



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:28 AM UTC

PDB ID : 2RBE / pdb_00002rbe
Title : The discovery of 2-anilinothiazolones as 11beta-HSD1 inhibitors
Authors : Zhang, J.; Jordan, S.R.; Li, V.
Deposited on : 2007-09-18
Resolution : 1.90 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

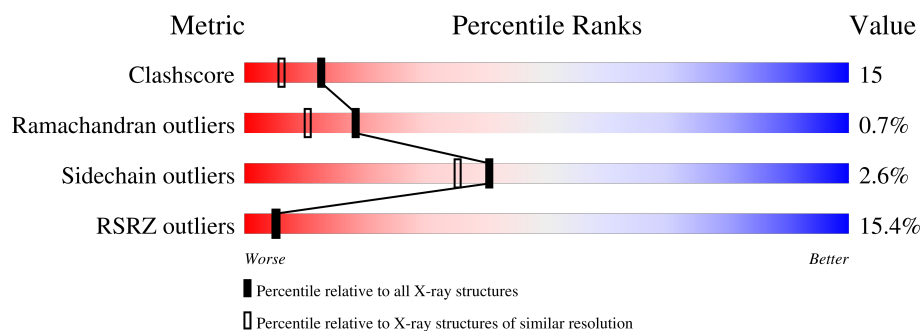
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	275	32% 62% 31% 6%
1	B	275	12% 62% 27% 7%
1	C	275	4% 67% 24% 7%
1	D	275	10% 73% 18% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8618 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1988	1270	335	368	15			
1	B	255	Total	C	N	O	S	0	0	0
			1951	1247	331	358	15			
1	C	255	Total	C	N	O	S	0	0	0
			1954	1249	331	359	15			
1	D	261	Total	C	N	O	S	0	0	0
			2002	1277	338	372	15			

There are 32 discrepancies between the modelled and reference sequences:

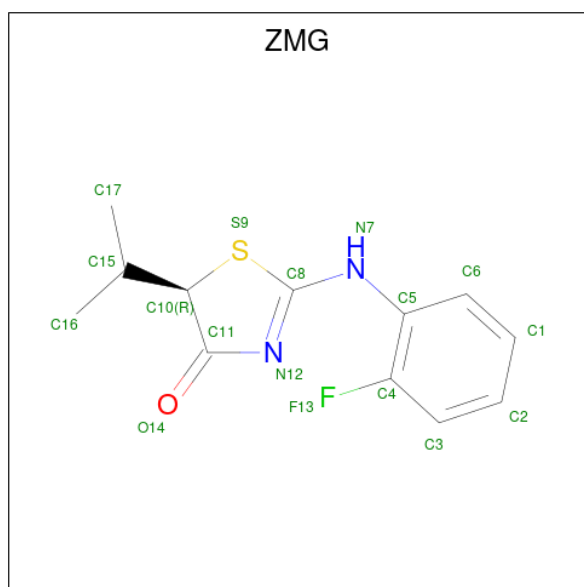
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	HIS	-	expression tag	UNP P28845
A	21	HIS	-	expression tag	UNP P28845
A	22	HIS	-	expression tag	UNP P28845
A	23	HIS	-	expression tag	UNP P28845
A	24	HIS	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	18	MET	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	HIS	-	expression tag	UNP P28845
B	21	HIS	-	expression tag	UNP P28845
B	22	HIS	-	expression tag	UNP P28845
B	23	HIS	-	expression tag	UNP P28845
B	24	HIS	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	18	MET	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	HIS	-	expression tag	UNP P28845
C	21	HIS	-	expression tag	UNP P28845
C	22	HIS	-	expression tag	UNP P28845

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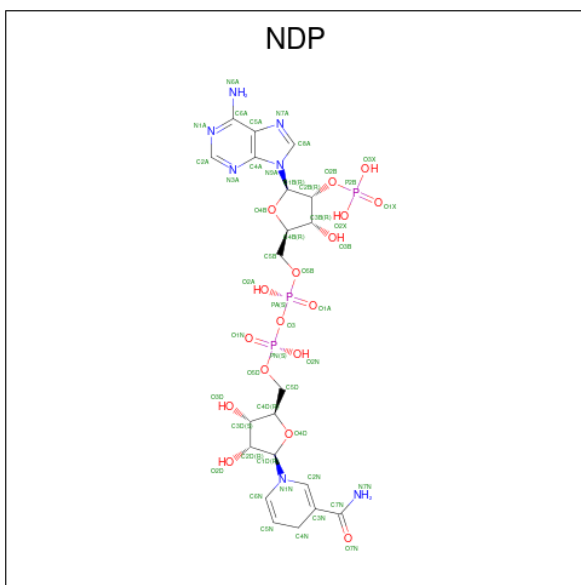
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP P28845
C	24	HIS	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	18	MET	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	HIS	-	expression tag	UNP P28845
D	21	HIS	-	expression tag	UNP P28845
D	22	HIS	-	expression tag	UNP P28845
D	23	HIS	-	expression tag	UNP P28845
D	24	HIS	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is (5R)-2-[(2-fluorophenyl)amino]-5-(1-methylethyl)-1,3-thiazol-4(5H)-one (CCD ID: ZMG) (formula: C₁₂H₁₃FN₂OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	B	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	C	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	D	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0

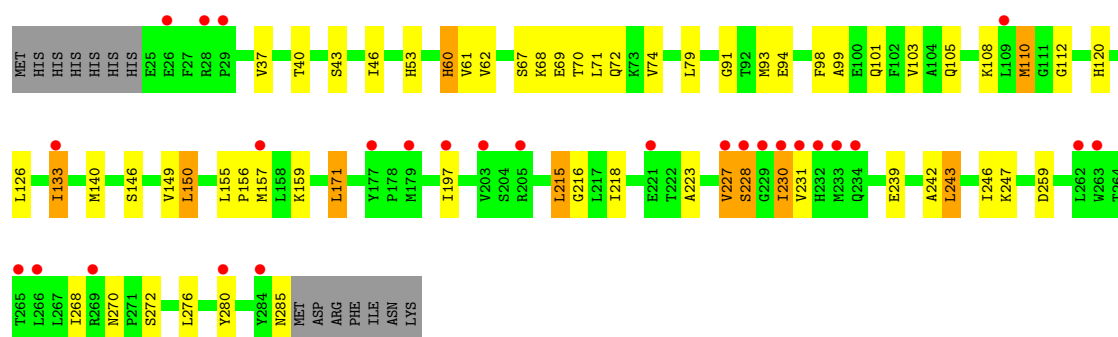
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 47	C 21	N 6	O 17	P 3	0	0
3	B	1	Total 47	C 21	N 6	O 17	P 3	0	0
3	C	1	Total 47	C 21	N 6	O 17	P 3	0	0
3	D	1	Total 47	C 21	N 6	O 17	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0
4	B	114	Total O 114 114	0	0
4	C	143	Total O 143 143	0	0
4	D	128	Total O 128 128	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.91Å 138.66Å 155.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (50.00-1.90) 91.4 (50.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.264 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8618	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: ZMG, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2021	0.79	1/2727 (0.0%)
1	B	0.38	1/1984 (0.1%)	0.85	5/2678 (0.2%)
1	C	0.38	0/1987	0.85	3/2682 (0.1%)
1	D	0.38	1/2036 (0.0%)	0.85	5/2749 (0.2%)
All	All	0.37	2/8028 (0.0%)	0.84	14/10836 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	MET	SD-CE	-5.49	1.65	1.79
1	B	110	MET	SD-CE	-5.08	1.66	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	GLU	N-CA-C	-7.17	104.33	113.23
1	C	94	GLU	N-CA-C	-7.17	104.00	112.89
1	D	37	VAL	N-CA-C	6.53	117.89	108.48
1	B	94	GLU	N-CA-C	-6.29	105.09	112.89
1	B	37	VAL	N-CA-C	6.07	117.50	108.46
1	D	171	LEU	N-CA-C	-5.91	104.84	111.28
1	C	162	ASN	N-CA-C	-5.83	103.35	111.52
1	B	171	LEU	N-CA-C	-5.78	105.07	111.71
1	D	67	SER	N-CA-C	5.49	117.17	108.67
1	C	37	VAL	N-CA-C	5.44	116.57	108.46
1	A	94	GLU	N-CA-C	-5.37	106.23	112.89
1	B	216	GLY	N-CA-C	-5.27	104.51	112.41
1	B	61	VAL	N-CA-C	5.14	116.05	108.45
1	D	60	HIS	N-CA-C	-5.02	101.06	109.24

