



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:12 PM UTC

PDB ID : 2XDR / pdb_00002xdr
Title : CRYSTALLOGRAPHIC STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE MUTANT E252A FROM PSEUDOMONAS AERUGINOSA
Authors : Diaz-Sanchez, A.G.; Gonzalez-Segura, L.; Rudino-Pinera, E.; Lira-Rocha, A.; Munoz-Clares, R.A.
Deposited on : 2010-05-06
Resolution : 2.30 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

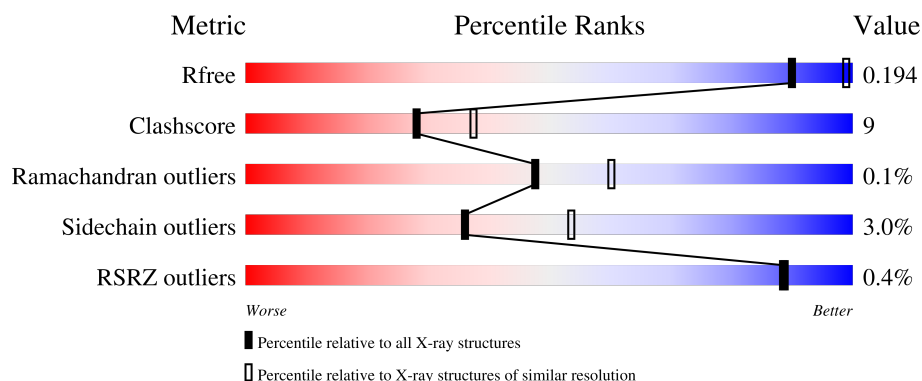
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	489	85% 13% .
1	B	489	% 83% 15% .
1	C	489	% 82% 17% .
1	D	489	86% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TOE	A	1492	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17057 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 BETAINE ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	6	0
			3782	2373	665	729	15			
1	B	489	Total	C	N	O	S	0	4	0
			3775	2369	667	724	15			
1	C	489	Total	C	N	O	S	0	5	0
			3792	2379	669	728	16			
1	D	489	Total	C	N	O	S	0	6	0
			3815	2390	675	735	15			

There are 4 discrepancies between the modelled and reference sequences:

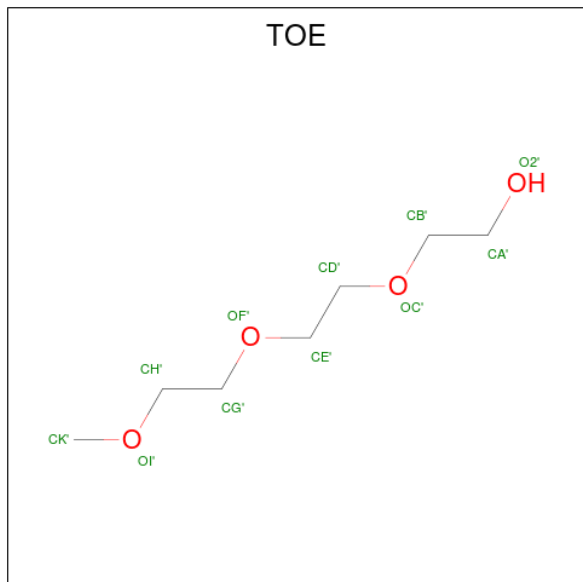
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	GLU	engineered mutation	UNP Q9HTJ1
B	252	ALA	GLU	engineered mutation	UNP Q9HTJ1
C	252	ALA	GLU	engineered mutation	UNP Q9HTJ1
D	252	ALA	GLU	engineered mutation	UNP Q9HTJ1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: $C_7H_{16}O_4$).

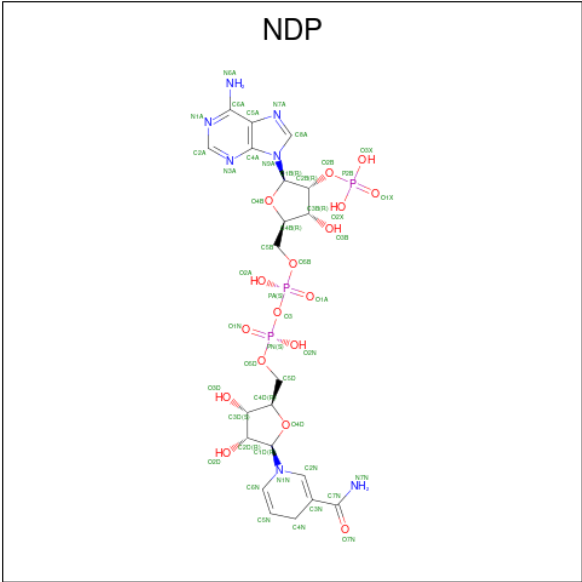


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	C	2	Total	K	0	0
			2	2		
4	D	2	Total	K	0	0
			2	2		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

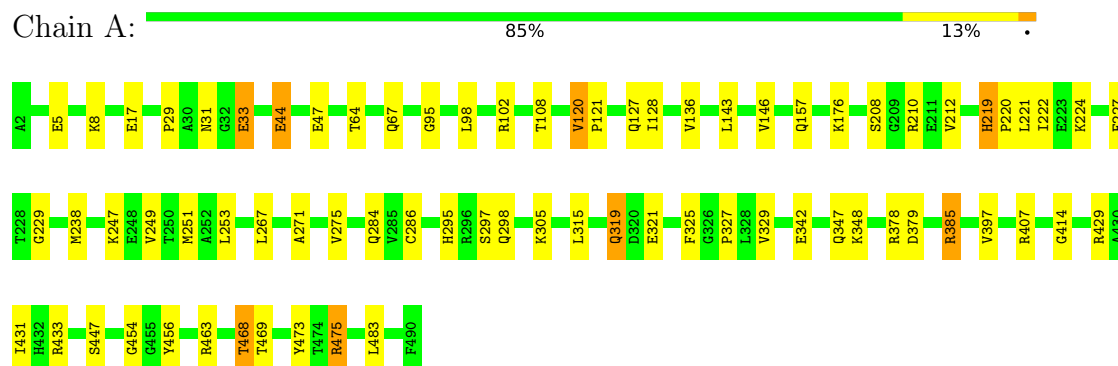
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	545	Total	O	0	0
			545	545		
6	B	390	Total	O	0	0
			390	390		
6	C	337	Total	O	0	0
			337	337		
6	D	410	Total	O	0	0
			410	410		

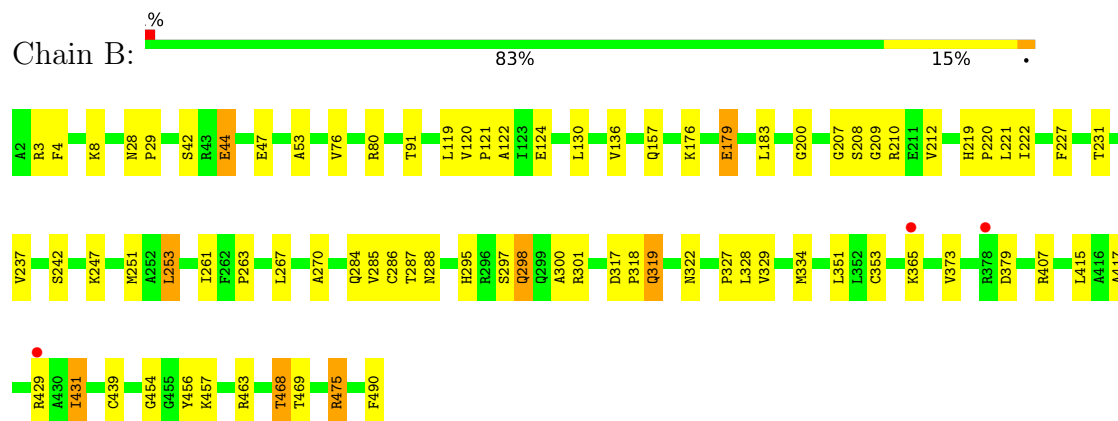
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

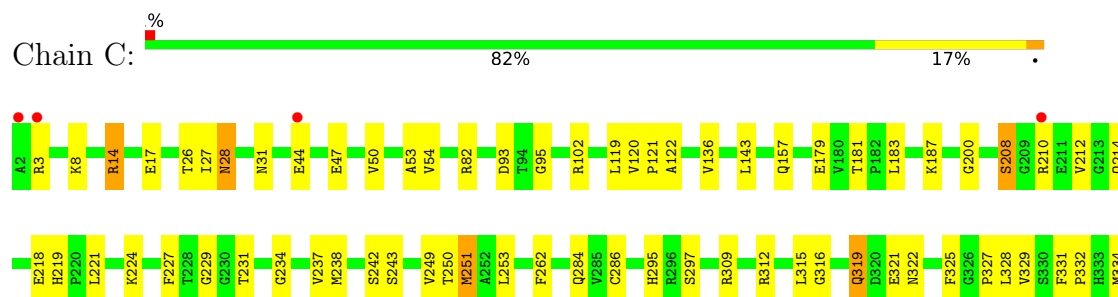
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE

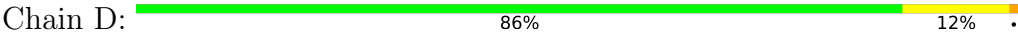


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE





● Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.56Å 151.56Å 242.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 2.30 29.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.88-2.30) 97.6 (29.88-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.160 , 0.200 0.153 , 0.194	Depositor DCC
R_{free} test set	7020 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17057	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: GOL, K, TOE, 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	0.43	0/3853	0.77	3/5221 (0.1%)
1	B	0.38	0/3843	0.75	3/5207 (0.1%)
1	C	0.37	0/3860	0.75	6/5229 (0.1%)
1	D	0.40	0/3883	0.76	3/5259 (0.1%)
All	All	0.39	0/15439	0.75	15/20916 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	HIS	CA-C-N	7.01	127.00	119.28
1	D	219	HIS	C-N-CA	7.01	127.00	119.28
1	C	457	LYS	CB-CA-C	-5.88	109.77	116.54
1	C	28	ASN	CA-C-N	5.68	125.35	119.56
1	C	28	ASN	C-N-CA	5.68	125.35	119.56
1	A	219	HIS	CA-C-N	5.42	125.51	119.87
1	A	219	HIS	C-N-CA	5.42	125.51	119.87
1	B	183	LEU	N-CA-C	5.39	116.97	111.14
1	B	457	LYS	CB-CA-C	-5.36	109.41	115.79
1	D	457	LYS	CB-CA-C	-5.35	109.42	115.79
1	A	120	VAL	CB-CA-C	-5.25	108.72	113.70
1	B	130	LEU	N-CA-C	-5.14	106.69	113.12
1	C	183	LEU	N-CA-C	5.11	116.53	110.97
1	C	262	PHE	CA-C-N	5.06	124.78	119.82
1	C	262	PHE	C-N-CA	5.06	124.78	119.82

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	3782	0	3753	69	1
1	B	3775	0	3751	67	0
1	C	3792	0	3765	79	0
1	D	3815	0	3779	57	0
2	A	6	0	8	1	0
2	B	24	0	32	4	0
2	C	30	0	40	6	0
2	D	24	0	32	3	0
3	A	11	0	16	7	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	27	0	11	3	0
5	B	27	0	11	2	0
5	C	27	0	11	3	0
5	D	27	0	11	2	0
6	A	545	0	0	22	0
6	B	390	0	0	15	0
6	C	337	0	0	14	0
6	D	410	0	0	13	0
All	All	17057	0	15220	271	1

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 9.

