A	602	NDP	O3D-C3D-C4D	-3.07	102.26	111.08
3	C	602	NDP	O2A-PA-O1A	3.00	126.41	112.44
3	C	602	NDP	C3N-C2N-N1N	-3.00	118.81	123.20
3	A	602	NDP	C6N-N1N-C2N	2.97	122.50	119.32
3	C	602	NDP	O3-PA-O1A	-2.97	101.78	110.70
3	C	602	NDP	O3X-P2B-O2X	2.92	118.75	107.80
3	D	602	NDP	O2X-P2B-O2B	-2.87	94.68	105.85
3	A	602	NDP	C3N-C2N-N1N	-2.85	119.03	123.20
3	B	602	NDP	C3B-C2B-C1B	-2.77	97.51	102.81
3	D	602	NDP	O4D-C1D-N1N	2.72	113.27	108.08
3	C	602	NDP	C4A-N9A-C8A	2.67	108.55	105.74
3	C	602	NDP	C2D-C1D-N1N	-2.67	106.74	113.31
3	C	602	NDP	C3B-C2B-C1B	-2.67	97.70	102.81
3	B	602	NDP	C2D-C1D-N1N	-2.61	106.90	113.31
3	D	602	NDP	C1D-N1N-C2N	-2.53	116.98	121.14
3	C	602	NDP	O3B-C3B-C4B	-2.48	103.96	111.08
3	D	602	NDP	P2B-O2B-C2B	-2.42	116.96	123.43
3	C	602	NDP	O2N-PN-O1N	2.37	123.49	112.44
3	C	602	NDP	O4B-C1B-C2B	-2.37	102.50	106.59
3	C	602	NDP	C5A-C4A-N9A	-2.36	103.24	105.81
3	D	602	NDP	O3D-C3D-C4D	-2.35	104.32	111.08
3	C	602	NDP	C4B-O4B-C1B	-2.35	104.27	109.47
3	C	602	NDP	C2B-C1B-N9A	2.30	117.54	113.75
3	B	602	NDP	O3B-C3B-C4B	-2.27	104.56	111.08