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	1988	0	2034	79	0
1	B	1951	0	2007	73	0
1	C	1954	0	2008	58	0
1	D	2002	0	2046	54	0
2	A	17	0	13	0	0
2	B	17	0	13	0	0
2	C	17	0	13	0	0
2	D	17	0	13	0	0
3	A	47	0	25	2	0
3	B	47	0	25	2	0
3	C	47	0	25	2	0
3	D	47	0	25	2	0
4	A	82	0	0	1	0
4	B	114	0	0	4	0
4	C	143	0	0	0	0
4	D	128	0	0	0	0
All	All	8618	0	8247	249	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 15.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HE2	1:D:140:MET:HE2	1.39	1.04
1:B:46:ILE:HD11	1:B:218:ILE:HG21	1.39	1.02
1:A:140:MET:HE2	1:B:140:MET:HE2	1.41	1.01
3:D:504:NDP:C2A	3:D:504:NDP:C6A	2.37	1.01
3:C:503:NDP:C6A	3:C:503:NDP:C2A	2.37	1.00
3:A:501:NDP:C6A	3:A:501:NDP:C2A	2.37	1.00
3:B:502:NDP:C6A	3:B:502:NDP:C2A	2.38	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ILE:HD11	1:D:218:ILE:HG21	1.50	0.93
1:B:62:VAL:HG23	1:B:110:MET:HE3	1.50	0.93
1:C:227:VAL:HG13	1:C:231:VAL:HB	1.46	0.93
1:D:112:GLY:HA2	1:D:157:MET:HE2	1.52	0.92
1:A:62:VAL:HG23	1:A:110:MET:HE3	1.53	0.91
1:D:62:VAL:HG23	1:D:110:MET:HE3	1.57	0.84
1:A:46:ILE:HD11	1:A:218:ILE:HG21	1.60	0.83
1:C:67:SER:HB2	1:C:70:THR:HG22	1.61	0.82
1:B:103:VAL:HG21	1:B:153:ALA:CB	2.10	0.82
1:A:227:VAL:HG13	1:A:231:VAL:HB	1.63	0.81
1:A:54:LEU:HA	1:A:57:MET:HE3	1.64	0.80
1:A:57:MET:HE1	1:A:246:ILE:HG21	1.64	0.80
1:C:126:LEU:HB3	1:C:179:MET:HE2	1.62	0.79
1:A:128:LEU:HG	1:A:179:MET:HE1	1.66	0.78
1:B:167:VAL:HG23	1:B:212:LEU:HA	1.65	0.77
1:A:247:LYS:HD3	1:A:248:GLY:N	1.99	0.76
1:B:103:VAL:HG21	1:B:153:ALA:HB1	1.67	0.74
1:C:104:ALA:O	1:C:108:LYS:HG2	1.87	0.74
1:C:227:VAL:CG1	1:C:231:VAL:HB	2.17	0.74
1:C:99:ALA:HB1	1:C:150:LEU:HD13	1.71	0.72
1:C:67:SER:HB2	1:C:70:THR:CG2	2.21	0.69
1:A:46:ILE:HG22	1:A:50:MET:HE2	1.75	0.69
1:D:133:ILE:HD13	1:D:133:ILE:O	1.95	0.67
1:A:96:MET:SD	1:A:145:LEU:HD22	2.36	0.66
1:B:243:LEU:HD22	1:B:247:LYS:HD2	1.77	0.66
1:C:32:LEU:HD22	1:C:57:MET:SD	2.37	0.65
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.12	0.65
1:D:61:VAL:CA	1:D:110:MET:HE1	2.27	0.65
1:C:43:SER:HB2	1:C:70:THR:CG2	2.26	0.64
1:A:167:VAL:HG23	1:A:212:LEU:HD12	1.78	0.64
1:A:225:LYS:NZ	1:A:225:LYS:HB3	2.12	0.64
1:A:224:MET:HE3	1:A:224:MET:HA	1.80	0.64
1:D:60:HIS:C	1:D:110:MET:HE1	2.22	0.64
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.80	0.64
1:D:60:HIS:HB3	1:D:110:MET:HE2	1.79	0.64
1:B:46:ILE:HG22	1:B:50:MET:HE2	1.81	0.63
1:B:103:VAL:HG21	1:B:153:ALA:HB3	1.81	0.63
1:B:156:PRO:O	1:B:160:GLN:HG3	1.99	0.62
1:D:227:VAL:HG12	1:D:228:SER:N	2.14	0.62
1:A:36:LYS:HB3	1:A:110:MET:SD	2.39	0.62
1:A:118:LEU:HD22	1:A:150:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.80	0.62
1:B:30:GLU:HG3	1:B:33:GLN:NE2	2.14	0.62
1:B:171:LEU:HG	1:B:216:GLY:HA2	1.82	0.62
1:A:167:VAL:HG23	1:A:212:LEU:HA	1.82	0.62
1:B:61:VAL:CA	1:B:110:MET:HE1	2.30	0.62
1:C:133:ILE:HD13	1:D:149:VAL:HG22	1.81	0.62
1:A:155:LEU:HG	1:A:159:LYS:HE3	1.82	0.61
1:C:32:LEU:HD23	1:C:54:LEU:HD23	1.82	0.61
1:B:29:PRO:HA	1:B:57:MET:HE3	1.83	0.61
1:A:273:ARG:HG3	1:B:175:VAL:HG22	1.83	0.60
1:B:216:GLY:HA3	1:B:259:ASP:OD1	2.02	0.60
1:C:67:SER:CB	1:C:70:THR:HG22	2.31	0.59
1:B:103:VAL:CG2	1:B:153:ALA:HB1	2.33	0.59
1:C:37:VAL:HG11	1:C:54:LEU:HD13	1.84	0.58
1:A:32:LEU:HD23	1:A:35:LYS:HG3	1.86	0.58
1:B:167:VAL:CG2	1:B:212:LEU:HA	2.34	0.58
1:A:101:GLN:O	1:A:105:GLN:HG3	2.04	0.57
1:A:217:LEU:HD11	1:A:227:VAL:HG21	1.86	0.57
1:A:175:VAL:HG22	1:B:273:ARG:HG3	1.87	0.57
1:A:219:ASP:OD2	1:A:237:PRO:HA	2.04	0.57
1:C:43:SER:HB2	1:C:70:THR:HG21	1.85	0.57
1:D:243:LEU:HD22	1:D:247:LYS:HE3	1.86	0.57
1:A:220:THR:HG22	1:A:222:THR:H	1.68	0.57
1:B:255:GLU:HG2	4:B:706:HOH:O	2.04	0.57
1:C:126:LEU:HD13	1:C:180:VAL:HG13	1.85	0.57
1:C:122:THR:O	1:C:124:THR:HG23	2.04	0.56
1:C:216:GLY:HA3	1:C:259:ASP:OD1	2.05	0.56
1:D:126:LEU:HD23	1:D:230:ILE:HG21	1.87	0.56
1:B:60:HIS:HB3	1:B:110:MET:HE2	1.86	0.56
1:B:68:LYS:HG2	1:B:72:GLN:HE21	1.70	0.56
1:D:61:VAL:N	1:D:110:MET:HE1	2.20	0.56
1:B:60:HIS:C	1:B:110:MET:HE1	2.31	0.55
1:C:32:LEU:HD23	1:C:54:LEU:CD2	2.36	0.55
1:B:224:MET:HE3	1:B:224:MET:HA	1.89	0.54
1:B:46:ILE:HD13	1:B:238:LYS:HB2	1.88	0.54
1:B:167:VAL:HG23	1:B:212:LEU:HD12	1.90	0.54
1:C:194:PHE:HA	1:C:197:ILE:HG12	1.90	0.54
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.90	0.54
1:C:144:PHE:CD2	1:C:145:LEU:HD22	2.43	0.54
1:C:171:LEU:HD13	1:D:280:TYR:OH	2.08	0.54
1:A:277:GLU:HG2	1:B:175:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:N	1:B:110:MET:HE1	2.23	0.54
1:A:261:SER:O	1:A:265:THR:HG23	2.08	0.53
1:C:179:MET:HE1	1:C:230:ILE:HG21	1.90	0.53
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.88	0.53
1:B:79:LEU:HD13	1:B:86:ALA:HB3	1.90	0.53
1:C:155:LEU:HG	1:C:159:LYS:HE3	1.89	0.53
1:C:103:VAL:HG21	1:C:153:ALA:CB	2.38	0.53
1:C:243:LEU:HD22	1:C:247:LYS:HD2	1.89	0.53
1:D:68:LYS:O	1:D:72:GLN:HG3	2.09	0.53
1:A:277:GLU:CG	1:B:175:VAL:HG13	2.39	0.53
1:B:71:LEU:HA	1:B:74:VAL:HG22	1.90	0.53
1:C:76:SER:O	1:C:80:GLU:HG3	2.10	0.52
1:A:231:VAL:HG12	1:A:233:MET:HG2	1.90	0.52
1:D:60:HIS:C	1:D:110:MET:CE	2.82	0.52
1:A:71:LEU:O	1:A:74:VAL:HG12	2.10	0.52
1:B:243:LEU:O	1:B:247:LYS:HG3	2.10	0.52
1:B:71:LEU:O	1:B:74:VAL:HG22	2.10	0.52
1:A:230:ILE:N	1:A:230:ILE:HD12	2.24	0.51
1:B:270:ASN:C	1:B:270:ASN:HD22	2.18	0.51
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.91	0.51
1:A:225:LYS:HB3	1:A:225:LYS:HZ3	1.74	0.51
1:D:171:LEU:HD13	1:D:268:ILE:HD13	1.92	0.51
1:A:71:LEU:O	1:A:75:VAL:HG23	2.11	0.51
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.93	0.51
1:C:231:VAL:HG12	1:C:233:MET:HG2	1.93	0.51
1:D:133:ILE:HD13	1:D:133:ILE:C	2.36	0.51
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.93	0.51
1:D:276:LEU:HG	1:D:280:TYR:CE2	2.45	0.51
1:A:145:LEU:HD23	1:A:145:LEU:O	2.12	0.50
1:C:53:HIS:HE1	1:C:239:GLU:O	1.93	0.50
1:D:93:MET:HG3	1:D:120:HIS:CE1	2.46	0.50
1:A:29:PRO:HG2	1:A:30:GLU:OE2	2.10	0.50
1:A:92:THR:OG1	1:A:94:GLU:HG3	2.12	0.50
1:B:96:MET:HE3	1:B:141:GLU:HG3	1.93	0.50
1:B:99:ALA:HB1	1:B:150:LEU:HD13	1.93	0.50
1:A:128:LEU:HD23	1:A:179:MET:SD	2.52	0.50
1:C:30:GLU:O	1:C:33:GLN:HG2	2.12	0.50
1:C:43:SER:HB2	1:C:70:THR:HG23	1.92	0.50
1:D:71:LEU:HA	1:D:74:VAL:HG12	1.94	0.50
1:C:103:VAL:CG2	1:C:153:ALA:HB1	2.41	0.49
1:C:178:PRO:O	1:C:179:MET:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LYS:O	1:C:203:VAL:HG23	2.11	0.49
1:B:66:ARG:HD2	1:D:105:GLN:HE22	1.77	0.49
1:B:100:GLU:O	1:B:103:VAL:HG22	2.12	0.49
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.95	0.49
1:B:118:LEU:HD22	1:B:150:LEU:HD23	1.95	0.49
1:D:216:GLY:HA3	1:D:259:ASP:OD1	2.11	0.49
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.48	0.49
1:A:284:TYR:HA	1:B:230:ILE:O	2.13	0.48
1:B:251:LEU:HD12	1:B:253:GLN:HE21	1.78	0.48
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.14	0.48
1:C:264:THR:HG23	1:D:280:TYR:OH	2.14	0.48
1:C:275:ILE:O	1:C:279:LEU:HD13	2.13	0.48
1:A:171:LEU:HD23	1:A:214:VAL:HG12	1.95	0.48
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.95	0.48
1:D:61:VAL:HA	1:D:110:MET:HE1	1.95	0.48
1:D:99:ALA:HB1	1:D:150:LEU:HD13	1.95	0.48
1:A:118:LEU:CD2	1:A:150:LEU:HD23	2.42	0.47
1:A:276:LEU:HD11	1:A:280:TYR:CZ	2.49	0.47
1:B:61:VAL:HA	1:B:110:MET:HE1	1.93	0.47
1:C:171:LEU:HD22	1:C:268:ILE:HD13	1.94	0.47
1:D:71:LEU:O	1:D:74:VAL:HG12	2.13	0.47
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.49	0.47
1:B:195:SER:O	1:B:199:LYS:HG2	2.14	0.47
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.80	0.47
1:D:285:ASN:C	1:D:285:ASN:HD22	2.21	0.47
1:A:77:HIS:O	1:A:81:LEU:HG	2.15	0.47
1:C:103:VAL:HG21	1:C:153:ALA:HB1	1.96	0.47
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.97	0.47
1:B:221:GLU:O	1:B:225:LYS:HE2	2.15	0.46
1:B:242:ALA:O	1:B:246:ILE:HG12	2.15	0.46
1:A:225:LYS:NZ	1:A:225:LYS:CB	2.77	0.46
1:A:247:LYS:HD3	1:A:247:LYS:C	2.40	0.46
1:D:53:HIS:HE1	1:D:239:GLU:O	1.98	0.46
1:A:53:HIS:O	1:A:57:MET:HG3	2.16	0.46
1:C:32:LEU:HD21	1:C:246:ILE:CG2	2.46	0.46
1:A:99:ALA:HB1	1:A:150:LEU:HD13	1.97	0.46
1:B:108:LYS:CA	1:B:108:LYS:HE2	2.46	0.46
1:D:108:LYS:NZ	1:D:108:LYS:HB3	2.31	0.46
1:D:242:ALA:O	1:D:246:ILE:HG12	2.16	0.46
1:C:124:THR:HG22	1:C:135:HIS:HE1	1.81	0.46
1:C:194:PHE:CD1	1:C:197:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HG	1:C:216:GLY:HA2	1.97	0.45
1:C:129:PHE:HB3	1:D:197:ILE:CD1	2.46	0.45
1:D:103:VAL:CG2	1:D:150:LEU:HD12	2.47	0.45
1:D:216:GLY:O	3:D:504:NDP:H42N	2.16	0.45
1:D:223:ALA:O	1:D:227:VAL:HG23	2.16	0.45
1:A:193:PHE:O	1:A:197:ILE:HG12	2.16	0.45
4:B:693:HOH:O	1:D:101:GLN:HG3	2.16	0.45
1:A:276:LEU:HG	1:A:280:TYR:CE2	2.52	0.45
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.99	0.45
1:B:36:LYS:HB2	1:B:113:LEU:HA	1.98	0.45
1:C:174:LYS:HB2	1:C:268:ILE:HD11	1.97	0.45
1:D:108:LYS:HB3	1:D:108:LYS:HZ3	1.82	0.45
1:B:120:HIS:HE1	1:B:146:SER:OG	1.99	0.45
1:D:61:VAL:N	1:D:110:MET:CE	2.80	0.45
1:A:91:GLY:HA3	1:A:98:PHE:CZ	2.52	0.44
1:A:220:THR:HG22	1:A:222:THR:N	2.30	0.44
1:D:227:VAL:HG12	1:D:228:SER:H	1.81	0.44
1:A:106:ALA:O	1:A:110:MET:HG2	2.17	0.44
1:D:71:LEU:O	1:D:74:VAL:CG1	2.65	0.44
1:B:29:PRO:HA	1:B:57:MET:CE	2.48	0.44
1:D:171:LEU:HD23	1:D:215:LEU:C	2.42	0.44
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.17	0.44
1:A:94:GLU:OE1	1:A:138:LYS:NZ	2.50	0.44
1:B:47:GLY:HA2	1:B:50:MET:HE3	1.99	0.44
1:A:145:LEU:HD23	1:A:145:LEU:C	2.42	0.44
1:A:223:ALA:O	1:A:227:VAL:HG23	2.17	0.44
1:A:231:VAL:HG13	1:A:233:MET:HE3	1.98	0.44
1:B:178:PRO:O	1:B:179:MET:HB2	2.18	0.44
1:A:158:LEU:HD22	1:A:163:GLY:HA3	1.99	0.44
1:B:39:VAL:HG12	1:B:42:ALA:HB2	2.00	0.44
1:C:255:GLU:OE1	1:C:257:TYR:OH	2.35	0.44
1:A:216:GLY:O	3:A:501:NDP:H42N	2.18	0.43
1:B:74:VAL:HG23	1:B:75:VAL:N	2.32	0.43
1:B:164:SER:HB3	4:B:683:HOH:O	2.18	0.43
1:A:37:VAL:HG13	1:A:61:VAL:HG12	2.00	0.43
1:C:31:MET:C	1:C:32:LEU:HD12	2.44	0.43
1:A:280:TYR:C	1:A:282:THR:H	2.26	0.43
1:C:68:LYS:HG3	1:C:88:TYR:HE2	1.83	0.43
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.54	0.43
1:D:126:LEU:HD21	1:D:231:VAL:HG23	2.00	0.43
1:A:244:GLU:HA	1:A:247:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:CG1	1:A:176:ALA:N	2.82	0.43
1:D:103:VAL:HG23	1:D:150:LEU:HD12	2.01	0.43
1:D:155:LEU:HB3	1:D:156:PRO:HD3	1.99	0.43
1:A:39:VAL:HG12	1:A:42:ALA:HB2	2.01	0.42
1:C:40:THR:O	1:C:119:ASN:HB3	2.19	0.42
1:A:175:VAL:HG13	1:B:277:GLU:CG	2.49	0.42
1:B:32:LEU:HB2	1:B:57:MET:HE2	2.01	0.42
1:D:69:GLU:CD	1:D:69:GLU:H	2.27	0.42
1:D:227:VAL:HG13	1:D:231:VAL:HB	2.01	0.42
1:B:119:ASN:OD1	3:B:502:NDP:H4D	2.19	0.42
1:B:262:LEU:HD12	1:B:262:LEU:N	2.34	0.42
1:C:144:PHE:HD2	1:C:145:LEU:HD22	1.82	0.42
1:C:227:VAL:CG1	1:C:227:VAL:O	2.67	0.42
1:B:36:LYS:HD2	1:B:110:MET:HB2	2.01	0.42
1:D:43:SER:HB2	1:D:70:THR:CG2	2.49	0.42
1:B:108:LYS:HE2	1:B:108:LYS:N	2.34	0.42
1:B:167:VAL:HG23	1:B:167:VAL:O	2.19	0.42
1:C:207:ASN:HD22	1:C:207:ASN:HA	1.67	0.41
1:A:171:LEU:HG	1:A:216:GLY:HA2	2.02	0.41
1:A:277:GLU:HG2	1:B:175:VAL:CG1	2.50	0.41
1:D:270:ASN:C	1:D:270:ASN:HD22	2.27	0.41
1:A:217:LEU:CD1	1:A:227:VAL:HG21	2.48	0.41
1:B:126:LEU:HD11	1:B:227:VAL:HG12	2.02	0.41
1:B:157:MET:HG3	4:B:698:HOH:O	2.19	0.41
1:A:262:LEU:N	1:A:262:LEU:HD12	2.35	0.41
1:A:160:GLN:OE1	1:C:98:PHE:HB2	2.20	0.41
1:A:270:ASN:HD21	1:A:272:SER:HB2	1.85	0.41
1:A:220:THR:HG23	4:A:617:HOH:O	2.20	0.41
1:C:216:GLY:O	3:C:503:NDP:H42N	2.21	0.40
1:D:120:HIS:HE1	1:D:146:SER:OG	2.04	0.40
1:A:140:MET:HE2	1:B:140:MET:CE	2.28	0.40
1:C:37:VAL:CG1	1:C:54:LEU:HD13	2.50	0.40
1:C:215:LEU:HD21	1:C:245:ILE:HD11	2.04	0.40
1:A:280:TYR:OH	1:B:264:THR:HG23	2.21	0.40
1:B:155:LEU:CG	1:B:159:LYS:HE3	2.50	0.40
1:C:156:PRO:O	1:C:160:GLN:HG3	2.21	0.40
1:B:32:LEU:O	1:B:34:GLY:N	2.53	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	256/275 (93%)	237 (93%)	18 (7%)	1 (0%)	30	22
1	B	253/275 (92%)	242 (96%)	9 (4%)	2 (1%)	16	8
1	C	253/275 (92%)	243 (96%)	9 (4%)	1 (0%)	30	22
1	D	259/275 (94%)	247 (95%)	9 (4%)	3 (1%)	10	4
All	All	1021/1100 (93%)	969 (95%)	45 (4%)	7 (1%)	18	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	B	33	GLN
1	B	219	ASP
1	D	227	VAL
1	D	228	SER
1	C	219	ASP
1	D	230	ILE