All (271) 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:301[B]:ARG:HH21	1:B:301[B]:ARG:HG3	1.07	1.15
1:A:98:LEU:HD22	6:A:2374:HOH:O	1.55	1.04
1:A:219:HIS:HD2	1:A:221:LEU:H	1.14	0.94
1:C:27:ILE:HG22	1:C:28:ASN:H	1.30	0.93
1:B:301[B]:ARG:HG3	1:B:301[B]:ARG:NH2	1.85	0.85
1:D:284:GLN:HE22	1:D:329:VAL:H	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:HIS:HD2	1:D:221:LEU:H	1.26	0.83
1:C:143:LEU:HD23	1:C:475:ARG:HG2	1.60	0.82
6:C:2115:HOH:O	1:D:468:THR:HG22	1.78	0.81
1:B:298:GLN:HA	1:B:301[B]:ARG:NH2	1.96	0.81
1:B:261:ILE:HD13	1:B:270:ALA:HB1	1.63	0.80
1:B:176:LYS:HD2	1:B:212:VAL:HG13	1.63	0.79
1:C:400:ASP:HB3	6:C:2251:HOH:O	1.83	0.78
1:C:219:HIS:HD2	1:C:221:LEU:H	1.31	0.77
1:C:27:ILE:HG22	1:C:28:ASN:N	1.98	0.77
1:B:298:GLN:HA	1:B:301[B]:ARG:HH22	1.49	0.77
1:A:468:THR:HG22	6:B:2182:HOH:O	1.85	0.77
1:A:468:THR:HG23	6:A:2513:HOH:O	1.85	0.76
6:A:2224:HOH:O	1:B:468:THR:HG22	1.85	0.75
1:A:286[A]:CYS:SG	6:A:2310:HOH:O	2.43	0.74
1:A:157:GLN:OE1	3:A:1492:TOE:H4	1.87	0.74
1:B:286[A]:CYS:SG	6:B:2251:HOH:O	2.46	0.74
1:A:176:LYS:HD2	1:A:212:VAL:HG13	1.70	0.74
1:B:219:HIS:HD2	1:B:221:LEU:H	1.34	0.73
1:B:379:ASP:OD2	1:B:407:ARG:HD2	1.88	0.73
1:A:284:GLN:HE22	1:A:329:VAL:H	1.33	0.73
1:B:284:GLN:HE22	1:B:329:VAL:H	1.37	0.72
1:A:219:HIS:CD2	1:A:221:LEU:H	2.05	0.72
1:C:187:LYS:NZ	2:C:1491:GOL:H12	2.06	0.71
1:C:284:GLN:HE22	1:C:329:VAL:H	1.38	0.71
1:B:267:LEU:HD11	1:B:298:GLN:HG2	1.73	0.71
1:D:157:GLN:OE1	2:D:1492:GOL:H12	1.91	0.70
1:C:219:HIS:CD2	1:C:221:LEU:H	2.10	0.70
1:C:27:ILE:CG2	1:C:28:ASN:H	2.05	0.69
1:D:219:HIS:CD2	1:D:221:LEU:H	2.10	0.69
1:A:447:SER:H	3:A:1492:TOE:H16	1.57	0.68
1:D:468:THR:HG23	6:D:2373:HOH:O	1.93	0.67
2:B:1494:GOL:H31	6:B:2384:HOH:O	1.93	0.67
1:D:379:ASP:OD2	1:D:407:ARG:HD2	1.93	0.67
1:B:219:HIS:CD2	1:B:221:LEU:H	2.12	0.67
1:A:456:TYR:CZ	1:B:475:ARG:HD3	2.31	0.66
1:A:295:HIS:CD2	1:A:297:SER:H	2.15	0.65
1:A:29:PRO:HG3	6:A:2388:HOH:O	1.97	0.65
1:A:475:ARG:HD3	1:B:456:TYR:CZ	2.32	0.65
2:D:1491:GOL:H31	6:D:2399:HOH:O	1.97	0.64
1:B:212:VAL:HB	6:B:2074:HOH:O	1.97	0.64
1:C:446:GLU:OE1	6:C:2289:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14[B]:ARG:HH11	1:D:14[B]:ARG:CG	2.10	0.64
1:A:447:SER:H	3:A:1492:TOE:CK'	2.11	0.64
1:A:143:LEU:HD23	1:A:475:ARG:HG2	1.79	0.63
1:C:234:GLY:C	1:C:251[B]:MET:HE1	2.24	0.63
1:D:295:HIS:CD2	1:D:297:SER:H	2.17	0.63
2:D:1491:GOL:H11	6:D:2399:HOH:O	1.99	0.63
1:B:47:GLU:OE1	1:B:219:HIS:HE1	1.82	0.62
1:A:212:VAL:HB	6:A:2090:HOH:O	1.99	0.62
2:A:1491:GOL:H12	3:A:1492:TOE:H5	1.82	0.62
1:C:187:LYS:HZ3	2:C:1491:GOL:H12	1.62	0.62
1:C:157:GLN:OE1	2:C:1492:GOL:H12	2.00	0.62
1:C:295:HIS:HD2	1:C:297:SER:OG	1.83	0.61
1:C:31:ASN:O	1:C:365:LYS:HG2	2.00	0.61
1:C:456:TYR:CZ	1:D:475:ARG:HD3	2.35	0.61
1:D:284:GLN:HE22	1:D:329:VAL:N	1.97	0.61
1:D:5:GLU:HG2	6:D:2398:HOH:O	2.01	0.60
1:A:483:LEU:O	1:D:429[C]:ARG:NH2	2.35	0.59
1:A:284:GLN:HE22	1:A:329:VAL:N	2.00	0.59
1:D:261:ILE:HD12	1:D:270:ALA:HB1	1.84	0.59
1:A:229:GLY:O	1:A:253:LEU:HA	2.02	0.59
1:D:14[B]:ARG:HH11	1:D:14[B]:ARG:HG2	1.67	0.59
1:B:468:THR:HG23	6:B:2359:HOH:O	2.02	0.58
1:C:238:MET:HE3	1:C:249[A]:VAL:HG21	1.85	0.58
1:C:231:THR:HA	1:C:253:LEU:HD13	1.85	0.58
1:C:50:VAL:O	1:C:54:VAL:HG23	2.04	0.58
1:B:208:SER:HB2	6:B:2242:HOH:O	2.04	0.57
1:C:328:LEU:HD12	1:C:334:MET:HA	1.86	0.57
1:A:475:ARG:NH1	6:A:2520:HOH:O	2.04	0.57
1:B:231:THR:HA	1:B:253:LEU:HG	1.86	0.57
2:B:1493:GOL:H12	6:B:2007:HOH:O	2.04	0.57
1:C:234:GLY:CA	1:C:251[B]:MET:HE1	2.35	0.57
1:C:295:HIS:CD2	1:C:297:SER:H	2.24	0.56
1:B:463:ARG:HB2	6:B:2359:HOH:O	2.06	0.56
1:C:284:GLN:HE22	1:C:329:VAL:N	2.04	0.56
1:D:47:GLU:OE1	1:D:219:HIS:HE1	1.89	0.56
1:B:328:LEU:HD12	1:B:334:MET:HA	1.88	0.56
1:D:44[A]:GLU:HG3	6:D:2091:HOH:O	2.05	0.56
1:D:82:ARG:NH2	6:D:2155:HOH:O	2.32	0.56
1:A:102:ARG:NH2	1:A:321:GLU:HG2	2.20	0.55
1:A:379:ASP:OD2	1:A:407:ARG:HD2	2.07	0.55
1:B:157:GLN:OE1	2:B:1492:GOL:H12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249[A]:VAL:HG22	6:C:2182:HOH:O	2.06	0.55
1:B:176:LYS:HD2	1:B:212:VAL:CG1	2.34	0.55
1:C:242:SER:OG	1:D:238:MET:HE2	2.07	0.55
1:C:251[B]:MET:HE3	1:C:253:LEU:HD21	1.89	0.55
1:B:179:GLU:HG3	1:B:207:GLY:O	2.06	0.55
1:C:237:VAL:HG12	1:C:251[A]:MET:HE1	1.88	0.54
1:D:14[B]:ARG:HG2	1:D:14[B]:ARG:NH1	2.21	0.54
1:A:397:VAL:O	1:A:407:ARG:NH2	2.39	0.54
1:A:227:PHE:HE1	5:A:5502:NDP:O4B	1.89	0.54
1:B:210:ARG:HG3	6:B:2242:HOH:O	2.06	0.54
1:D:229:GLY:O	1:D:253:LEU:HA	2.08	0.54
1:B:219:HIS:CD2	1:B:220:PRO:HD2	2.43	0.54
1:B:122:ALA:HB2	1:C:119:LEU:HD21	1.90	0.53
1:C:397:VAL:O	1:C:407:ARG:NH2	2.41	0.53
1:D:249:VAL:HG11	1:D:251:MET:HE3	1.89	0.53
1:B:301[B]:ARG:HH21	1:B:301[B]:ARG:CG	1.96	0.53
1:B:227:PHE:HE1	5:B:5502:NDP:O4B	1.91	0.53
1:C:412:GLU:HG2	6:C:2132:HOH:O	2.09	0.52
1:D:318:PRO:HG3	1:D:327:PRO:HD2	1.91	0.52
1:C:227:PHE:HE1	5:C:5502:NDP:O4B	1.93	0.52
1:D:397:VAL:O	1:D:407:ARG:NH2	2.43	0.52
1:B:4:PHE:CD1	2:B:1493:GOL:H2	2.45	0.52
1:D:250:THR:HG21	6:D:2371:HOH:O	2.10	0.52
1:D:43:ARG:NH2	1:D:218[B]:GLU:OE1	2.43	0.51
1:A:429:ARG:HD3	6:A:2480:HOH:O	2.10	0.51
1:C:218:GLU:HG2	6:C:2178:HOH:O	2.10	0.51
1:A:47:GLU:OE1	1:A:219:HIS:HE1	1.93	0.51
1:A:319:GLN:HA	6:A:2374:HOH:O	2.10	0.51
1:B:42:SER:OG	1:B:44:GLU:HG2	2.10	0.51
1:C:417:ALA:O	1:C:439:CYS:HA	2.11	0.51
1:D:143:LEU:HD23	1:D:475:ARG:HG2	1.93	0.50
1:A:379:ASP:OD2	1:A:407:ARG:CD	2.59	0.50
1:C:378:ARG:NH1	6:C:2235:HOH:O	2.43	0.50
1:B:379:ASP:OD1	1:B:407:ARG:NH1	2.45	0.50
1:C:102:ARG:NH2	1:C:321:GLU:HG2	2.27	0.50
5:A:5502:NDP:H52A	6:A:2543:HOH:O	2.11	0.50
1:B:469:THR:HA	6:B:2361:HOH:O	2.12	0.50
1:C:102:ARG:HH21	1:C:321:GLU:HG2	1.76	0.50
1:C:219:HIS:CD2	1:C:221:LEU:HB2	2.46	0.50
1:A:210:ARG:HD3	6:A:2544:HOH:O	2.12	0.49
1:C:319:GLN:HE21	1:C:319:GLN:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HG12	1:B:251:MET:HE1	1.94	0.49
1:D:219:HIS:CD2	1:D:220:PRO:HD2	2.47	0.49
1:B:295:HIS:HD2	1:B:297:SER:OG	1.96	0.49
1:C:315:LEU:C	1:C:315:LEU:HD23	2.38	0.49
1:B:379:ASP:CG	1:B:407:ARG:HH11	2.20	0.49
1:D:14[B]:ARG:CG	1:D:14[B]:ARG:NH1	2.74	0.49
