



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 8VHA / pdb_00008vha
Title : Crystal Structure of Human IDH1 R132Q in complex with NADPH and Alpha-Ketoglutarate
Authors : Mealka, M.; Sohl, C.D.; Huxford, T.
Deposited on : 2023-12-31
Resolution : 2.28 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

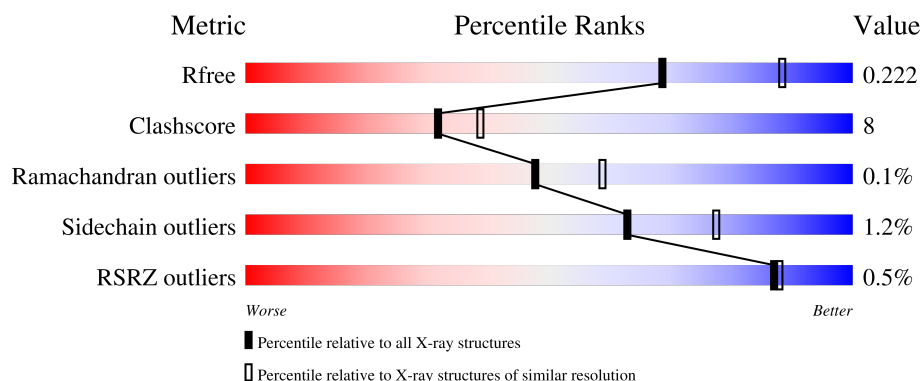
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	430	
1	B	430	
1	C	430	
1	D	430	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13870 atoms, of which 106 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	1	0
			3286	2087	557	623	19			
1	B	411	Total	C	N	O	S	0	1	0
			3262	2073	552	619	18			
1	C	412	Total	C	N	O	S	0	1	0
			3266	2077	550	620	19			
1	D	412	Total	C	N	O	S	0	0	0
			3260	2072	551	619	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP O75874
A	-14	HIS	-	expression tag	UNP O75874
A	-13	HIS	-	expression tag	UNP O75874
A	-12	HIS	-	expression tag	UNP O75874
A	-11	HIS	-	expression tag	UNP O75874
A	-10	HIS	-	expression tag	UNP O75874
A	-9	SER	-	expression tag	UNP O75874
A	-8	SER	-	expression tag	UNP O75874
A	-7	GLY	-	expression tag	UNP O75874
A	-6	LEU	-	expression tag	UNP O75874
A	-5	VAL	-	expression tag	UNP O75874
A	-4	PRO	-	expression tag	UNP O75874
A	-3	ARG	-	expression tag	UNP O75874
A	-2	GLY	-	expression tag	UNP O75874
A	-1	SER	-	expression tag	UNP O75874
A	0	HIS	-	expression tag	UNP O75874
A	132	GLN	ARG	engineered mutation	UNP O75874
B	-15	HIS	-	expression tag	UNP O75874
B	-14	HIS	-	expression tag	UNP O75874
B	-13	HIS	-	expression tag	UNP O75874
B	-12	HIS	-	expression tag	UNP O75874