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	216/232 (93%)	212 (98%)	4 (2%)	50	47
1	B	212/232 (91%)	203 (96%)	9 (4%)	26	19
1	C	212/232 (91%)	208 (98%)	4 (2%)	50	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	218/232 (94%)	213 (98%)	5 (2%)	44	40
All	All	858/928 (92%)	836 (97%)	22 (3%)	40	35

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	150	LEU
1	A	224	MET
1	A	247	LYS
1	B	73	LYS
1	B	79	LEU
1	B	108	LYS
1	B	110	MET
1	B	131	ASP
1	B	150	LEU
1	B	224	MET
1	B	233	MET
1	B	243	LEU
1	C	141	GLU
1	C	150	LEU
1	C	207	ASN
1	C	243	LEU
1	D	79	LEU
1	D	133	ILE
1	D	150	LEU
1	D	215	LEU
1	D	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	120	HIS
1	A	123	ASN
1	A	162	ASN
1	A	270	ASN
1	B	33	GLN
1	B	53	HIS
1	B	72	GLN
1	B	101	GLN

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Mol	Chain	Res	Type
1	B	105	GLN
1	B	120	HIS
1	B	162	ASN
1	B	207	ASN
1	B	234	GLN
1	B	253	GLN
1	B	270	ASN
1	C	33	GLN
1	C	53	HIS
1	C	72	GLN
1	C	105	GLN
1	C	123	ASN
1	C	127	ASN
1	C	135	HIS
1	C	160	GLN
1	C	162	ASN
1	C	207	ASN
1	C	234	GLN
1	C	253	GLN
1	D	53	HIS
1	D	72	GLN
1	D	77	HIS
1	D	105	GLN
1	D	120	HIS
1	D	123	ASN
1	D	127	ASN
1	D	135	HIS
1	D	207	ASN
1	D	253	GLN
1	D	270	ASN
1	D	285	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZMG	B	602	-	17,18,18	1.36	3 (17%)	18,25,25	1.32	2 (11%)
2	ZMG	D	604	-	17,18,18	1.48	4 (23%)	18,25,25	1.29	2 (11%)
3	NDP	B	502	-	47,50,52	1.65	6 (12%)	60,76,80	1.05	3 (5%)
3	NDP	D	504	-	47,50,52	1.59	7 (14%)	60,76,80	0.97	2 (3%)
3	NDP	A	501	-	47,50,52	1.56	6 (12%)	60,76,80	1.14	3 (5%)
2	ZMG	C	603	-	17,18,18	1.48	2 (11%)	18,25,25	1.42	3 (16%)
2	ZMG	A	601	-	17,18,18	1.37	1 (5%)	18,25,25	1.09	1 (5%)
3	NDP	C	503	-	47,50,52	1.67	8 (17%)	60,76,80	1.11	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZMG	B	602	-	-	0/8/20/20	0/2/2/2
2	ZMG	D	604	-	-	0/8/20/20	0/2/2/2
3	NDP	B	502	-	-	6/34/77/77	0/4/4/5
3	NDP	D	504	-	-	4/34/77/77	0/4/4/5
3	NDP	A	501	-	-	2/34/77/77	0/4/4/5
2	ZMG	C	603	-	-	0/8/20/20	0/2/2/2
2	ZMG	A	601	-	-	0/8/20/20	0/2/2/2
3	NDP	C	503	-	-	5/34/77/77	0/4/4/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NDP	C6A-C5A	-6.59	1.39	1.50
3	D	504	NDP	C6A-C5A	-6.19	1.39	1.50
3	C	503	NDP	C6A-C5A	-6.07	1.40	1.50
3	A	501	NDP	C6A-C5A	-6.01	1.40	1.50
3	C	503	NDP	C4N-C3N	-5.14	1.40	1.50
3	B	502	NDP	C4N-C3N	-4.91	1.40	1.50
3	D	504	NDP	C4N-C3N	-4.91	1.40	1.50
3	A	501	NDP	C4N-C3N	-4.77	1.41	1.50
3	B	502	NDP	C4N-C5N	-3.71	1.39	1.49
3	A	501	NDP	C4N-C5N	-3.49	1.40	1.49
2	C	603	ZMG	C5-N7	-3.42	1.35	1.41
3	D	504	NDP	C4N-C5N	-3.23	1.40	1.49
3	C	503	NDP	C2N-C3N	3.18	1.43	1.35
3	C	503	NDP	C4N-C5N	-3.07	1.41	1.49
3	C	503	NDP	PN-O3	-2.94	1.56	1.59
2	D	604	ZMG	C5-C4	2.85	1.42	1.39
2	A	601	ZMG	C5-N7	-2.74	1.36	1.41
3	C	503	NDP	C6N-C5N	2.73	1.41	1.33
2	B	602	ZMG	C5-N7	-2.63	1.36	1.41
2	D	604	ZMG	C1-C6	2.37	1.43	1.38
3	B	502	NDP	C6N-C5N	2.35	1.40	1.33
2	D	604	ZMG	C8-N12	2.33	1.34	1.31
3	C	503	NDP	C6A-N6A	-2.31	1.34	1.48
3	D	504	NDP	C6N-C5N	2.31	1.40	1.33
3	D	504	NDP	C2N-C3N	2.29	1.41	1.35
3	B	502	NDP	C6A-N6A	-2.28	1.34	1.48
3	A	501	NDP	C2N-C3N	2.27	1.41	1.35
2	B	602	ZMG	C8-N12	2.26	1.34	1.31
3	A	501	NDP	C6A-N6A	-2.24	1.34	1.48
3	B	502	NDP	C2N-C3N	2.21	1.41	1.35
2	D	604	ZMG	C5-N7	-2.17	1.37	1.41
2	C	603	ZMG	C8-N7	-2.13	1.33	1.36
3	A	501	NDP	C6N-C5N	2.09	1.39	1.33
3	D	504	NDP	C6A-N6A	-2.08	1.35	1.48
3	D	504	NDP	PN-O3	-2.06	1.57	1.59
2	B	602	ZMG	C1-C6	2.01	1.42	1.38
3	C	503	NDP	O4D-C4D	-2.00	1.40	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NDP	C5A-C6A-N6A	4.43	122.77	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	504	NDP	C5A-C6A-N6A	4.25	122.38	113.08
3	C	503	NDP	C5A-C6A-N6A	4.21	122.29	113.08
2	B	602	ZMG	C10-C11-N12	-3.64	111.26	115.69
3	A	501	NDP	O2D-C2D-C1D	3.45	122.00	110.10
3	B	502	NDP	C5A-C6A-N6A	3.45	120.63	113.08
2	C	603	ZMG	C10-C11-N12	-3.29	111.69	115.69
2	C	603	ZMG	C6-C5-C4	3.11	120.63	117.23
2	D	604	ZMG	C10-C11-N12	-2.91	112.15	115.69
3	B	502	NDP	O3B-C3B-C4B	-2.82	102.97	111.08
3	C	503	NDP	O2D-C2D-C3D	2.66	120.35	111.82
2	A	601	ZMG	C10-C11-N12	-2.65	112.47	115.69
3	B	502	NDP	O2D-C2D-C1D	2.52	118.78	110.10
2	D	604	ZMG	O14-C11-C10	2.45	123.22	120.23
3	A	501	NDP	O4D-C1D-N1N	2.42	112.71	108.08
2	C	603	ZMG	O14-C11-C10	2.40	123.15	120.23
3	C	503	NDP	O3D-C3D-C2D	-2.31	104.42	111.82
3	C	503	NDP	O3B-C3B-C4B	-2.30	104.48	111.08
2	B	602	ZMG	O14-C11-C10	2.26	122.99	120.23
3	D	504	NDP	O4D-C4D-C3D	2.19	109.49	105.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