1:C:31:ASN:HB2	1:C:365:LYS:HD3	1.95	0.48
1:C:315:LEU:HA	1:C:325:PHE:O	2.13	0.48
1:D:14[B]:ARG:HH11	1:D:14[B]:ARG:CB	2.25	0.48
1:A:219:HIS:CD2	1:A:220:PRO:HD2	2.49	0.48
1:C:95:GLY:O	1:C:327:PRO:HD2	2.13	0.48
1:A:102:ARG:HH22	1:A:321:GLU:HG2	1.78	0.48
1:A:8:LYS:HE2	1:A:17:GLU:OE2	2.13	0.48
1:C:210:ARG:HG3	6:C:2334:HOH:O	2.14	0.48
5:C:5502:NDP:O3	6:C:2336:HOH:O	2.20	0.48
5:D:5502:NDP:H52A	6:D:2223:HOH:O	2.13	0.48
1:C:419:VAL:HG22	1:C:431:ILE:HD13	1.96	0.48
1:B:119:LEU:HD21	1:C:122:ALA:HB2	1.95	0.48
6:B:2194:HOH:O	1:C:433:ARG:HD2	2.13	0.48
1:C:475:ARG:HD3	1:D:456:TYR:CZ	2.49	0.48
1:D:152:TRP:CE3	1:D:329:VAL:HG11	2.49	0.47
1:D:301:ARG:HD3	6:D:2286:HOH:O	2.14	0.47
1:D:472:HIS:CE1	6:D:2374:HOH:O	2.67	0.47
1:A:321:GLU:HG3	6:A:2381:HOH:O	2.15	0.47
1:C:224:LYS:HE3	1:C:473:TYR:CZ	2.50	0.47
1:B:120:VAL:HB	1:B:121:PRO:HD3	1.95	0.47
1:B:353:CYS:HB2	1:B:373:VAL:H	1.80	0.47
1:C:120:VAL:HB	1:C:121:PRO:HD3	1.96	0.47
1:D:472:HIS:HE1	6:D:2374:HOH:O	1.98	0.47
1:A:146:VAL:HG12	1:A:224:LYS:HB3	1.97	0.46
1:B:286[B]:CYS:SG	1:B:287:THR:HG23	2.55	0.46
1:A:5:GLU:HG2	6:A:2002:HOH:O	2.15	0.46
1:A:44[A]:GLU:HG3	6:A:2097:HOH:O	2.15	0.46
1:B:318:PRO:HG3	1:B:327:PRO:HD2	1.98	0.46
1:C:8:LYS:HE2	1:C:17:GLU:OE2	2.15	0.46
1:D:249:VAL:CG1	1:D:251:MET:HE3	2.45	0.46
1:A:271:ALA:O	1:A:275[A]:VAL:HG22	2.15	0.46
1:C:348:LYS:NZ	6:C:2225:HOH:O	2.48	0.46
1:D:315:LEU:C	1:D:315:LEU:HD23	2.41	0.46
1:A:210:ARG:NH2	6:A:2294:HOH:O	2.48	0.46
1:B:76:VAL:O	1:B:80:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:HG22	6:A:2388:HOH:O	2.15	0.46
1:A:95:GLY:O	1:A:327:PRO:HD2	2.16	0.46
1:D:176:LYS:HD2	1:D:212:VAL:HG22	1.97	0.46
1:D:219:HIS:HA	1:D:220:PRO:HD3	1.75	0.46
1:C:47:GLU:OE1	1:C:219:HIS:HE1	1.98	0.46
1:D:14[B]:ARG:HH11	1:D:14[B]:ARG:HB3	1.80	0.46
1:B:285:VAL:HB	1:B:288:ASN:OD1	2.15	0.46
1:C:250:THR:C	1:C:251[B]:MET:HG2	2.41	0.45
1:B:319:GLN:HE21	1:B:319:GLN:HA	1.81	0.45
1:C:339:GLY:HA3	2:C:1495:GOL:H12	1.99	0.45
1:D:217:THR:HG21	1:D:237:VAL:HG13	1.99	0.45
1:D:327:PRO:HD3	1:D:368:TYR:CE1	2.51	0.45
1:B:301[B]:ARG:NH2	6:B:2279:HOH:O	2.49	0.45
1:B:208:SER:O	1:B:212:VAL:HG12	2.17	0.45
1:A:224:LYS:HE3	1:A:473:TYR:CE1	2.52	0.45
1:C:14:ARG:HE	1:C:14:ARG:HB3	1.60	0.45
1:C:234:GLY:O	1:C:251[B]:MET:HE1	2.17	0.45
1:A:222:ILE:O	1:A:247:LYS:HE3	2.17	0.45
1:D:14[B]:ARG:NH2	6:D:2023:HOH:O	2.50	0.45
1:B:44:GLU:H	1:B:44:GLU:CD	2.24	0.45
1:C:53:ALA:HA	1:C:200:GLY:O	2.16	0.45
1:C:295:HIS:HE1	1:C:399:ASP:O	2.00	0.44
1:A:267:LEU:HB3	1:A:305:LYS:HD2	1.99	0.44
1:A:342:GLU:HG2	6:A:2400:HOH:O	2.16	0.44
1:C:229:GLY:O	1:C:253:LEU:HA	2.17	0.44
1:B:53:ALA:HA	1:B:200:GLY:O	2.17	0.44
1:A:454:GLY:HA3	1:A:463:ARG:HD3	2.00	0.44
1:C:44[A]:GLU:HG3	6:C:2033:HOH:O	2.16	0.44
1:A:127:GLN:C	1:A:128:ILE:HG13	2.42	0.44
1:C:214:GLN:O	1:C:218:GLU:HG3	2.17	0.44
5:C:5502:NDP:H52A	6:C:2335:HOH:O	2.17	0.44
1:B:365:LYS:HB3	1:B:365:LYS:HE3	1.73	0.44
1:A:219:HIS:HA	1:A:220:PRO:HD3	1.73	0.44
1:C:187:LYS:HZ1	2:C:1491:GOL:H12	1.81	0.44
1:C:331:PHE:N	1:C:332:PRO:CD	2.81	0.44
1:A:120:VAL:HB	1:A:121:PRO:HD3	2.00	0.43
1:D:284:GLN:NE2	1:D:329:VAL:H	2.06	0.43
1:B:417:ALA:O	1:B:439:CYS:HA	2.19	0.43
1:C:243:SER:HB3	1:D:239:ALA:HB2	2.00	0.43
3:A:1492:TOE:H2	6:A:2342:HOH:O	2.19	0.43
1:D:147:ALA:HB3	1:D:225:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:OD1	1:A:33:GLU:HB3	2.18	0.43
3:A:1492:TOE:H15	6:A:2086:HOH:O	2.18	0.43
1:B:263:PRO:HD2	6:B:2331:HOH:O	2.19	0.43
1:C:295:HIS:CD2	1:C:297:SER:OG	2.68	0.43
1:A:227:PHE:HB3	1:A:251:MET:HE2	2.00	0.43
1:B:284:GLN:HE22	1:B:329:VAL:N	2.12	0.43
1:C:179:GLU:OE1	1:C:208:SER:HB2	2.17	0.43
1:C:464:GLU:OE1	2:C:1493:GOL:H31	2.18	0.43
1:A:102:ARG:HH22	1:A:321:GLU:CG	2.32	0.42
1:A:385:ARG:HB3	1:A:385:ARG:HH11	1.84	0.42
1:C:82:ARG:HD3	6:C:2077:HOH:O	2.18	0.42
1:C:93:ASP:O	1:C:181:THR:HG22	2.19	0.42
1:A:108:THR:HG21	3:A:1492:TOE:H12	2.01	0.42
1:A:347:GLN:O	1:A:348:LYS:HB2	2.18	0.42
1:B:454:GLY:HA3	1:B:463:ARG:HD3	2.01	0.42
1:C:379:ASP:OD2	1:C:407:ARG:CD	2.67	0.42
1:C:379:ASP:OD2	1:C:407:ARG:HD2	2.18	0.42
1:C:475:ARG:H	1:C:475:ARG:HG3	1.58	0.42
1:A:275[B]:VAL:HG12	1:B:490:PHE:CD2	2.53	0.42
1:D:263:PRO:HA	1:D:298:GLN:OE1	2.19	0.42
1:A:295:HIS:HD2	1:A:297:SER:OG	2.02	0.42
1:B:351:LEU:HD11	1:B:353:CYS:O	2.19	0.42
1:B:300:ALA:HB3	6:B:2279:HOH:O	2.20	0.42
1:C:286[A]:CYS:SG	6:C:2175:HOH:O	2.62	0.42
1:C:295:HIS:HD2	1:C:297:SER:H	1.67	0.42
1:B:28:ASN:HA	1:B:29:PRO:HD2	1.96	0.42
1:B:222:ILE:O	1:B:247:LYS:HE3	2.20	0.42
1:D:245:SER:O	1:D:246:LEU:HB2	2.20	0.42
1:A:64:THR:OG1	1:A:67:GLN:HG3	2.20	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.84	0.42
1:A:315:LEU:HA	1:A:325:PHE:O	2.20	0.41
1:D:227:PHE:HB3	1:D:251:MET:HE2	2.02	0.41
1:A:238:MET:HB3	1:B:242:SER:HB3	2.01	0.41
1:B:286[B]:CYS:SG	1:B:415:LEU:HD21	2.60	0.41
1:D:83:ASN:ND2	1:D:106:ILE:HB	2.35	0.41
1:D:419:VAL:HG22	1:D:431:ILE:HD13	2.02	0.41
1:A:208[A]:SER:O	1:A:212:VAL:HG12	2.20	0.41
1:B:124:GLU:OE1	1:D:126:GLU:OE2	2.37	0.41
1:B:317:ASP:HA	1:B:318:PRO:HD3	1.96	0.41
1:C:315:LEU:HD23	1:C:316:GLY:N	2.35	0.41
1:C:431:ILE:HG13	1:C:439:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ALA:HB3	6:D:2288:HOH:O	2.19	0.41
1:C:31:ASN:O	1:C:365:LYS:O	2.39	0.41
1:C:309:ARG:O	1:C:312:ARG:HG2	2.21	0.41
1:D:295:HIS:HD2	1:D:297:SER:H	1.65	0.41
1:A:284:GLN:NE2	1:A:329:VAL:H	2.09	0.41
1:C:3[C]:ARG:H	1:C:3[C]:ARG:HG2	1.57	0.41
1:A:433:ARG:HD2	6:A:2484:HOH:O	2.20	0.41
1:B:431:ILE:HD12	1:B:431:ILE:HA	1.88	0.41
1:A:238:MET:HG3	1:A:249:VAL:HG21	2.04	0.40
1:A:227:PHE:CE1	5:A:5502:NDP:O4B	2.72	0.40
1:A:298:GLN:NE2	6:A:2327:HOH:O	2.40	0.40
1:B:209:GLY:HA3	5:B:5502:NDP:C4A	2.51	0.40
1:B:295:HIS:CD2	1:B:297:SER:H	2.39	0.40
1:D:227:PHE:CE1	5:D:5502:NDP:O4B	2.74	0.40
1:A:98:LEU:HD21	1:A:102:ARG:NH1	2.36	0.40
1:D:351:LEU:HD21	1:D:354:GLY:O	2.20	0.40
1:D:454:GLY:HA3	1:D:463:ARG:HD3	2.02	0.40
1:A:469:THR:HA	6:A:2516:HOH:O	2.21	0.40
1:B:468:THR:CG2	6:B:2359:HOH:O	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ARG:NH1	1:A:378:ARG:NH1[6_555]	2.15	0.05