3	D	602	NDP	O2A-PA-O1A	2.27	122.99	112.44
3	A	602	NDP	O3B-C3B-C4B	-2.26	104.59	111.08
3	C	602	NDP	O2X-P2B-O2B	-2.24	97.12	105.85
3	A	602	NDP	O2A-PA-O1A	2.23	122.82	112.44
3	B	602	NDP	O2A-PA-O1A	2.21	122.70	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	NDP	C5B-C4B-C3B	-2.13	107.53	115.21
3	B	602	NDP	O3X-P2B-O2X	2.10	115.68	107.80
3	D	602	NDP	C3B-C2B-C1B	-2.07	98.83	102.81
3	A	602	NDP	O7N-C7N-C3N	-2.02	117.09	120.90
3	B	602	NDP	C5A-C6A-N6A	-2.01	118.30	123.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C3B-C2B-O2B-P2B
3	C	602	NDP	C5B-O5B-PA-O1A
3	B	602	NDP	C3B-C2B-O2B-P2B
3	D	602	NDP	C3B-C2B-O2B-P2B
3	B	602	NDP	C3B-C4B-C5B-O5B
3	B	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C1B-C2B-O2B-P2B
3	D	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	O4D-C1D-N1N-C2N
3	B	602	NDP	O4D-C1D-N1N-C2N
3	D	602	NDP	O4D-C1D-N1N-C2N
3	B	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	C1B-C2B-O2B-P2B
3	C	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C3B-C4B-C5B-O5B

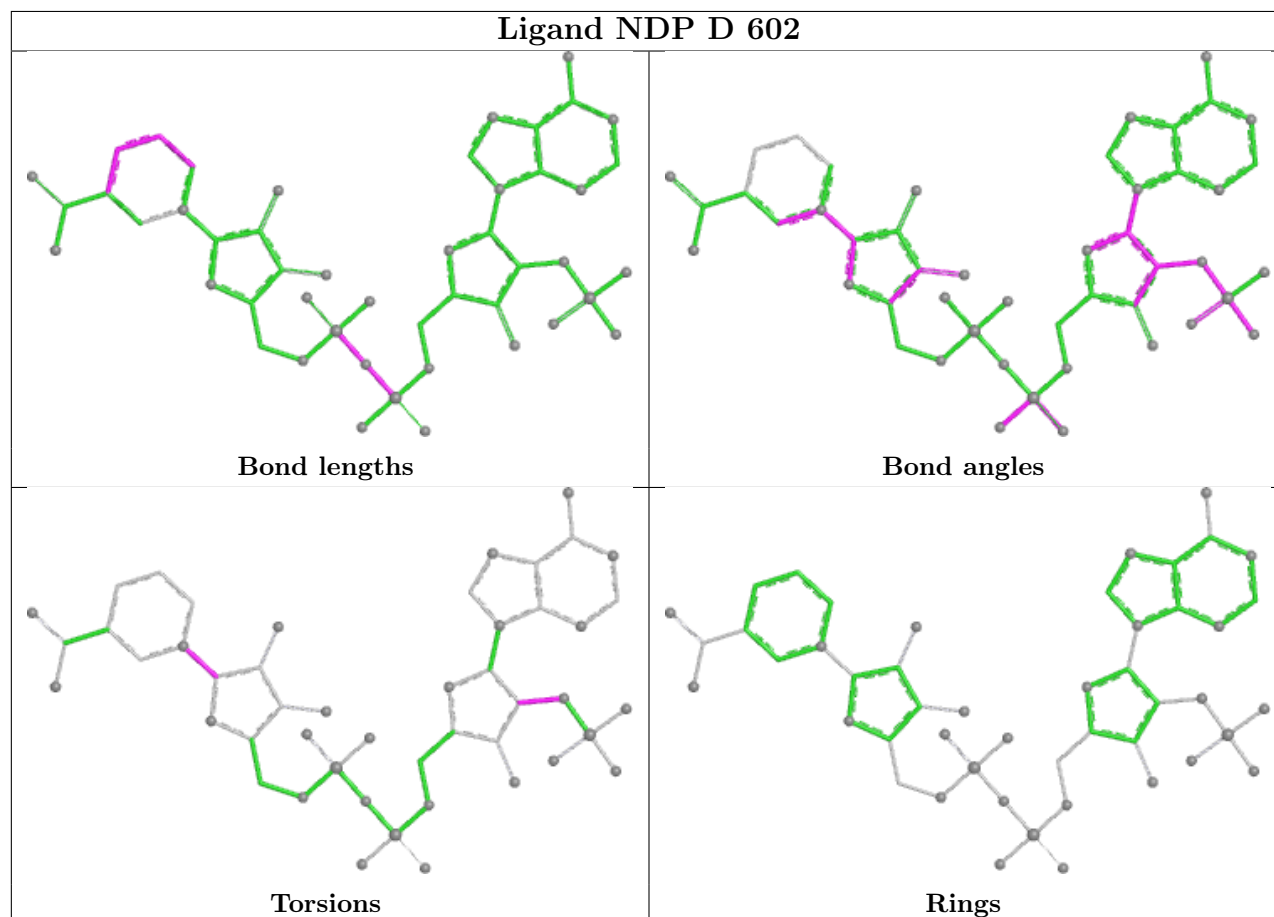
There are no ring outliers.