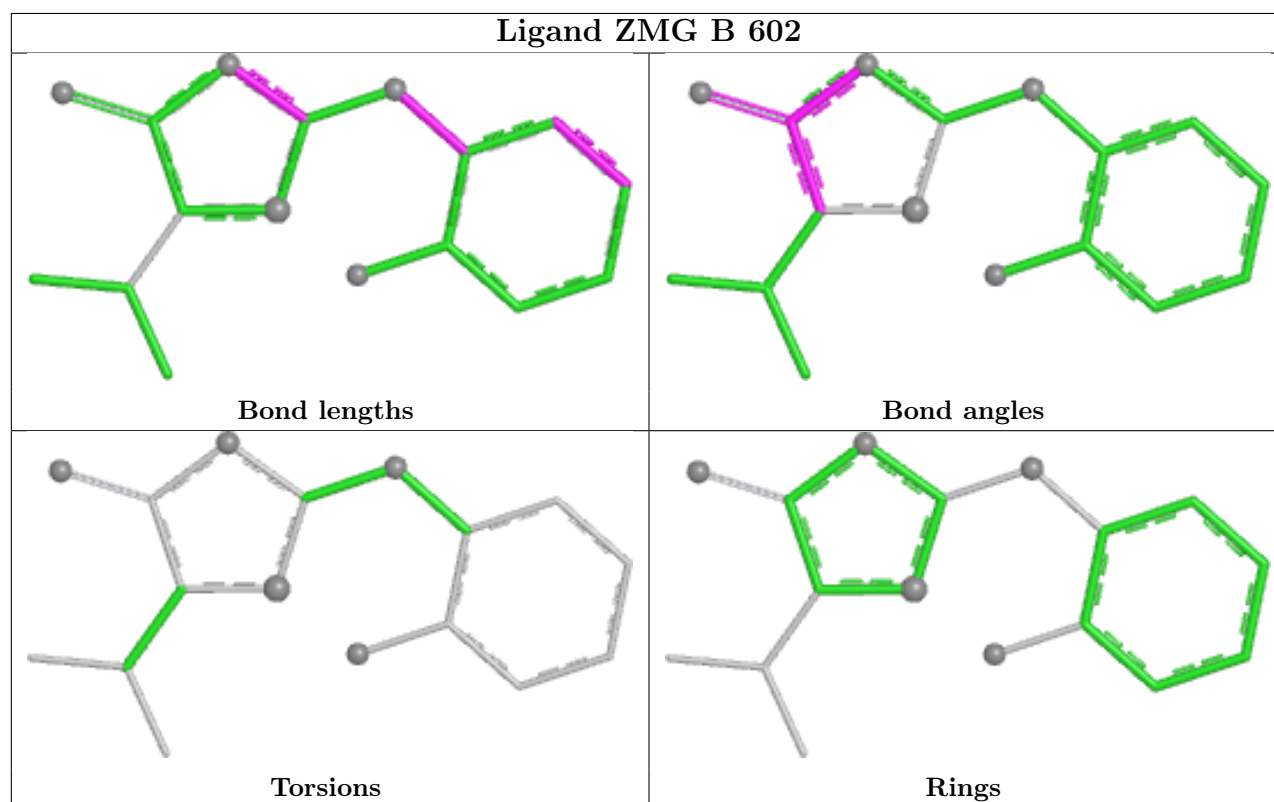
Mol	Chain	Res	Type	Atoms
3	B	502	NDP	C5D-O5D-PN-O2N
3	A	501	NDP	O4D-C1D-N1N-C6N
3	B	502	NDP	O4D-C1D-N1N-C6N
3	C	503	NDP	O4D-C1D-N1N-C6N
3	D	504	NDP	O4D-C1D-N1N-C6N
3	C	503	NDP	PN-O3-PA-O1A
3	B	502	NDP	C5D-O5D-PN-O3
3	B	502	NDP	C5D-O5D-PN-O1N
3	C	503	NDP	C3B-C2B-O2B-P2B
3	D	504	NDP	C3B-C2B-O2B-P2B
3	B	502	NDP	PN-O3-PA-O2A
3	D	504	NDP	PN-O3-PA-O2A
3	B	502	NDP	O4B-C4B-C5B-O5B
3	C	503	NDP	C1B-C2B-O2B-P2B
3	D	504	NDP	C1B-C2B-O2B-P2B
3	A	501	NDP	PN-O3-PA-O2A
3	C	503	NDP	PN-O3-PA-O2A

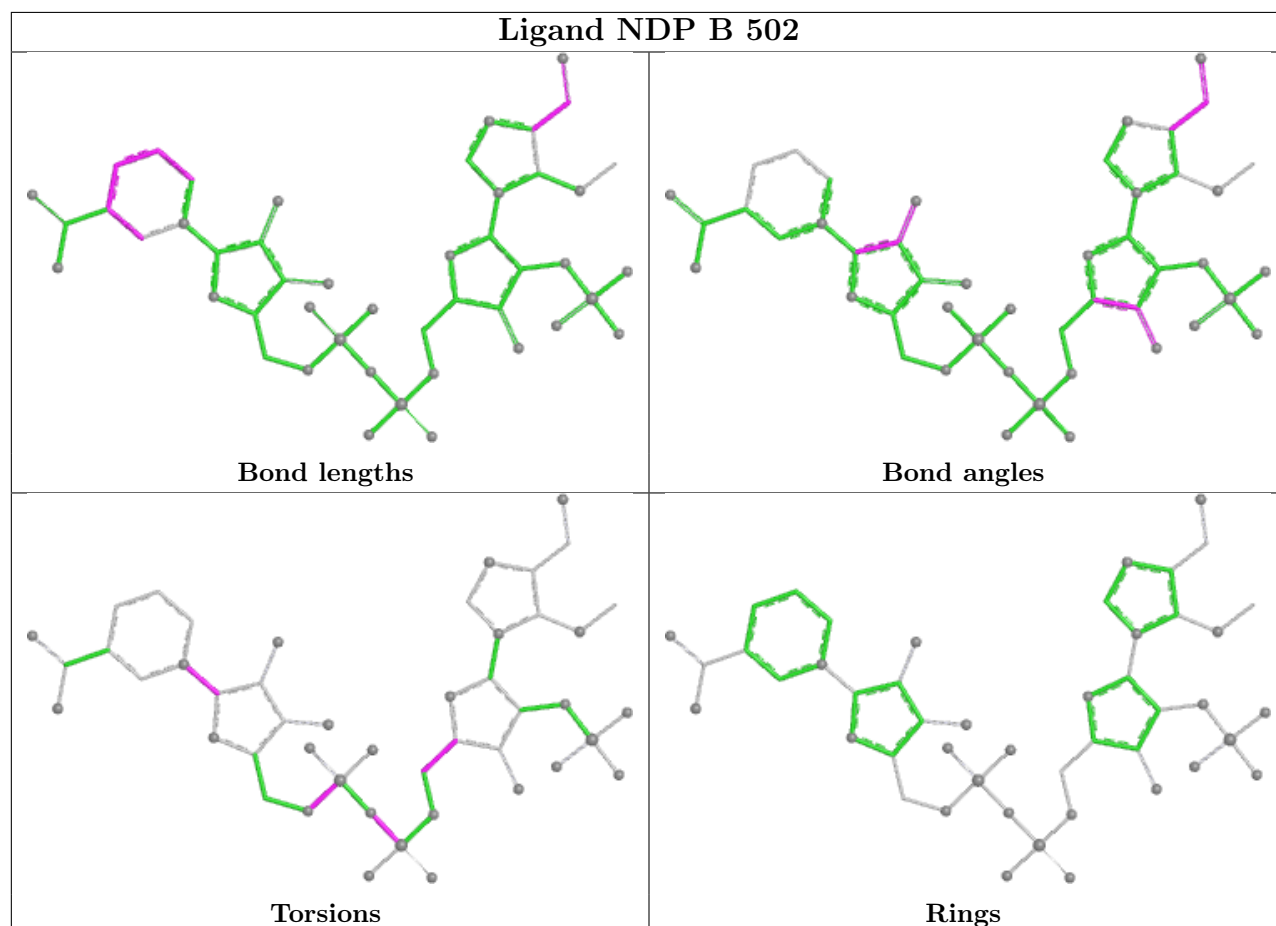
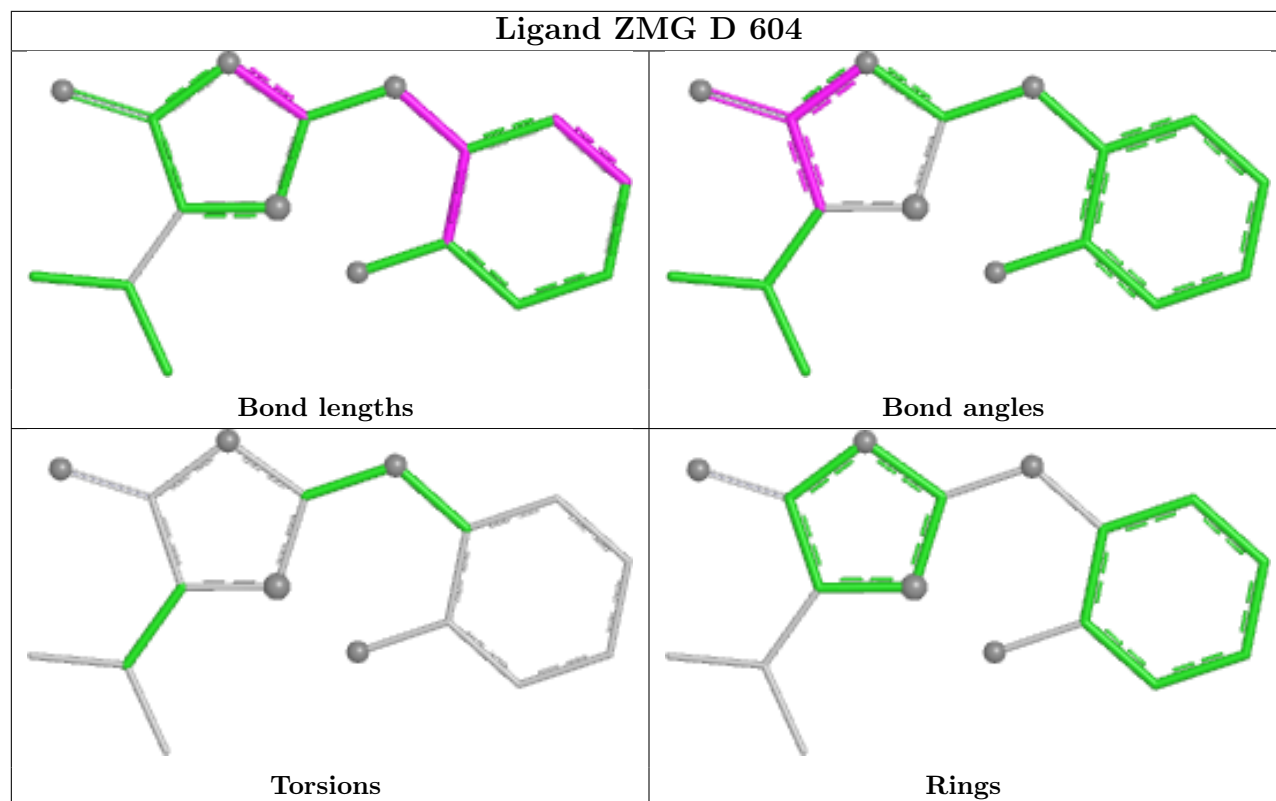
There are no ring outliers.