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	493/489 (101%)	476 (97%)	16 (3%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	491/489 (100%)	472 (96%)	19 (4%)	0	100	100
1	C	493/489 (101%)	474 (96%)	19 (4%)	0	100	100
1	D	495/489 (101%)	478 (97%)	16 (3%)	1 (0%)	43	55
All	All	1972/1956 (101%)	1900 (96%)	70 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	GLY
1	D	414	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/389 (102%)	386 (98%)	9 (2%)	44	63
1	B	393/389 (101%)	377 (96%)	16 (4%)	27	41
1	C	395/389 (102%)	382 (97%)	13 (3%)	33	50
1	D	397/389 (102%)	384 (97%)	13 (3%)	33	50
All	All	1580/1556 (102%)	1529 (97%)	51 (3%)	36	51

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	44[A]	GLU
1	A	44[B]	GLU
1	A	136	VAL
1	A	319	GLN
1	A	385	ARG
1	A	431	ILE
1	A	468	THR
1	A	475	ARG

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Mol	Chain	Res	Type
1	B	3	ARG
1	B	8	LYS
1	B	44	GLU
1	B	91	THR
1	B	136[A]	VAL
1	B	136[B]	VAL
1	B	179	GLU
1	B	253	LEU
1	B	298	GLN
1	B	319	GLN
1	B	322	ASN
1	B	429[A]	ARG
1	B	429[B]	ARG
1	B	431	ILE
1	B	468	THR
1	B	475	ARG
1	C	14	ARG
1	C	26	THR
1	C	136	VAL
1	C	208	SER
1	C	212	VAL
1	C	251[A]	MET
1	C	251[B]	MET
1	C	319	GLN
1	C	322	ASN
1	C	348	LYS
1	C	385	ARG
1	C	431	ILE
1	C	475	ARG
1	D	26	THR
1	D	40	ARG
1	D	136	VAL
1	D	211	GLU
1	D	212	VAL
1	D	214[A]	GLN
1	D	214[B]	GLN
1	D	250	THR
1	D	251	MET
1	D	319	GLN
1	D	431	ILE
1	D	468	THR
1	D	475	ARG

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

Mol	Chain	Res	Type
1	A	219	HIS
1	A	284	GLN
1	A	295	HIS
1	A	319	GLN
1	B	127	GLN
1	B	219	HIS
1	B	284	GLN
1	B	295	HIS
1	B	319	GLN
1	C	7	GLN
1	C	219	HIS
1	C	284	GLN
1	C	295	HIS
1	C	319	GLN
1	D	219	HIS
1	D	284	GLN
1	D	295	HIS

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 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 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$
2	GOL	C	1494	-	5,5,5	0.52	0	5,5,5	1.30	1 (20%)
3	TOE	A	1492	-	10,10,10	0.53	0	9,9,9	1.38	0
2	GOL	C	1491	-	5,5,5	0.59	0	5,5,5	1.27	0
2	GOL	D	1494	-	5,5,5	0.52	0	5,5,5	1.10	0
2	GOL	B	1491	-	5,5,5	0.53	0	5,5,5	1.47	1 (20%)
5	NDP	D	5502	-	29,29,52	2.82	13 (44%)	44,45,80	2.02	15 (34%)
5	NDP	A	5502	-	29,29,52	2.84	13 (44%)	44,45,80	2.06	13 (29%)
2	GOL	D	1491	-	5,5,5	0.57	0	5,5,5	1.34	0
5	NDP	C	5502	-	29,29,52	2.85	13 (44%)	44,45,80	2.15	17 (38%)
2	GOL	A	1491	-	5,5,5	0.57	0	5,5,5	1.51	1 (20%)
2	GOL	C	1495	-	5,5,5	0.60	0	5,5,5	1.30	0
2	GOL	D	1493	-	5,5,5	0.61	0	5,5,5	1.44	1 (20%)
5	NDP	B	5502	-	29,29,52	2.87	13 (44%)	44,45,80	2.07	17 (38%)
2	GOL	D	1492	-	5,5,5	0.56	0	5,5,5	1.25	0
2	GOL	B	1494	-	5,5,5	0.57	0	5,5,5	1.32	0
2	GOL	C	1493	-	5,5,5	0.54	0	5,5,5	1.38	0
2	GOL	B	1493	-	5,5,5	0.57	0	5,5,5	1.30	0
2	GOL	B	1492	-	5,5,5	0.58	0	5,5,5	1.33	0
2	GOL	C	1492	-	5,5,5	0.56	0	5,5,5	1.32	0