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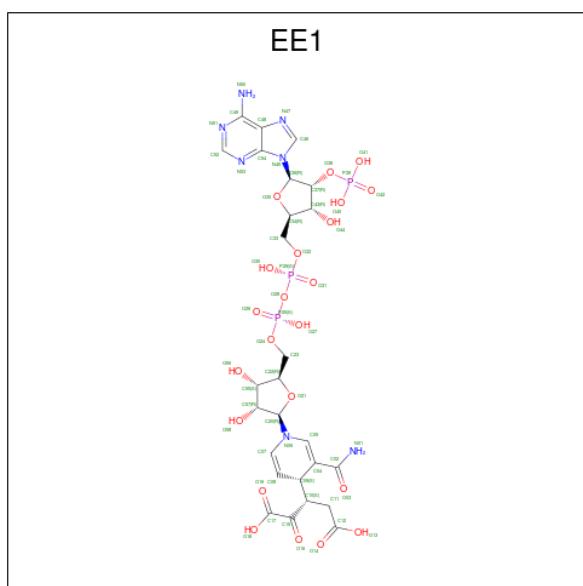
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP O75874
B	-10	HIS	-	expression tag	UNP O75874
B	-9	SER	-	expression tag	UNP O75874
B	-8	SER	-	expression tag	UNP O75874
B	-7	GLY	-	expression tag	UNP O75874
B	-6	LEU	-	expression tag	UNP O75874
B	-5	VAL	-	expression tag	UNP O75874
B	-4	PRO	-	expression tag	UNP O75874
B	-3	ARG	-	expression tag	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	SER	-	expression tag	UNP O75874
B	0	HIS	-	expression tag	UNP O75874
B	132	GLN	ARG	engineered mutation	UNP O75874
C	-15	HIS	-	expression tag	UNP O75874
C	-14	HIS	-	expression tag	UNP O75874
C	-13	HIS	-	expression tag	UNP O75874
C	-12	HIS	-	expression tag	UNP O75874
C	-11	HIS	-	expression tag	UNP O75874
C	-10	HIS	-	expression tag	UNP O75874
C	-9	SER	-	expression tag	UNP O75874
C	-8	SER	-	expression tag	UNP O75874
C	-7	GLY	-	expression tag	UNP O75874
C	-6	LEU	-	expression tag	UNP O75874
C	-5	VAL	-	expression tag	UNP O75874
C	-4	PRO	-	expression tag	UNP O75874
C	-3	ARG	-	expression tag	UNP O75874
C	-2	GLY	-	expression tag	UNP O75874
C	-1	SER	-	expression tag	UNP O75874
C	0	HIS	-	expression tag	UNP O75874
C	132	GLN	ARG	engineered mutation	UNP O75874
D	-15	HIS	-	expression tag	UNP O75874
D	-14	HIS	-	expression tag	UNP O75874
D	-13	HIS	-	expression tag	UNP O75874
D	-12	HIS	-	expression tag	UNP O75874
D	-11	HIS	-	expression tag	UNP O75874
D	-10	HIS	-	expression tag	UNP O75874
D	-9	SER	-	expression tag	UNP O75874
D	-8	SER	-	expression tag	UNP O75874
D	-7	GLY	-	expression tag	UNP O75874
D	-6	LEU	-	expression tag	UNP O75874
D	-5	VAL	-	expression tag	UNP O75874
D	-4	PRO	-	expression tag	UNP O75874

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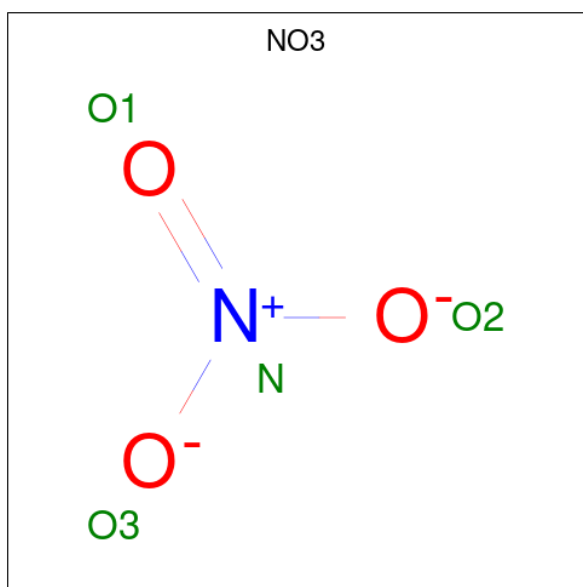
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP O75874
D	-2	GLY	-	expression tag	UNP O75874
D	-1	SER	-	expression tag	UNP O75874
D	0	HIS	-	expression tag	UNP O75874
D	132	GLN	ARG	engineered mutation	UNP O75874

- Molecule 2 is (3 {S})-3-[(4 {S})-3-aminocarbonyl-1-[(2 {R},3 {R},4 {S},5 {R})-5-[[[(2 {R},3 {R},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3-oxidanyl-4-phosphonooxy-oxolan-2-yl] methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-3,4-bis(oxidanyl)oxolan-2-yl]-4 {H}-pyridin-4-yl]-2-oxidanylidene-pentanedioic acid (CCD ID: EE1) (formula: C₂₆H₃₄N₇O₂₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			86	26	28	7	22	3		
2	C	1	Total	C	H	N	O	P	0	0
			86	26	28	7	22	3		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).