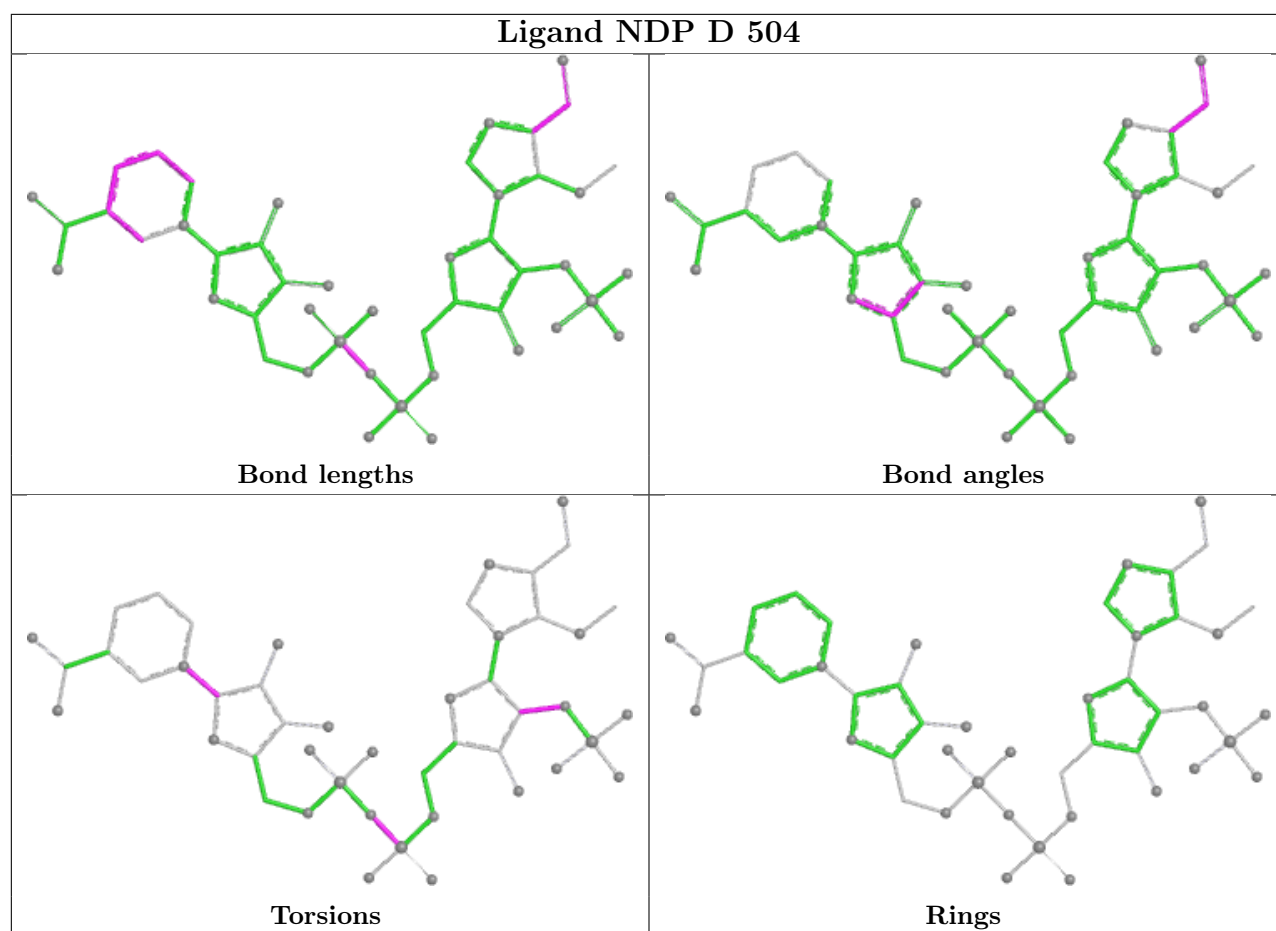
4 monomers are involved in 8 short contacts:

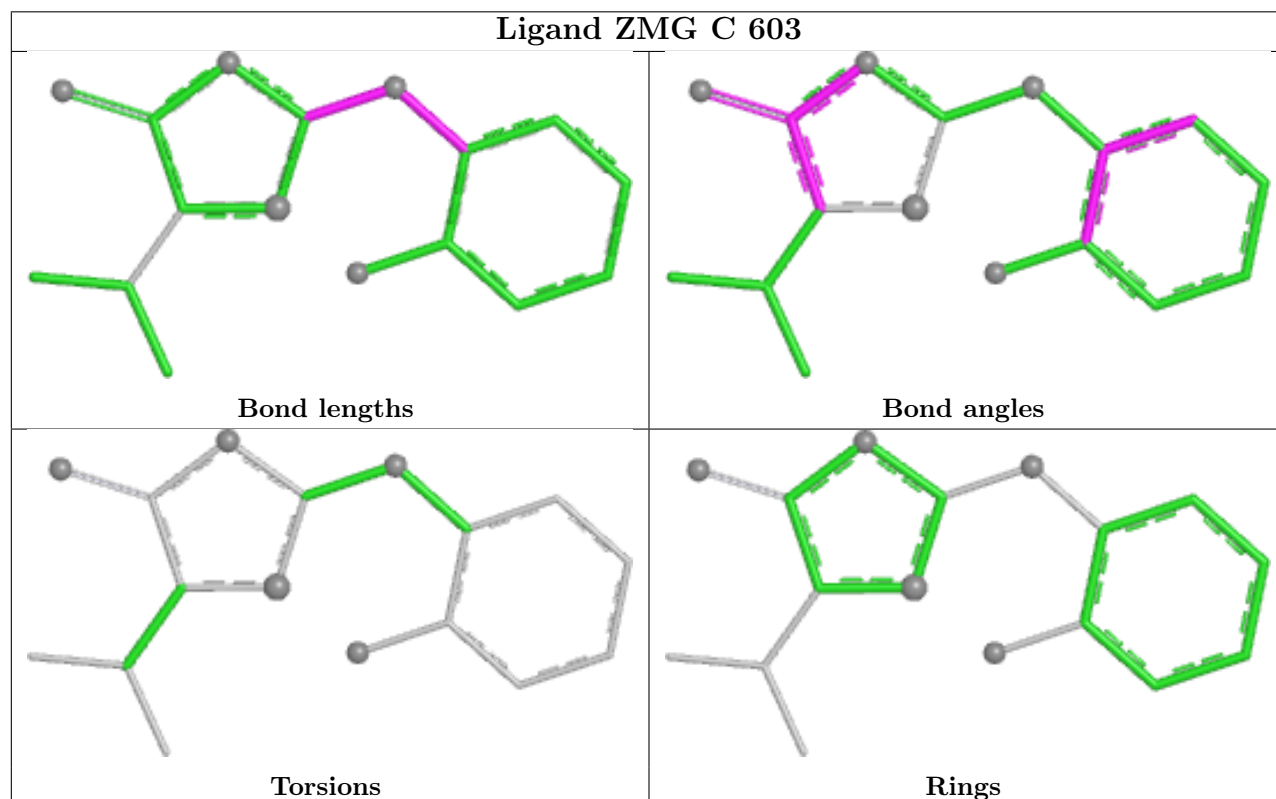
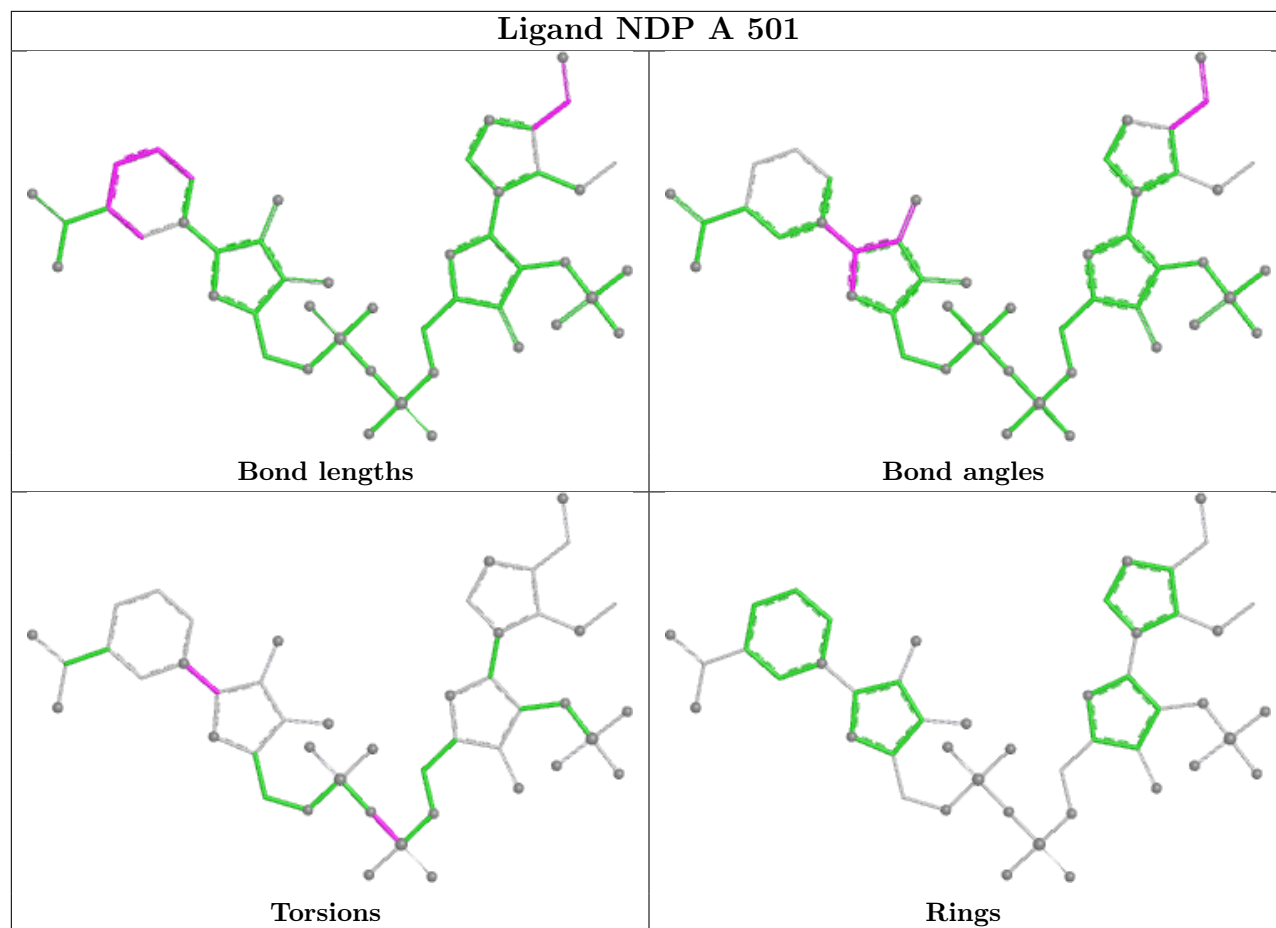
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NDP	2	0
3	D	504	NDP	2	0
3	A	501	NDP	2	0
3	C	503	NDP	2	0