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	GOL	C	1494	-	-	2/4/4/4	-
3	TOE	A	1492	-	-	4/8/8/8	-
2	GOL	C	1491	-	-	0/4/4/4	-
2	GOL	D	1494	-	-	1/4/4/4	-
2	GOL	B	1491	-	-	2/4/4/4	-
5	NDP	D	5502	-	-	3/15/31/77	0/3/3/5
5	NDP	A	5502	-	-	3/15/31/77	0/3/3/5
2	GOL	D	1491	-	-	3/4/4/4	-
5	NDP	C	5502	-	-	6/15/31/77	0/3/3/5
2	GOL	A	1491	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1495	-	-	0/4/4/4	-
2	GOL	D	1493	-	-	2/4/4/4	-
5	NDP	B	5502	-	-	3/15/31/77	0/3/3/5
2	GOL	D	1492	-	-	4/4/4/4	-
2	GOL	B	1494	-	-	2/4/4/4	-
2	GOL	C	1493	-	-	0/4/4/4	-
2	GOL	B	1493	-	-	1/4/4/4	-
2	GOL	B	1492	-	-	3/4/4/4	-
2	GOL	C	1492	-	-	2/4/4/4	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5502	NDP	C8A-N7A	7.09	1.45	1.31
5	B	5502	NDP	C8A-N7A	7.08	1.45	1.31
5	A	5502	NDP	C8A-N7A	7.01	1.45	1.31
5	D	5502	NDP	C8A-N7A	6.95	1.45	1.31
5	A	5502	NDP	C2A-N3A	5.34	1.43	1.33
5	D	5502	NDP	C2A-N3A	5.18	1.43	1.33
5	B	5502	NDP	C2A-N3A	5.14	1.43	1.33
5	B	5502	NDP	C6A-N6A	5.11	1.47	1.34
5	A	5502	NDP	C6A-N6A	5.10	1.47	1.34
5	C	5502	NDP	C2A-N3A	5.09	1.43	1.33
5	C	5502	NDP	C6A-N6A	5.07	1.47	1.34
5	D	5502	NDP	C6A-N6A	4.91	1.46	1.34
5	D	5502	NDP	PA-O1A	4.76	1.65	1.50
5	B	5502	NDP	PA-O1A	4.69	1.65	1.50
5	D	5502	NDP	P2B-O1X	4.59	1.64	1.50
5	C	5502	NDP	P2B-O1X	4.58	1.64	1.50
5	A	5502	NDP	PA-O1A	4.55	1.64	1.50
5	B	5502	NDP	P2B-O1X	4.49	1.64	1.50
5	C	5502	NDP	PA-O1A	4.44	1.64	1.50
5	A	5502	NDP	P2B-O1X	4.28	1.63	1.50
5	B	5502	NDP	P2B-O2B	4.06	1.66	1.59
5	B	5502	NDP	C3B-C4B	4.03	1.63	1.53
5	A	5502	NDP	P2B-O2B	3.94	1.66	1.59
5	D	5502	NDP	C3B-C4B	3.85	1.62	1.53
5	C	5502	NDP	P2B-O2B	3.85	1.66	1.59
5	C	5502	NDP	C3B-C4B	3.83	1.62	1.53
5	A	5502	NDP	C3B-C4B	3.81	1.62	1.53
5	D	5502	NDP	P2B-O2B	3.53	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5502	NDP	P2B-O2X	3.41	1.67	1.54
5	A	5502	NDP	P2B-O2X	3.37	1.67	1.54
5	C	5502	NDP	P2B-O2X	3.33	1.67	1.54
5	D	5502	NDP	P2B-O2X	3.26	1.66	1.54
5	D	5502	NDP	C4A-N9A	3.24	1.44	1.37
5	C	5502	NDP	C4A-N9A	3.17	1.44	1.37
5	A	5502	NDP	C4A-N9A	3.15	1.44	1.37
5	B	5502	NDP	C4A-N9A	3.05	1.44	1.37
5	B	5502	NDP	O4B-C4B	2.83	1.51	1.45
5	C	5502	NDP	O4B-C4B	2.83	1.51	1.45
5	A	5502	NDP	O4B-C4B	2.78	1.51	1.45
5	C	5502	NDP	P2B-O3X	-2.66	1.44	1.54
5	D	5502	NDP	O4B-C4B	2.65	1.50	1.45
5	D	5502	NDP	P2B-O3X	-2.64	1.45	1.54
5	B	5502	NDP	P2B-O3X	-2.62	1.45	1.54
5	A	5502	NDP	P2B-O3X	-2.62	1.45	1.54
5	C	5502	NDP	PA-O3	-2.58	1.45	1.54
5	B	5502	NDP	PA-O3	-2.45	1.45	1.54
5	A	5502	NDP	PA-O3	-2.39	1.45	1.54
5	D	5502	NDP	PA-O3	-2.37	1.46	1.54
5	D	5502	NDP	C2B-C1B	-2.34	1.47	1.53
5	A	5502	NDP	C2B-C1B	-2.19	1.47	1.53
5	B	5502	NDP	C2B-C1B	-2.18	1.47	1.53
5	C	5502	NDP	C2B-C1B	-2.09	1.48	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5502	NDP	N3A-C2A-N1A	-5.83	119.76	128.58
5	D	5502	NDP	N3A-C2A-N1A	-5.73	119.90	128.58
5	B	5502	NDP	N3A-C2A-N1A	-5.68	119.99	128.58
5	C	5502	NDP	N3A-C2A-N1A	-5.66	120.01	128.58
5	D	5502	NDP	C5A-C4A-N3A	-4.52	120.50	126.72
5	C	5502	NDP	C5A-C4A-N3A	-4.50	120.52	126.72
5	A	5502	NDP	C5A-C4A-N3A	-4.47	120.56	126.72
5	D	5502	NDP	N9A-C8A-N7A	-4.34	107.78	113.94
5	C	5502	NDP	N9A-C8A-N7A	-4.31	107.83	113.94
5	A	5502	NDP	N9A-C8A-N7A	-4.25	107.90	113.94
5	B	5502	NDP	N9A-C8A-N7A	-4.21	107.96	113.94
5	B	5502	NDP	C5A-C4A-N3A	-4.17	120.97	126.72
5	B	5502	NDP	C2B-C1B-N9A	-3.75	107.58	113.75
5	C	5502	NDP	O3B-C3B-C4B	3.57	121.33	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5502	NDP	O3B-C3B-C2B	3.42	120.77	111.19
5	A	5502	NDP	O3B-C3B-C4B	3.41	120.88	111.08
5	B	5502	NDP	O3B-C3B-C4B	3.39	120.82	111.08
5	D	5502	NDP	O3B-C3B-C4B	3.34	120.68	111.08
5	C	5502	NDP	C2A-N3A-C4A	3.15	119.53	111.83
5	D	5502	NDP	C2A-N3A-C4A	3.15	119.52	111.83
5	C	5502	NDP	O2B-C2B-C3B	3.12	122.86	111.68
5	A	5502	NDP	C2A-N3A-C4A	3.09	119.38	111.83
5	C	5502	NDP	C2B-C1B-N9A	-3.08	108.68	113.75
5	A	5502	NDP	O3B-C3B-C2B	3.05	119.71	111.19
5	B	5502	NDP	O2B-C2B-C3B	3.04	122.58	111.68
5	B	5502	NDP	C2A-N3A-C4A	3.00	119.16	111.83
5	C	5502	NDP	C5A-N7A-C8A	2.89	108.00	103.45
5	D	5502	NDP	C5A-N7A-C8A	2.86	107.94	103.45
5	A	5502	NDP	C2B-C1B-N9A	-2.84	109.07	113.75
5	A	5502	NDP	O2B-C2B-C3B	2.80	121.73	111.68
5	A	5502	NDP	O2B-C2B-C1B	2.80	119.90	110.05
5	A	5502	NDP	C5A-N7A-C8A	2.77	107.80	103.45
5	B	5502	NDP	C5A-N7A-C8A	2.73	107.74	103.45
5	C	5502	NDP	O3-PA-O5B	2.69	113.68	106.67
5	D	5502	NDP	C2B-C1B-N9A	-2.68	109.34	113.75
5	D	5502	NDP	O2B-C2B-C3B	2.66	121.23	111.68
5	D	5502	NDP	N3A-C4A-N9A	2.66	131.69	127.17
5	A	5502	NDP	N3A-C4A-N9A	2.65	131.67	127.17
5	C	5502	NDP	O2B-C2B-C1B	2.60	119.21	110.05
5	C	5502	NDP	O4B-C4B-C5B	2.56	117.54	109.33
5	D	5502	NDP	O4B-C4B-C3B	-2.51	100.17	105.15
5	C	5502	NDP	N3A-C4A-N9A	2.47	131.37	127.17
5	D	5502	NDP	O3B-C3B-C2B	2.46	118.08	111.19
5	B	5502	NDP	O4B-C4B-C3B	-2.46	100.27	105.15
5	B	5502	NDP	O2B-C2B-C1B	2.41	118.53	110.05
5	B	5502	NDP	O3B-C3B-C2B	2.40	117.92	111.19
2	A	1491	GOL	O3-C3-C2	2.36	121.00	110.38
5	A	5502	NDP	C4A-N9A-C8A	2.33	108.19	105.74
5	D	5502	NDP	C4A-N9A-C8A	2.32	108.17	105.74
5	B	5502	NDP	C4A-N9A-C8A	2.27	108.12	105.74
5	B	5502	NDP	O4B-C1B-N9A	2.26	112.43	108.09
5	C	5502	NDP	C4A-C5A-N7A	-2.25	108.01	110.58
5	B	5502	NDP	N3A-C4A-N9A	2.24	130.98	127.17
5	D	5502	NDP	C3B-C2B-C1B	-2.24	98.52	102.81
5	C	5502	NDP	C4A-N9A-C8A	2.21	108.06	105.74
2	B	1491	GOL	O3-C3-C2	2.17	120.16	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5502	NDP	O4B-C4B-C5B	2.16	116.27	109.33
5	B	5502	NDP	C4A-C5A-N7A	-2.14	108.13	110.58
2	D	1493	GOL	O1-C1-C2	2.14	120.00	110.38
5	C	5502	NDP	C5A-C4A-N9A	2.10	108.11	105.81
5	C	5502	NDP	O4B-C4B-C3B	-2.08	101.03	105.15
5	B	5502	NDP	C5A-C4A-N9A	2.05	108.05	105.81
5	A	5502	NDP	O4B-C4B-C3B	-2.04	101.10	105.15
5	D	5502	NDP	O4B-C1B-N9A	2.03	111.99	108.09
2	C	1494	GOL	O1-C1-C2	2.01	119.44	110.38
5	D	5502	NDP	C4A-C5A-N7A	-2.00	108.29	110.58