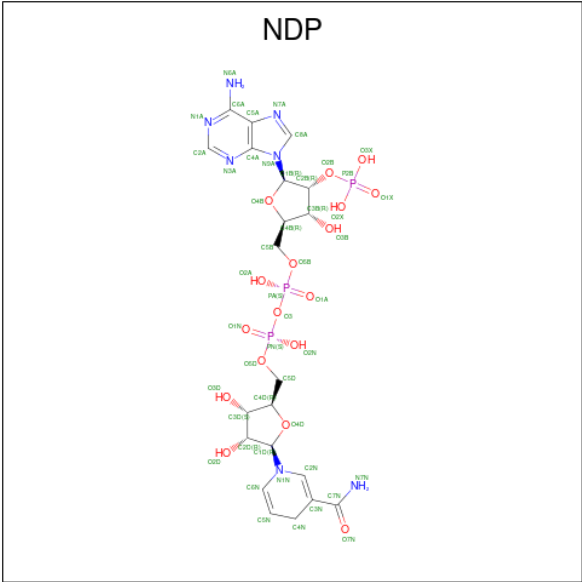


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

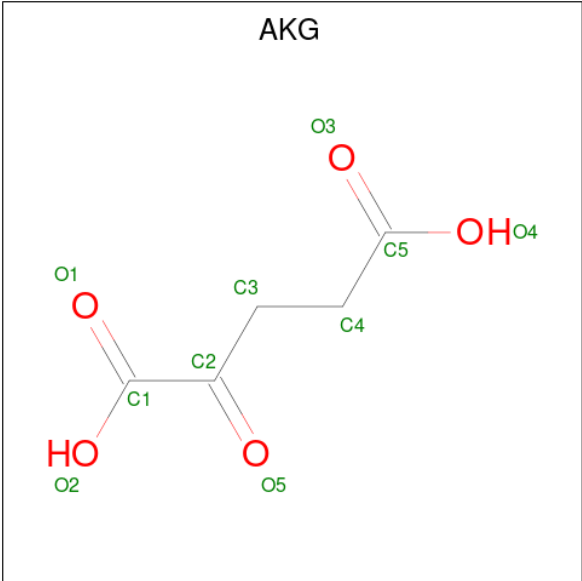
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



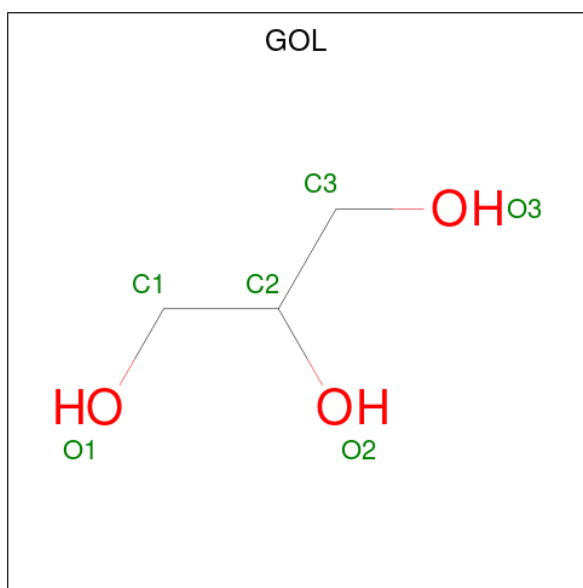
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
5	D	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		

- Molecule 6 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			14	5	4	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			14	3	8	3		