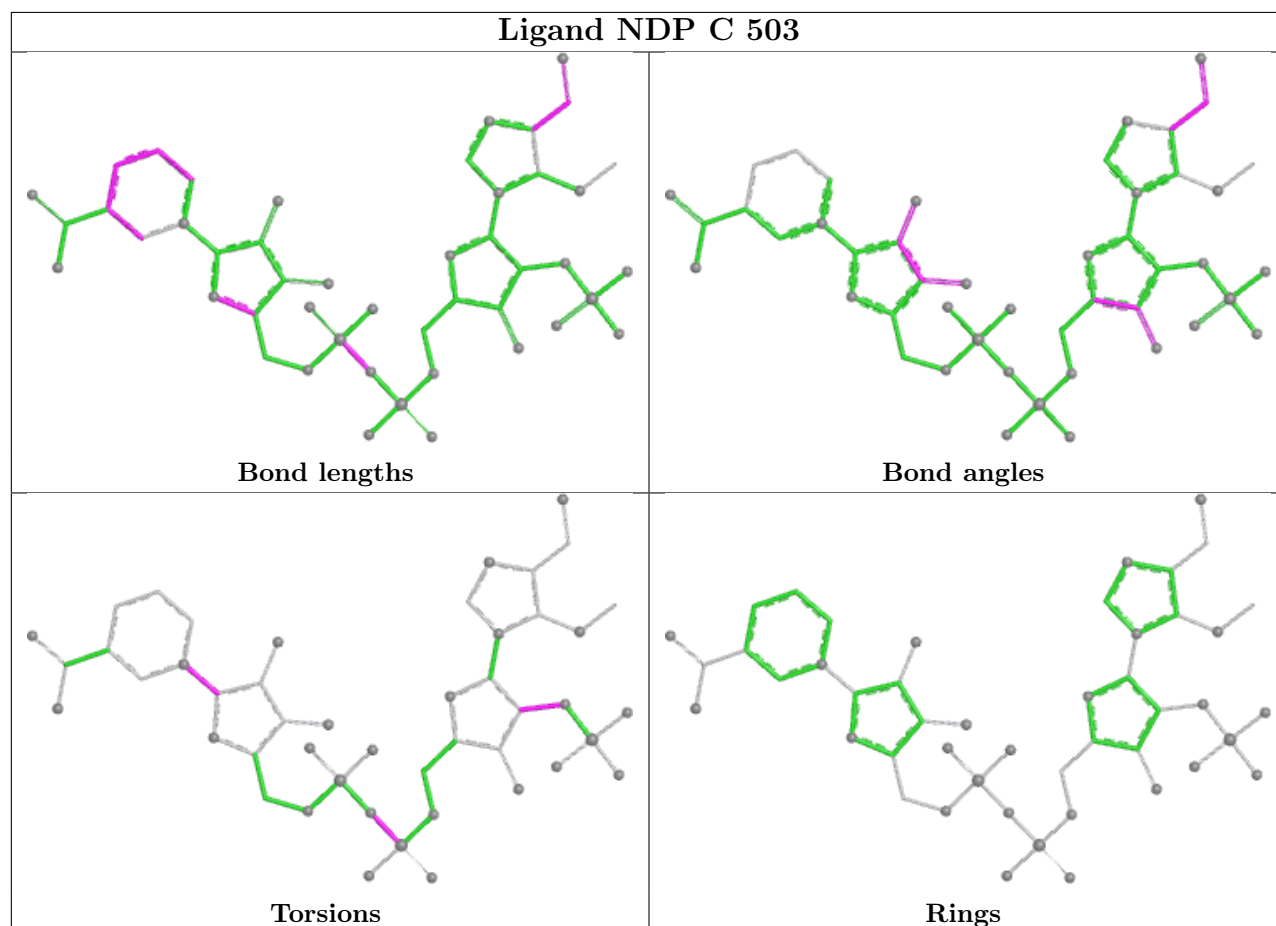
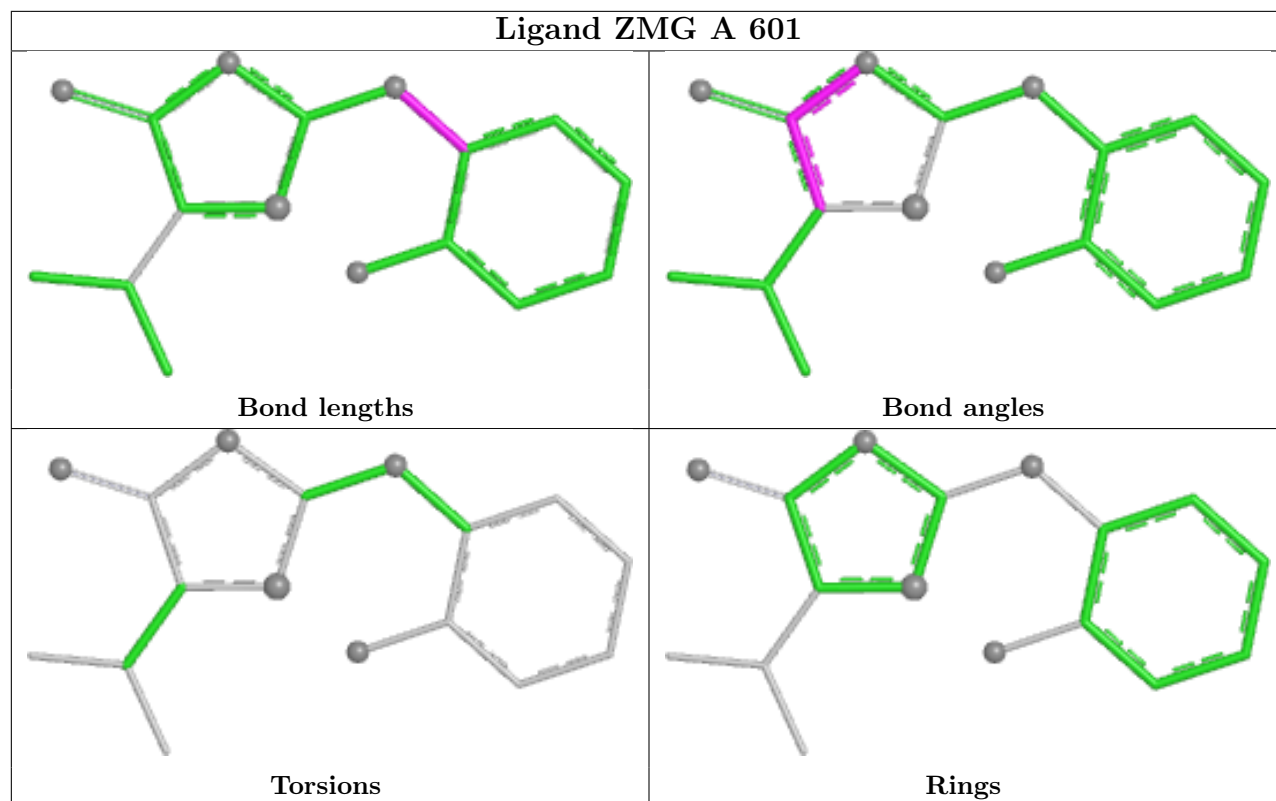
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	259/275 (94%)	1.66	88 (33%) 1 1	14, 38, 61, 77	0
1	B	255/275 (92%)	0.83	32 (12%) 8 8	15, 27, 44, 53	0
1	C	255/275 (92%)	0.49	12 (4%) 36 39	11, 23, 36, 52	0
1	D	261/275 (94%)	0.74	27 (10%) 12 12	11, 24, 43, 61	0
All	All	1030/1100 (93%)	0.93	159 (15%) 5 5	11, 27, 52, 77	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	HIS	9.6
1	D	231	VAL	8.3
1	D	232	HIS	7.8
1	A	230	ILE	7.7
1	D	230	ILE	6.2
1	A	229	GLY	6.1
1	D	229	GLY	5.5
1	D	228	SER	5.4
1	A	74	VAL	5.1
1	A	231	VAL	4.8
1	A	226	ALA	4.7
1	A	227	VAL	4.7
1	A	75	VAL	4.5
1	A	109	LEU	4.4
1	A	34	GLY	4.3
1	A	262	LEU	4.2
1	D	233	MET	4.2
1	A	163	GLY	4.2
1	A	89	ILE	4.1
1	A	71	LEU	4.1
1	A	282	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	284	TYR	3.9
1	A	81	LEU	3.9
1	A	84	ALA	3.8
1	A	177	TYR	3.7
1	D	227	VAL	3.7
1	D	262	LEU	3.6
1	C	280	TYR	3.6
1	A	27	PHE	3.6
1	A	32	LEU	3.5
1	A	235	ALA	3.5
1	A	60	HIS	3.5
1	A	207	ASN	3.4
1	A	114	ASP	3.3
1	C	203	VAL	3.3
1	B	30	GLU	3.3
1	A	79	LEU	3.3
1	A	263	TRP	3.3
1	A	233	MET	3.3
1	A	59	ALA	3.3
1	A	104	ALA	3.3
1	B	219	ASP	3.3
1	A	228	SER	3.3
1	A	37	VAL	3.2
1	C	171	LEU	3.2
1	A	265	THR	3.2
1	A	55	ALA	3.1
1	A	70	THR	3.1
1	A	52	TYR	3.1
1	D	234	GLN	3.1
1	A	42	ALA	3.1
1	A	54	LEU	3.0
1	A	206	VAL	3.0
1	B	160	GLN	3.0
1	B	32	LEU	3.0
1	A	107	GLY	3.0
1	A	72	GLN	3.0
1	C	205	ARG	3.0
1	D	280	TYR	2.9
1	B	203	VAL	2.9
1	A	43	SER	2.9
1	B	233	MET	2.9
1	A	73	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	232	HIS	2.8
1	A	69	GLU	2.8
1	B	132	ASP	2.8
1	B	239	GLU	2.8
1	A	29	PRO	2.8
1	A	77	HIS	2.8
1	A	88	TYR	2.7
1	A	48	ARG	2.7
1	D	205	ARG	2.7
1	A	134	HIS	2.7
1	A	63	VAL	2.7
1	B	27	PHE	2.7
1	B	280	TYR	2.7
1	D	265	THR	2.7
1	A	80	GLU	2.7
1	A	239	GLU	2.7
1	A	58	GLY	2.6
1	A	218	ILE	2.6
1	A	258	TYR	2.6
1	B	279	LEU	2.6
1	A	86	ALA	2.6
1	A	243	LEU	2.6
1	B	133	ILE	2.6
1	A	35	LYS	2.5
1	B	234	GLN	2.5
1	D	179	MET	2.5
1	A	100	GLU	2.5
1	C	26	GLU	2.5
1	D	203	VAL	2.5
1	D	29	PRO	2.5
1	D	177	TYR	2.5
1	B	130	HIS	2.5
1	A	38	ILE	2.5
1	A	123	ASN	2.4
1	B	33	GLN	2.4
1	A	133	ILE	2.4
1	A	111	GLY	2.4
1	D	266	LEU	2.4
1	B	255	GLU	2.4
1	A	126	LEU	2.4
1	A	251	LEU	2.4
1	A	205	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	205	ARG	2.4
1	B	231	VAL	2.4
1	C	279	LEU	2.3
1	A	280	TYR	2.3
1	A	97	THR	2.3
1	A	124	THR	2.3
1	A	33	GLN	2.3
1	A	162	ASN	2.3
1	D	157	MET	2.3
1	A	28	ARG	2.3
1	C	108	LYS	2.3
1	B	281	SER	2.3
1	B	73	LYS	2.3
1	A	106	ALA	2.3
1	A	85	SER	2.3
1	B	221	GLU	2.3
1	A	247	LYS	2.3
1	A	269	ARG	2.2
1	D	284	TYR	2.2
1	B	74	VAL	2.2
1	B	167	VAL	2.2
1	B	29	PRO	2.2
1	C	27	PHE	2.2
1	D	263	TRP	2.2
1	A	41	GLY	2.2
1	A	98	PHE	2.2
1	B	197	ILE	2.2
1	B	69	GLU	2.2
1	C	222	THR	2.2
1	A	112	GLY	2.2
1	A	266	LEU	2.2
1	B	79	LEU	2.2
1	D	109	LEU	2.2
1	A	44	LYS	2.2
1	D	269	ARG	2.2
1	D	133	ILE	2.1
1	B	180	VAL	2.1
1	C	70	THR	2.1
1	A	161	SER	2.1
1	B	128	LEU	2.1
1	D	28	ARG	2.1
1	D	26	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	LEU	2.1
1	C	29	PRO	2.1
1	A	125	SER	2.1
1	A	78	CYS	2.1
1	A	51	ALA	2.1
1	D	197	ILE	2.0
1	B	265	THR	2.0
1	B	123	ASN	2.0
1	A	175	VAL	2.0
1	C	32	LEU	2.0
1	D	221	GLU	2.0
1	A	197	ILE	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.