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1491	GOL	O1-C1-C2-C3
2	B	1491	GOL	O1-C1-C2-C3
2	B	1494	GOL	C1-C2-C3-O3
2	C	1492	GOL	C1-C2-C3-O3
2	C	1492	GOL	O2-C2-C3-O3
2	D	1491	GOL	C1-C2-C3-O3
2	D	1493	GOL	O1-C1-C2-C3
3	A	1492	TOE	OC'-CD'-CE'-OF'
5	B	5502	NDP	C3B-C2B-O2B-P2B
5	C	5502	NDP	C3B-C2B-O2B-P2B
5	B	5502	NDP	C1B-C2B-O2B-P2B
5	A	5502	NDP	C3B-C2B-O2B-P2B
5	D	5502	NDP	C3B-C2B-O2B-P2B
2	A	1491	GOL	C1-C2-C3-O3
2	B	1492	GOL	O1-C1-C2-C3
2	D	1491	GOL	O1-C1-C2-C3
2	D	1492	GOL	O1-C1-C2-C3
2	D	1492	GOL	C1-C2-C3-O3
2	D	1494	GOL	O1-C1-C2-C3
2	A	1491	GOL	O2-C2-C3-O3
2	B	1491	GOL	O1-C1-C2-O2
2	B	1494	GOL	O2-C2-C3-O3
2	D	1492	GOL	O2-C2-C3-O3
5	D	5502	NDP	C1B-C2B-O2B-P2B
2	A	1491	GOL	O1-C1-C2-O2
3	A	1492	TOE	O2'-CA'-CB'-OC'
5	D	5502	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	1494	GOL	O1-C1-C2-C3
2	C	1494	GOL	O1-C1-C2-O2
2	D	1492	GOL	O1-C1-C2-O2
5	C	5502	NDP	C1B-C2B-O2B-P2B
2	B	1492	GOL	O1-C1-C2-O2
3	A	1492	TOE	CD'-CE'-OF'-CG'
2	B	1493	GOL	O1-C1-C2-O2
3	A	1492	TOE	CE'-CD'-OC'-CB'
2	D	1493	GOL	O1-C1-C2-O2
5	C	5502	NDP	C2B-O2B-P2B-O1X
2	B	1492	GOL	O2-C2-C3-O3
5	C	5502	NDP	C2B-C1B-N9A-C8A
5	C	5502	NDP	C2B-O2B-P2B-O2X
5	C	5502	NDP	C2B-O2B-P2B-O3X
5	B	5502	NDP	C2B-C1B-N9A-C8A
5	A	5502	NDP	C2B-O2B-P2B-O1X
5	A	5502	NDP	C2B-C1B-N9A-C8A
2	D	1491	GOL	O2-C2-C3-O3

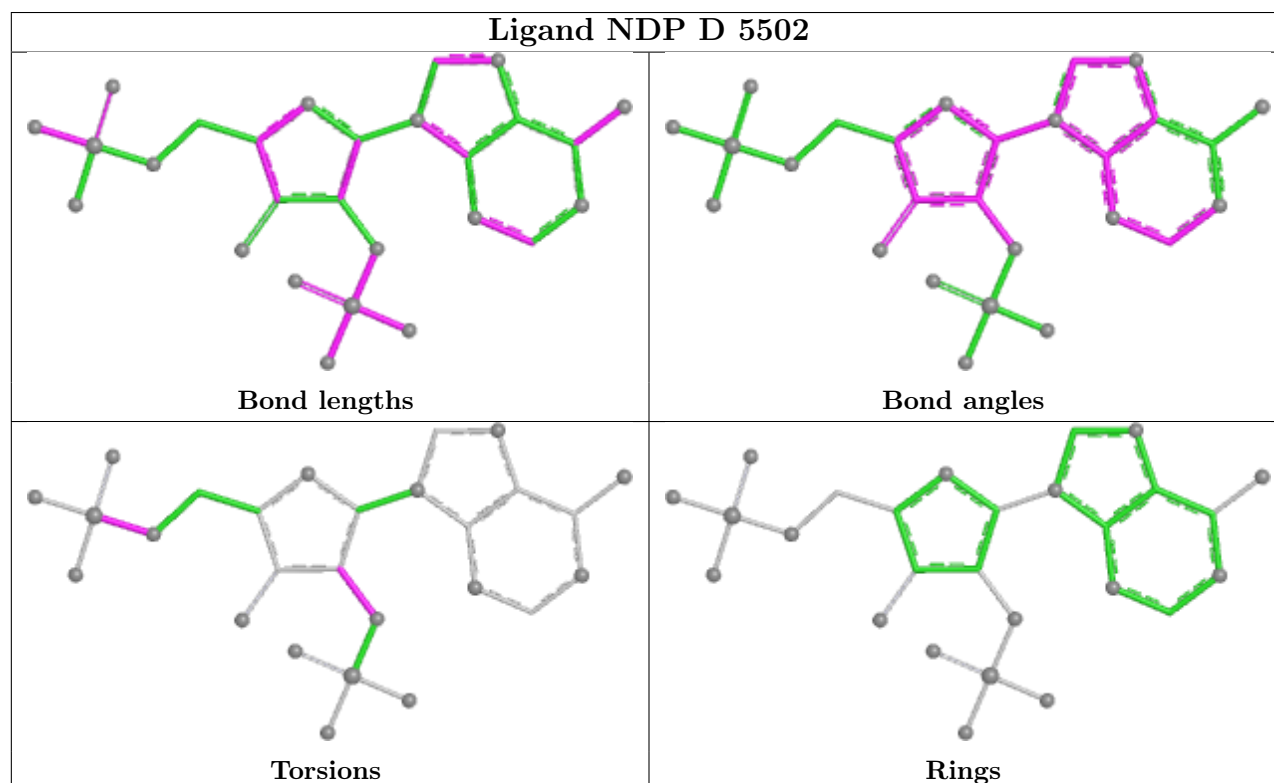
There are no ring outliers.

15 monomers are involved in 30 short contacts:

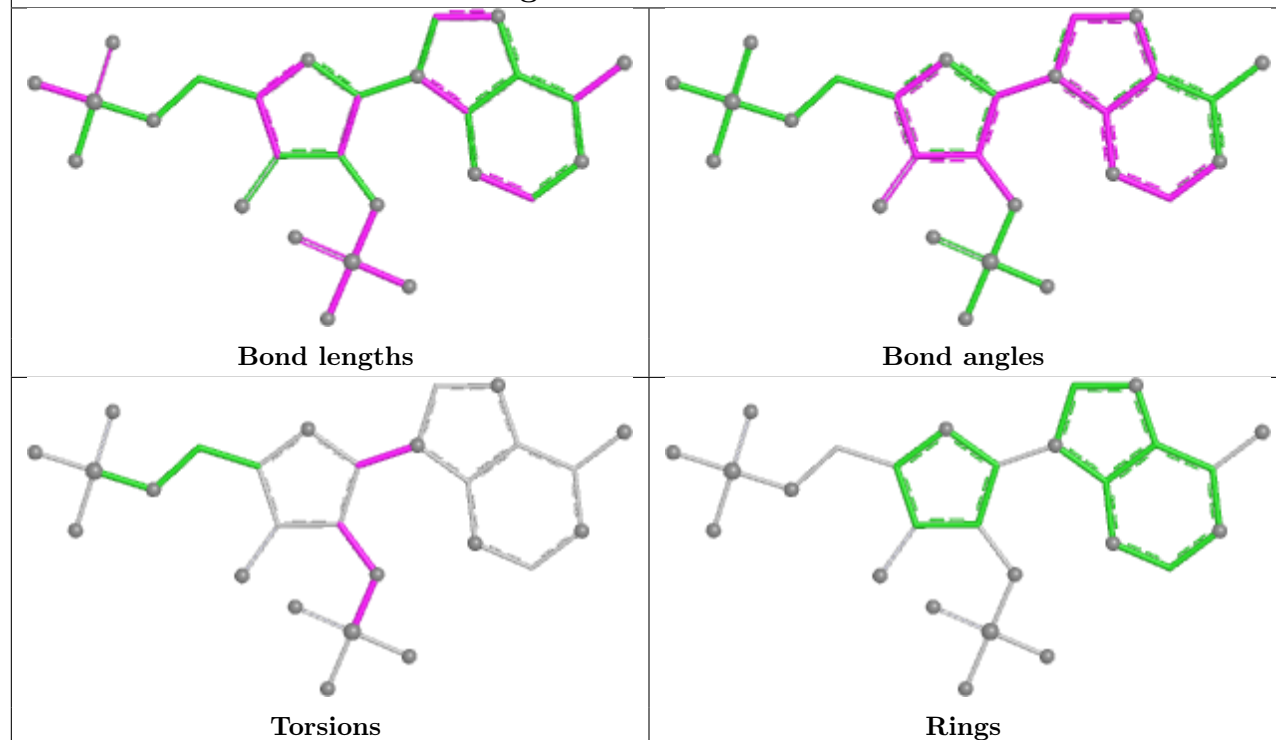
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1492	TOE	7	0
2	C	1491	GOL	3	0
5	D	5502	NDP	2	0
5	A	5502	NDP	3	0
2	D	1491	GOL	2	0
5	C	5502	NDP	3	0
2	A	1491	GOL	1	0
2	C	1495	GOL	1	0
5	B	5502	NDP	2	0
2	D	1492	GOL	1	0
2	B	1494	GOL	1	0
2	C	1493	GOL	1	0
2	B	1493	GOL	2	0
2	B	1492	GOL	1	0
2	C	1492	GOL	1	0