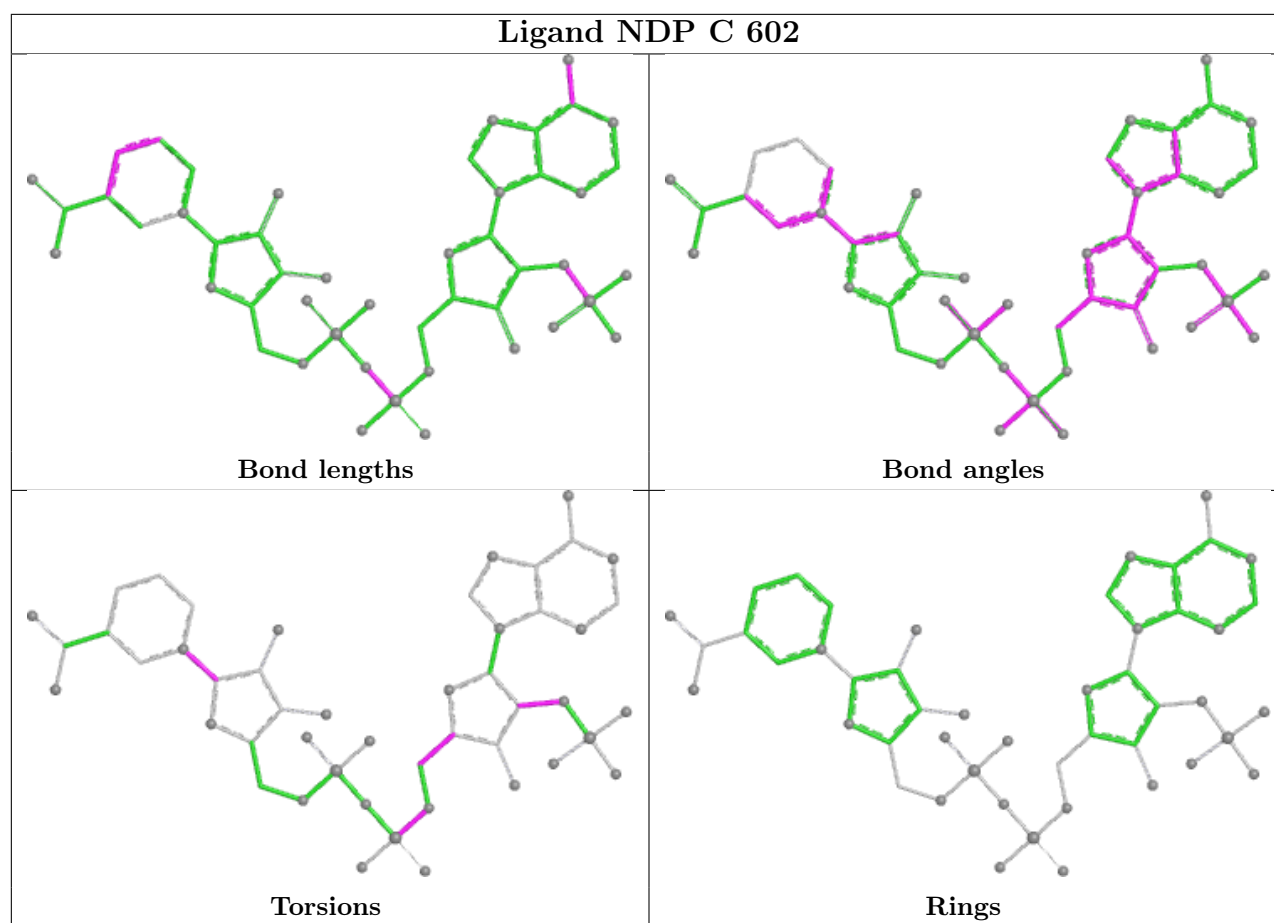
3 monomers are involved in 11 short contacts:

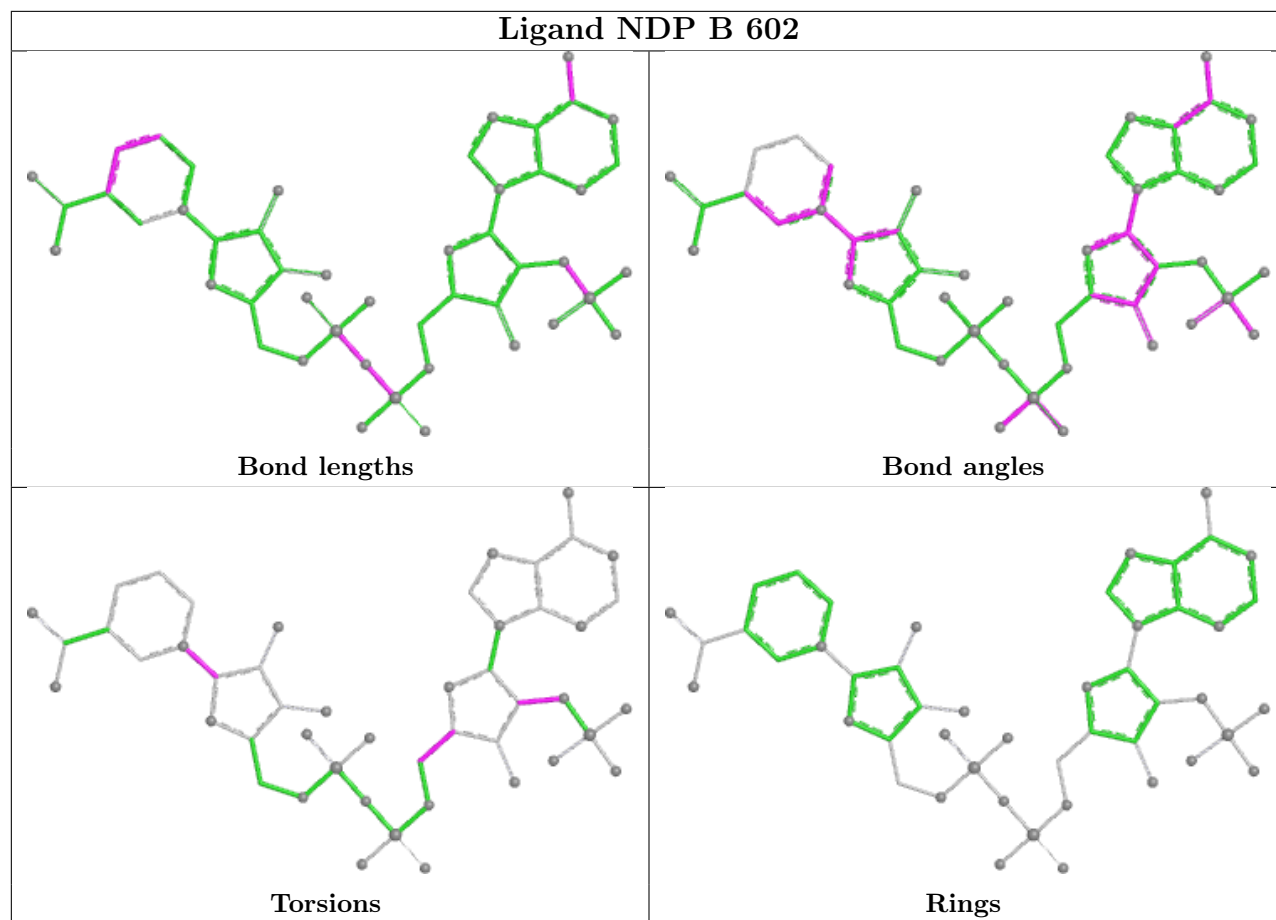
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	NDP	6	0
3	B	602	NDP	1	0
3	A	602	NDP	4	0

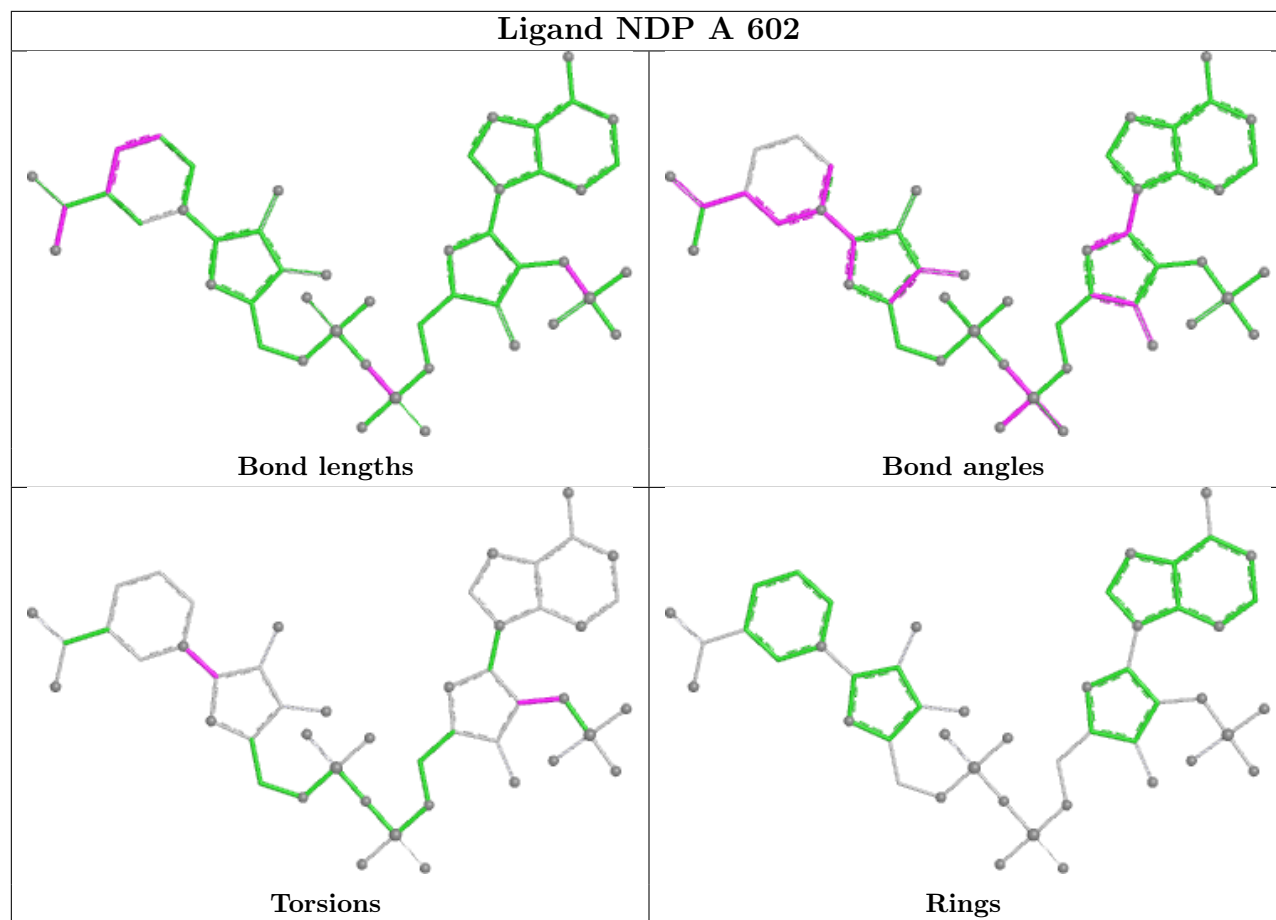
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	564/572 (98%)	0.03	4 (0%) 84 86	23, 36, 58, 74	0
1	B	564/572 (98%)	0.01	6 (1%) 78 80	22, 34, 56, 79	0
1	C	564/572 (98%)	0.47	56 (9%) 13 13	22, 38, 84, 118	0
1	D	564/572 (98%)	0.08	8 (1%) 73 75	22, 35, 61, 99	0
All	All	2256/2288 (98%)	0.15	74 (3%) 49 49	22, 35, 65, 118	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	VAL	5.6