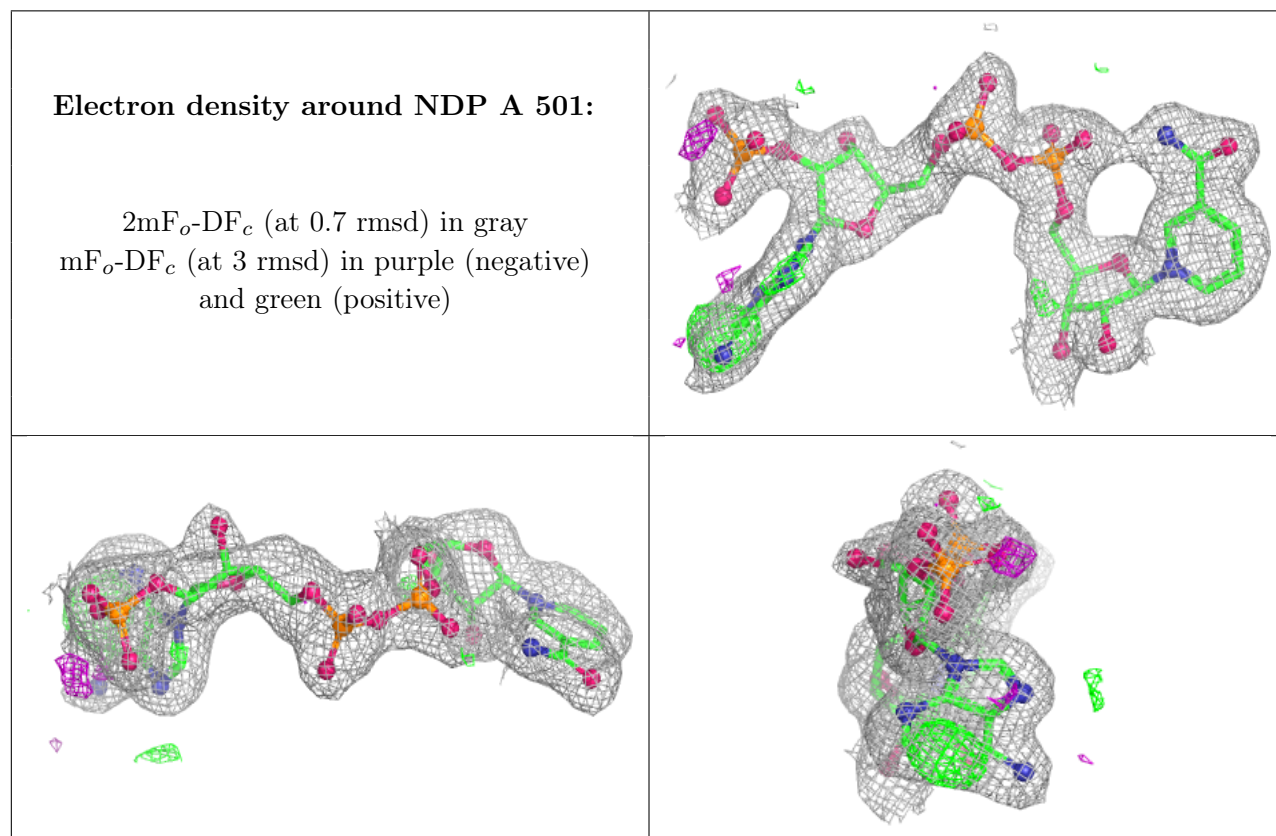
6.4 Ligands [i](#)

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	A	501	47/48	0.92	0.09	21,26,32,34	0
2	ZMG	A	601	17/17	0.94	0.10	27,31,34,34	0
3	NDP	B	502	47/48	0.94	0.07	17,21,23,28	0
2	ZMG	B	602	17/17	0.95	0.09	21,24,30,31	0
2	ZMG	D	604	17/17	0.95	0.09	20,25,27,27	0
2	ZMG	C	603	17/17	0.96	0.07	18,21,24,25	0
3	NDP	C	503	47/48	0.96	0.07	14,19,23,26	0
3	NDP	D	504	47/48	0.96	0.07	14,16,20,23	0

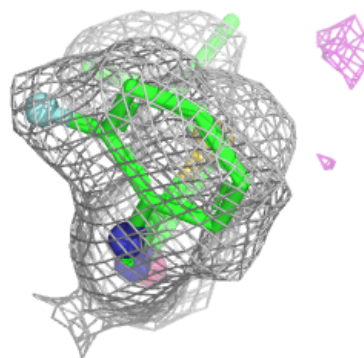
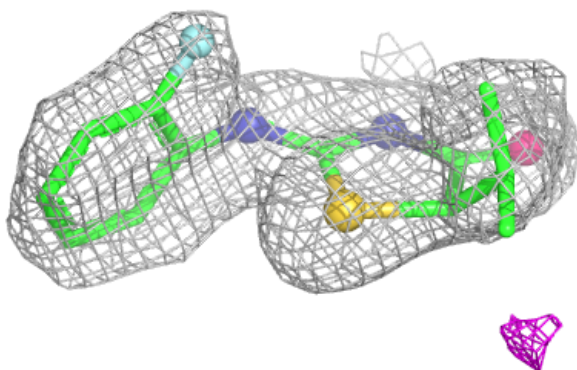
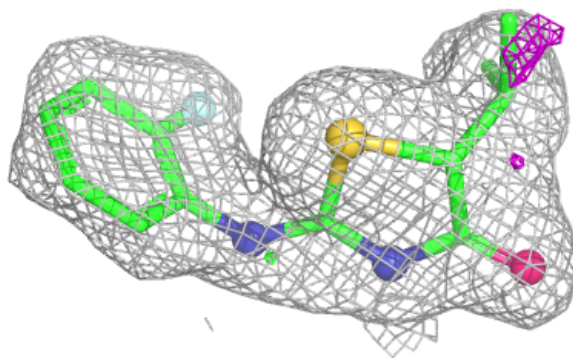
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