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

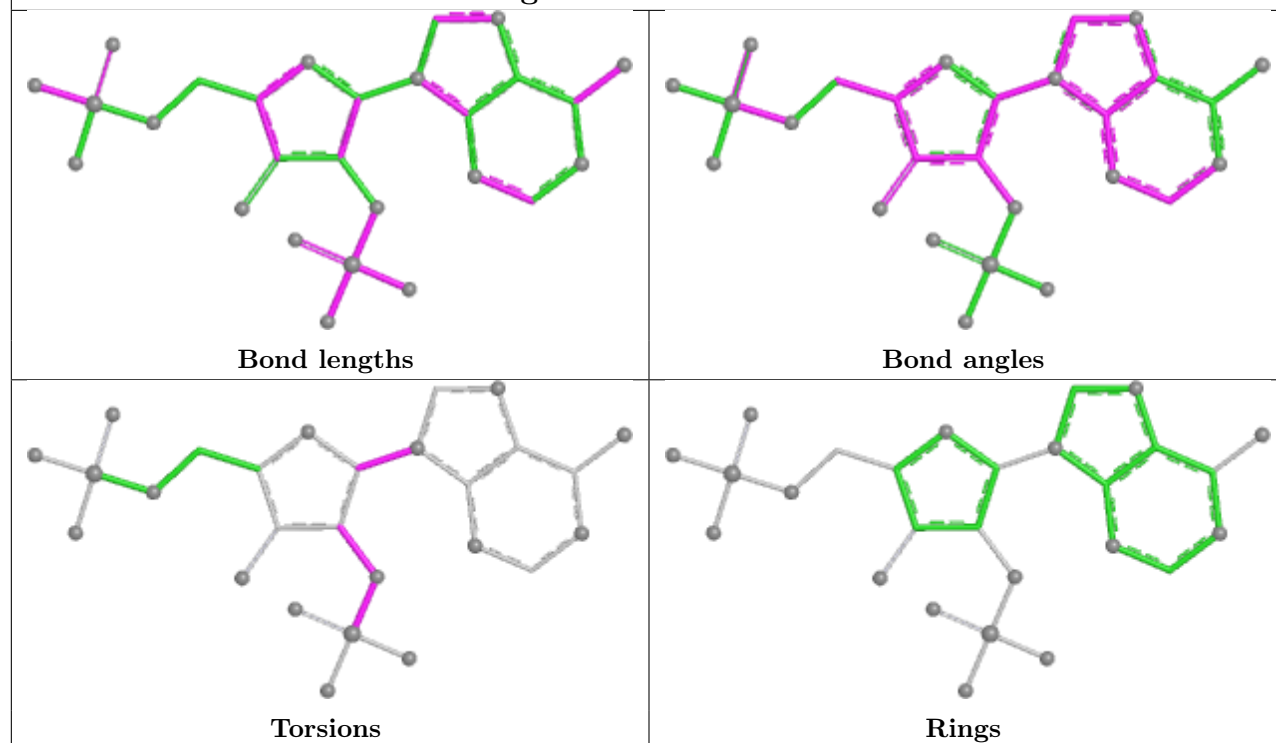
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

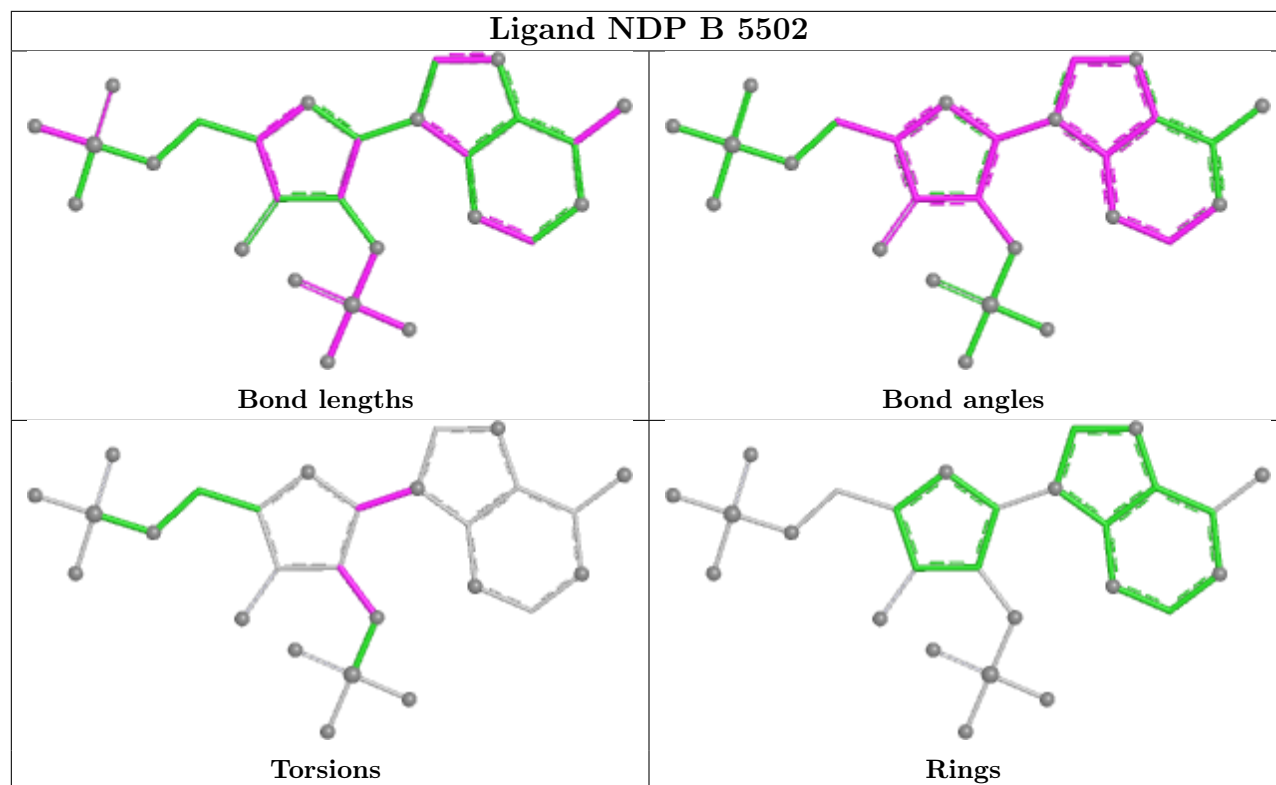


Ligand NDP A 5502



Ligand NDP C 5502





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	489/489 (100%)	-0.85	0 100 100	9, 25, 43, 78	6 (1%)
1	B	489/489 (100%)	-0.47	3 (0%) 85 86	7, 37, 62, 96	4 (0%)
1	C	489/489 (100%)	-0.51	5 (1%) 79 80	18, 39, 60, 92	5 (1%)
1	D	489/489 (100%)	-0.59	0 100 100	10, 33, 58, 79	6 (1%)
All	All	1956/1956 (100%)	-0.61	8 (0%) 88 89	7, 34, 59, 96	21 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3[A]	ARG	5.5
1	B	378	ARG	2.7
1	B	365	LYS	2.5
1	C	2	ALA	2.3
1	C	210	ARG	2.2
1	C	44[A]	GLU	2.2
1	B	429[A]	ARG	2.1
1	C	365	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 ⓘ

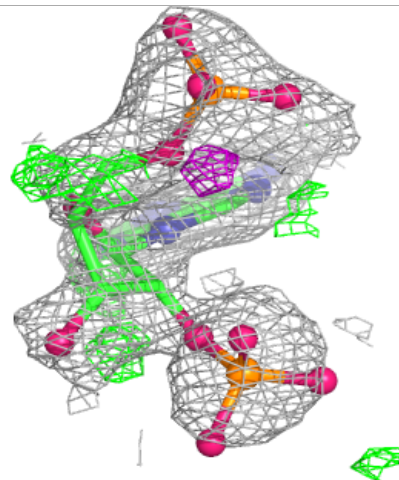
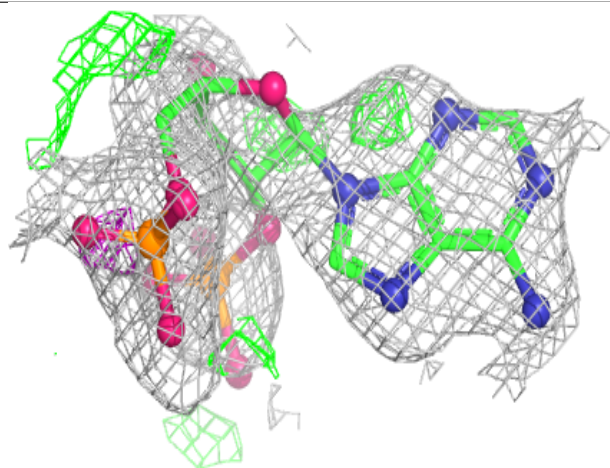
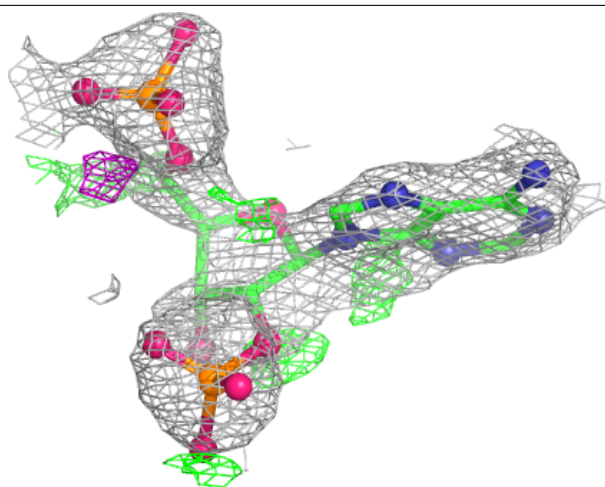
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	D	1493	6/6	0.81	0.17	57,60,76,84	0
2	GOL	C	1493	6/6	0.82	0.18	60,79,86,90	0
2	GOL	B	1491	6/6	0.82	0.20	61,64,66,71	0
2	GOL	C	1494	6/6	0.83	0.24	77,92,98,100	0
2	GOL	C	1491	6/6	0.85	0.12	70,72,75,78	0
2	GOL	C	1495	6/6	0.88	0.20	70,86,87,90	0
2	GOL	C	1492	6/6	0.88	0.14	49,58,68,73	0
5	NDP	B	5502	27/48	0.88	0.14	39,55,72,94	20
2	GOL	D	1494	6/6	0.89	0.14	53,56,60,62	0
4	K	C	1496	1/1	0.89	0.10	58,58,58,58	0
2	GOL	A	1491	6/6	0.89	0.14	36,48,55,60	0
5	NDP	C	5502	27/48	0.90	0.13	34,52,80,95	20
4	K	B	5500	1/1	0.91	0.11	68,68,68,68	0
3	TOE	A	1492	11/11	0.91	0.16	22,61,79,88	0
4	K	C	1497	1/1	0.92	0.12	74,74,74,74	0
5	NDP	A	5502	27/48	0.92	0.12	23,38,58,90	23
2	GOL	D	1492	6/6	0.93	0.12	54,67,71,74	0
2	GOL	B	1494	6/6	0.93	0.13	46,72,79,82	0
4	K	B	5501	1/1	0.94	0.08	50,50,50,50	0
2	GOL	D	1491	6/6	0.94	0.12	38,81,89,94	0
2	GOL	B	1493	6/6	0.94	0.11	62,65,67,68	0
4	K	D	1496	1/1	0.96	0.08	67,67,67,67	0
2	GOL	B	1492	6/6	0.96	0.09	61,63,73,76	0
4	K	A	1494	1/1	0.97	0.07	48,48,48,48	0
4	K	D	1495	1/1	0.97	0.06	41,41,41,41	0
4	K	A	1493	1/1	0.97	0.05	30,30,30,30	0
5	NDP	D	5502	27/48	0.97	0.07	22,33,54,87	12

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.