1	C	342	TRP	5.1
1	C	454	GLY	4.9
1	C	350	ILE	4.9
1	C	451	LEU	4.8
1	B	16	PRO	4.5
1	C	355	ALA	4.3
1	C	332	LEU	4.0
1	C	371	MET	4.0
1	C	453	ASN	3.9
1	C	16	PRO	3.9
1	C	260	VAL	3.7
1	C	364	PHE	3.6
1	C	378	VAL	3.5
1	C	579	LYS	3.5
1	C	374	LEU	3.5
1	C	345	ASP	3.5
1	C	452	PRO	3.4
1	C	377	ILE	3.3
1	C	407	PHE	3.3
1	C	393	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	368	HIS	3.2
1	C	390	ALA	3.2
1	C	343	LEU	3.2
1	C	366	HIS	3.2
1	C	344	VAL	3.1
1	B	74	HIS	3.1
1	A	579	LYS	3.1
1	C	263	PHE	3.0
1	C	333	PRO	3.0
1	C	380	GLU	3.0
1	C	455	GLN	3.0
1	D	579	LYS	3.0
1	C	19	ARG	3.0
1	A	540	TYR	3.0
1	C	358	THR	2.9
1	C	354	ARG	2.8
1	C	17	ARG	2.8
1	D	74	HIS	2.8
1	B	20	HIS	2.7
1	C	540	TYR	2.7
1	D	16	PRO	2.7
1	C	381	ILE	2.7
1	C	375	GLU	2.7
1	C	325	MET	2.6
1	A	353	GLY	2.6
1	B	19	ARG	2.6
1	D	453	ASN	2.5
1	C	340	LYS	2.5
1	C	397	SER	2.4
1	C	376	ALA	2.4
1	C	379	GLN	2.4
1	C	405	ALA	2.3
1	C	308	LEU	2.3
1	C	373	ASN	2.3
1	C	435	LYS	2.3
1	C	395	ALA	2.3
1	D	437	ARG	2.3
1	C	347	LYS	2.2
1	C	432	LYS	2.2
1	A	16	PRO	2.2
1	D	263	PHE	2.2
1	C	365	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	19	ARG	2.2
1	B	331	GLY	2.1
1	C	312	ALA	2.1
1	C	400	ILE	2.1
1	C	211	GLU	2.1
1	C	394	GLY	2.1
1	C	129	LYS	2.1
1	C	349	LEU	2.1
1	B	561	GLN	2.1
1	D	369	GLU	2.0
1	C	327	LEU	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](#)