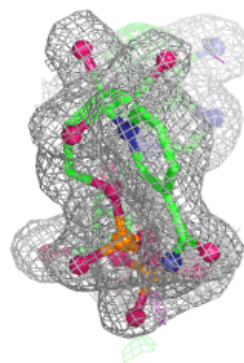
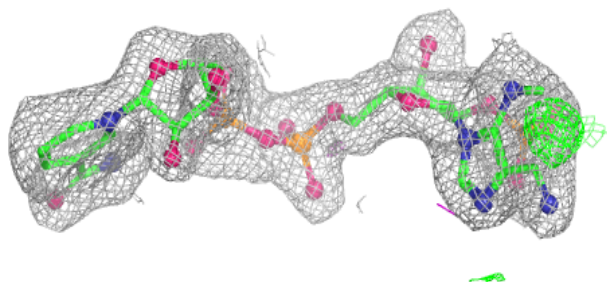
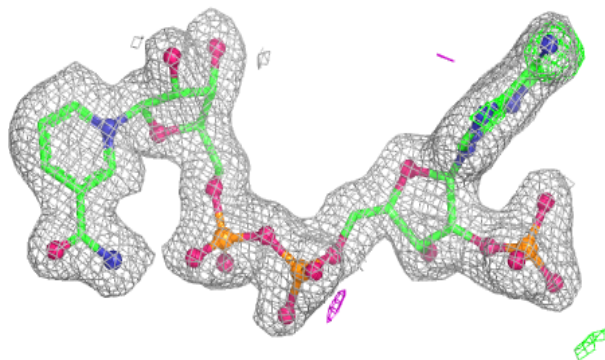


Electron density around ZMG A 601:

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

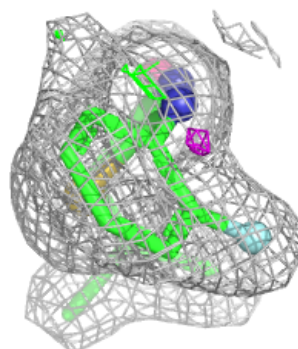
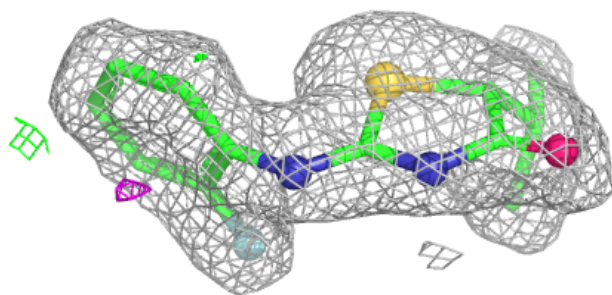
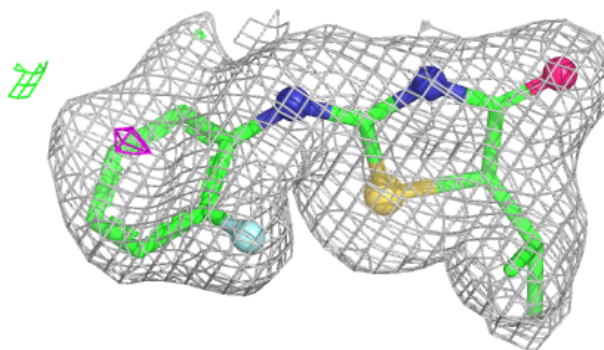
**Electron density around NDP B 502:**

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

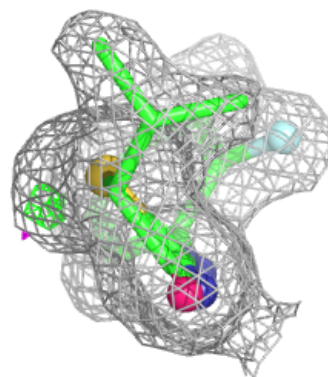
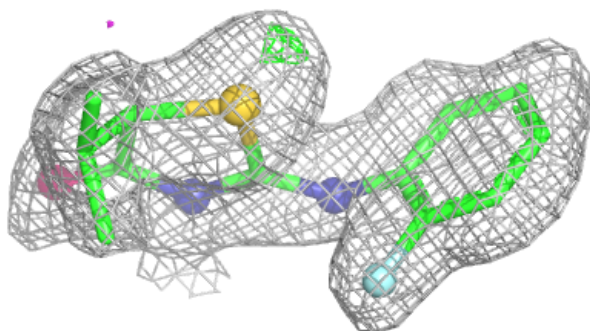
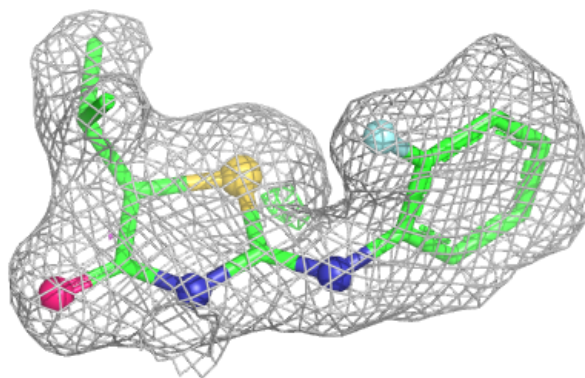


Electron density around ZMG B 602:

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

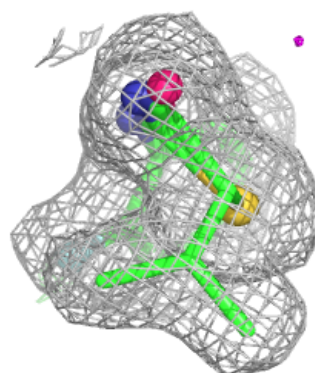
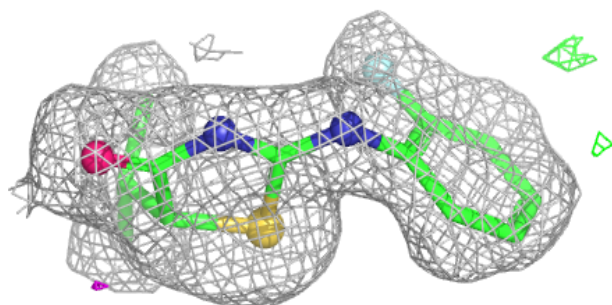
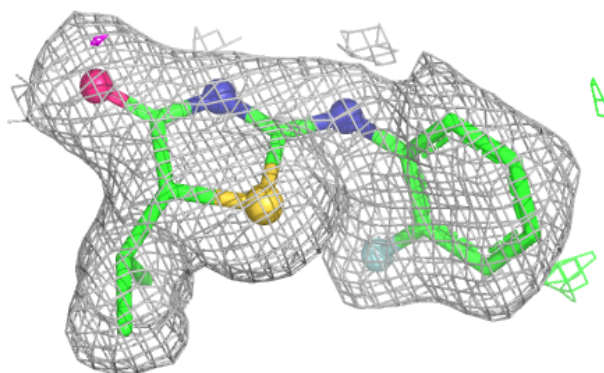
**Electron density around ZMG D 604:**

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

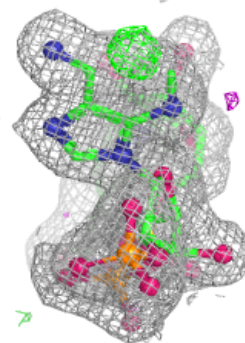
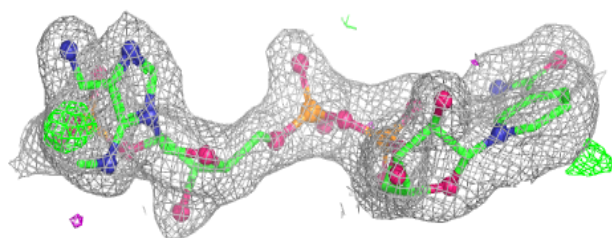
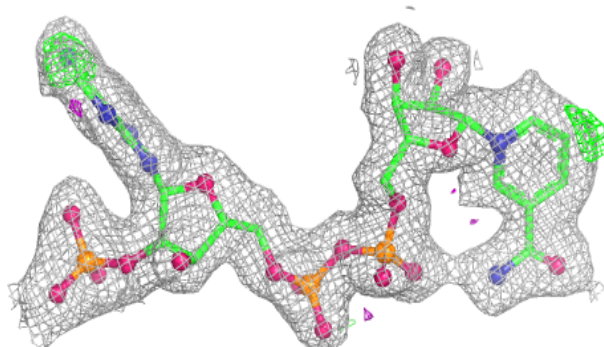


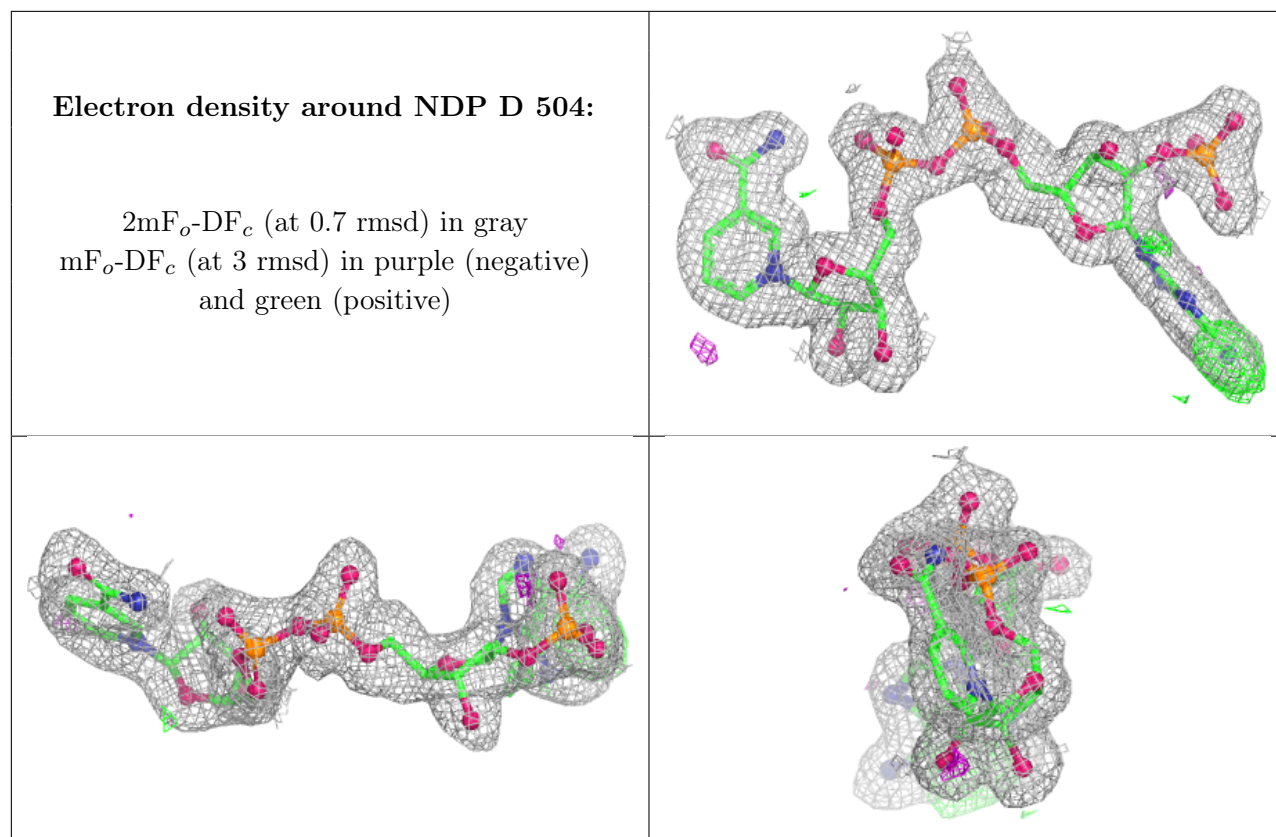
Electron density around ZMG C 603:

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

**Electron density around NDP C 503:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.