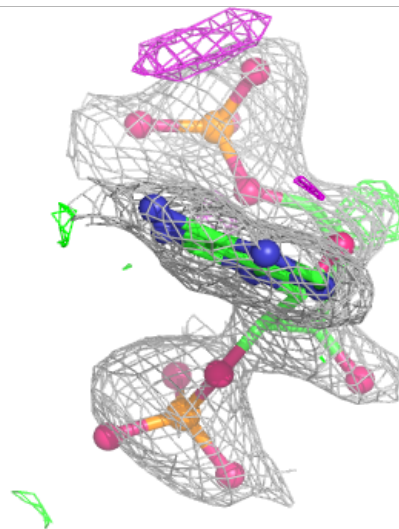
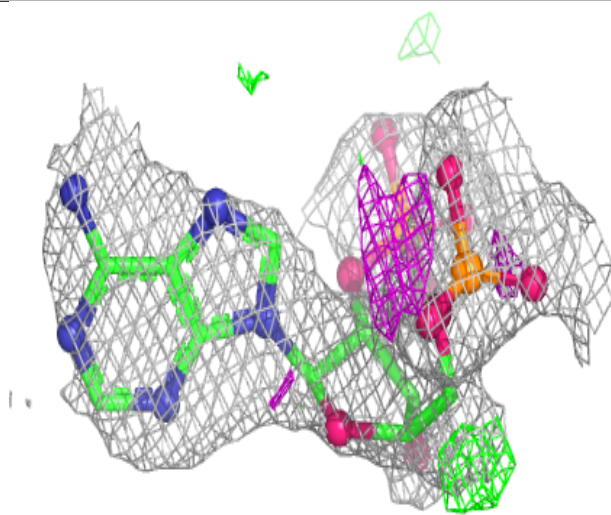
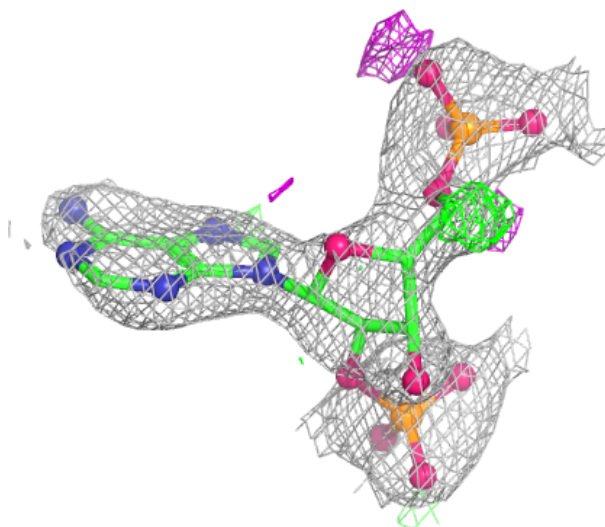
Electron density around NDP B 5502:

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



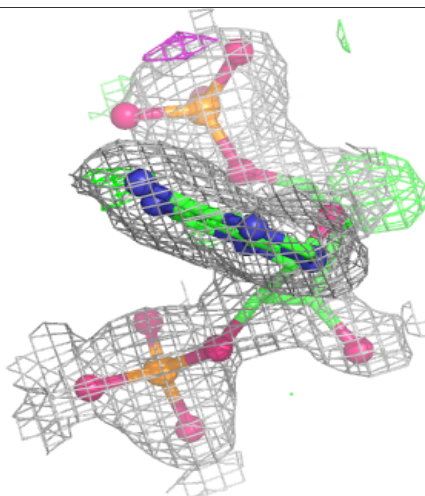
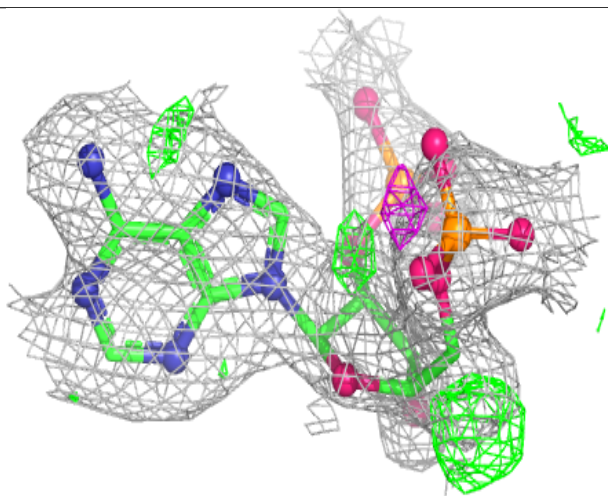
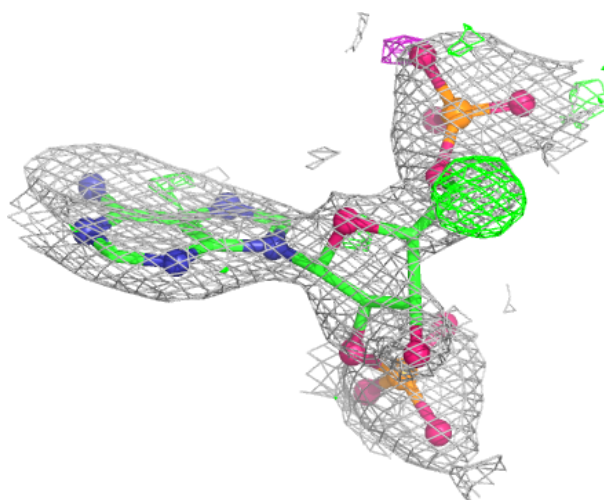
Electron density around NDP C 5502:

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



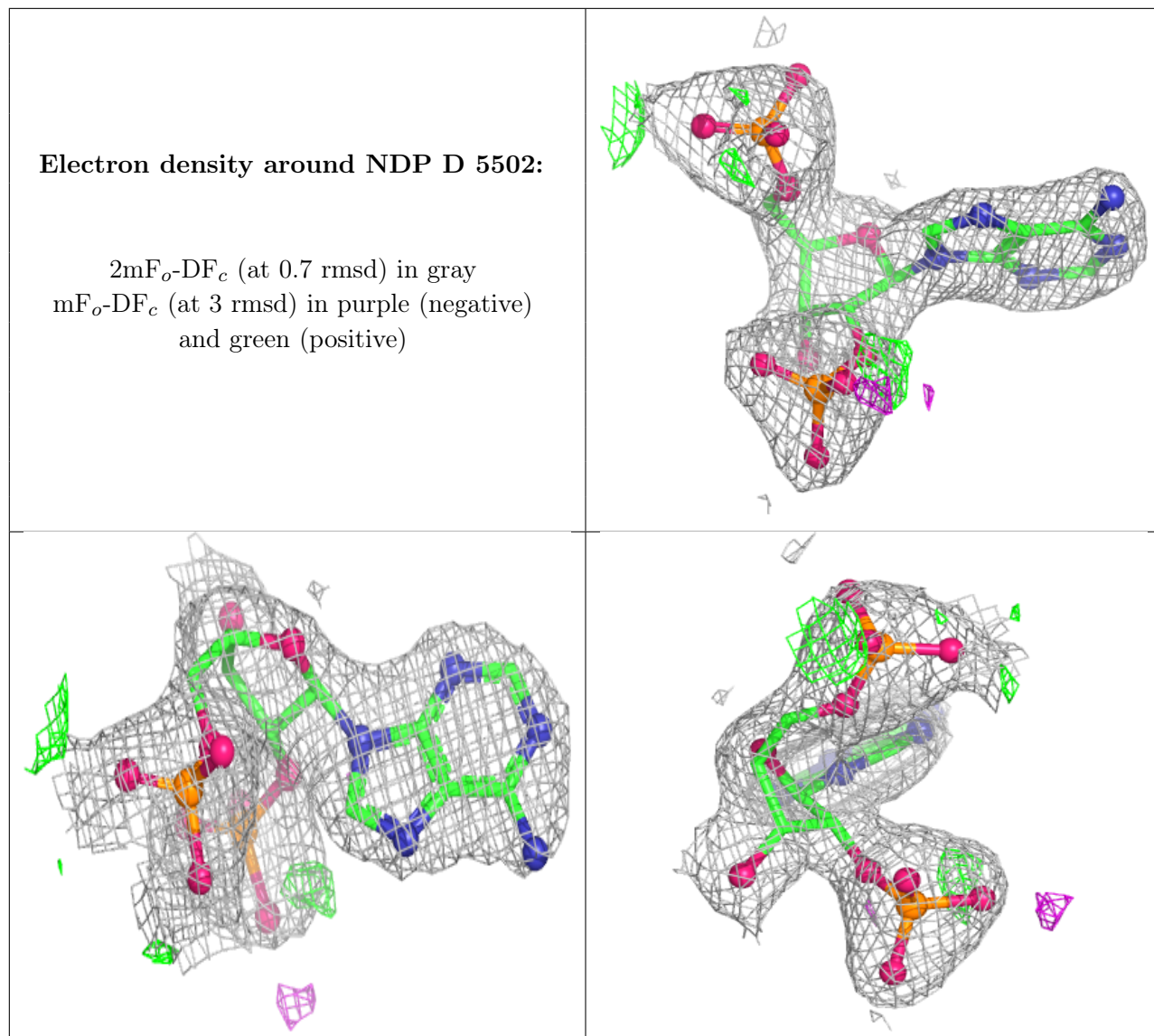
Electron density around NDP A 5502:

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



Electron density around NDP D 5502:

$2mF_o-DF_c$ (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.