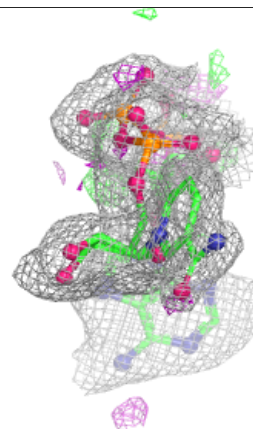
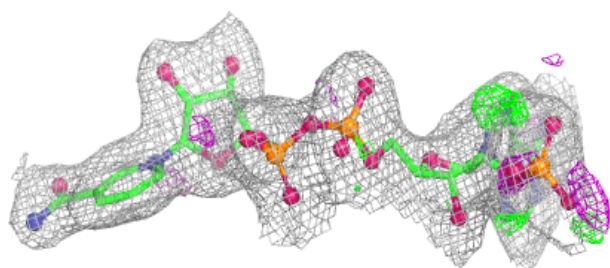
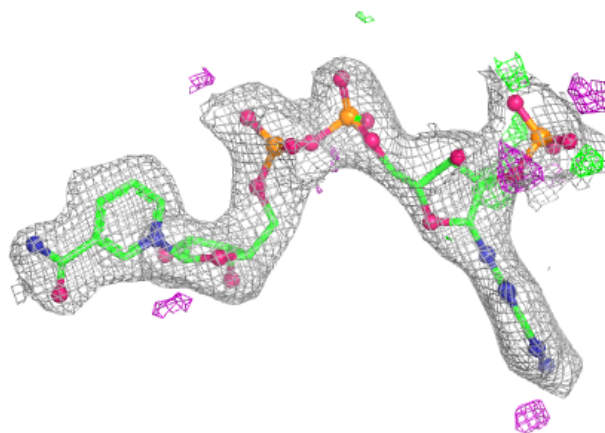
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	C	602	48/48	0.91	0.10	37,51,66,77	0
3	NDP	D	602	48/48	0.96	0.07	32,39,45,47	0
3	NDP	A	602	48/48	0.97	0.07	33,38,42,43	0
3	NDP	B	602	48/48	0.97	0.05	26,31,37,39	0
2	MN	C	601	1/1	0.99	0.02	34,34,34,34	0
2	MN	D	601	1/1	0.99	0.01	34,34,34,34	0
2	MN	A	601	1/1	1.00	0.01	36,36,36,36	0
2	MN	B	601	1/1	1.00	0.01	30,30,30,30	0

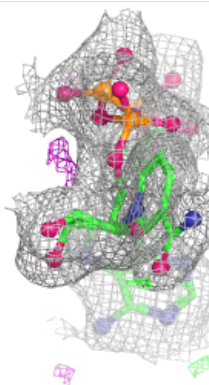
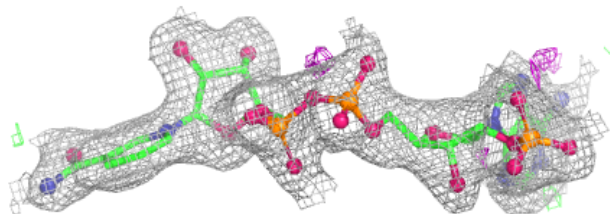
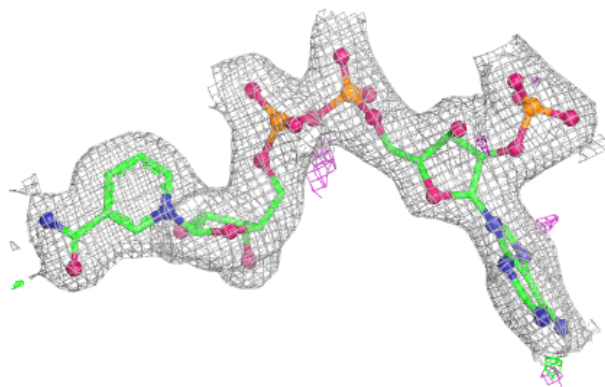
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP 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)

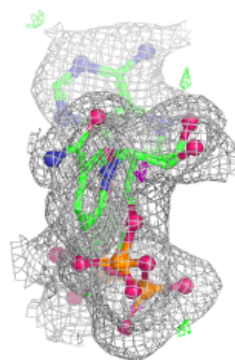
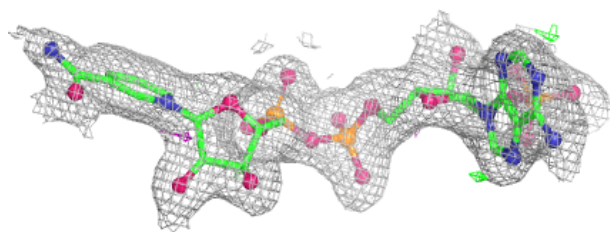
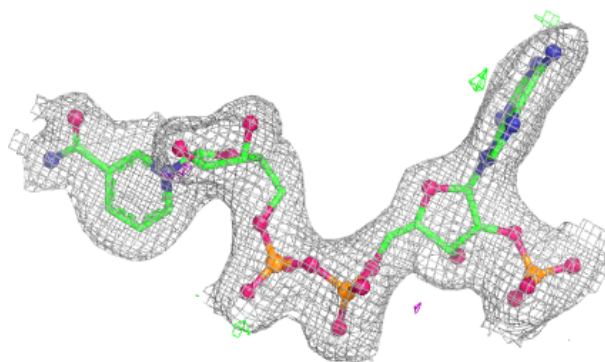
**Electron density around NDP D 602:**

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

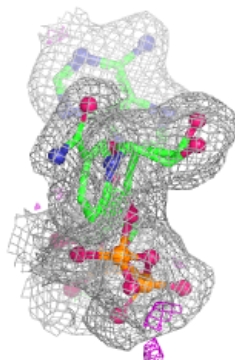
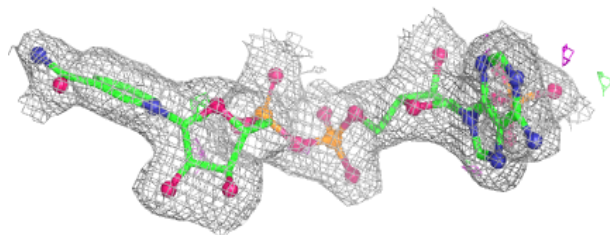
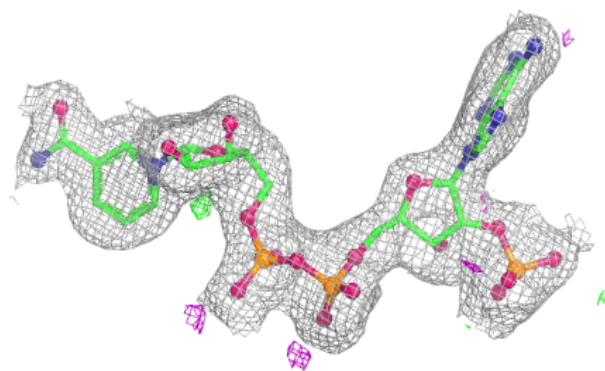


Electron density around NDP A 602:

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

**Electron density around NDP B 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.