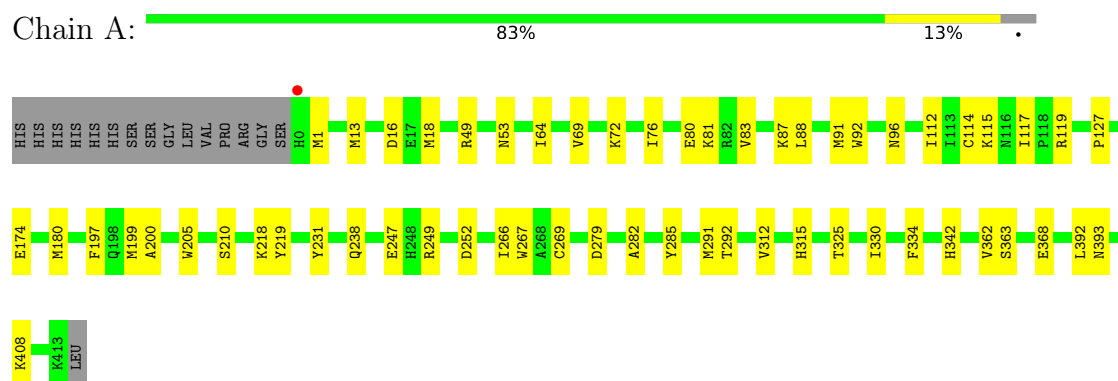
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	107	Total	O	0	0
			107	107		
8	B	130	Total	O	0	0
			130	130		
8	C	71	Total	O	0	0
			71	71		
8	D	154	Total	O	0	0
			154	154		

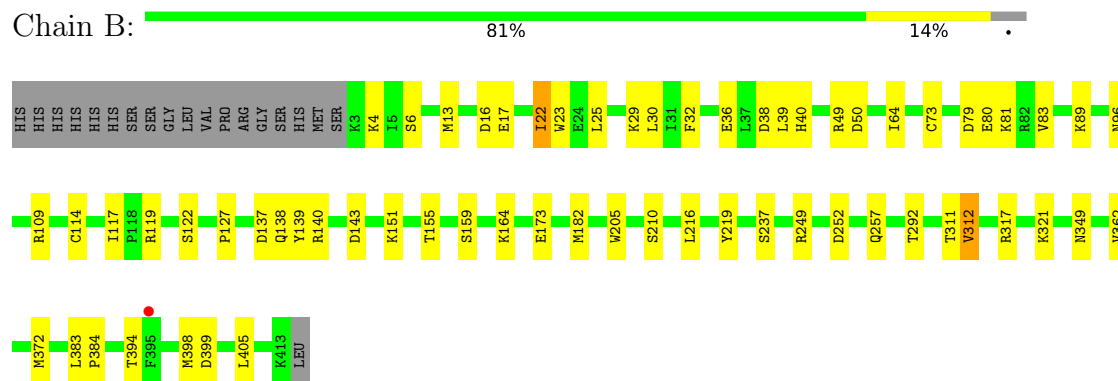
3 Residue-property plots [i](#)

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.

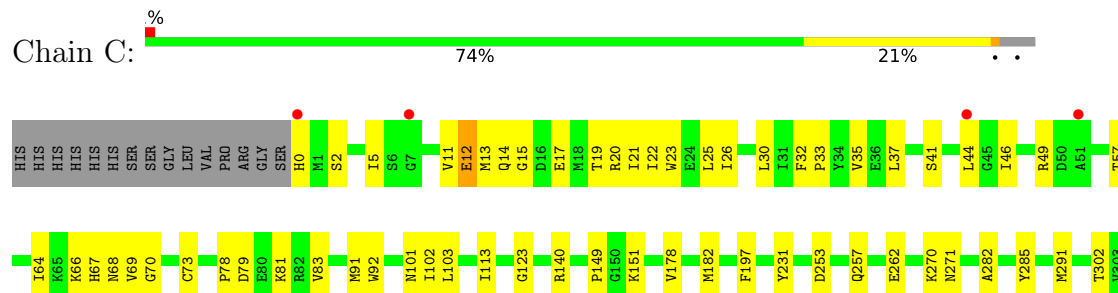
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

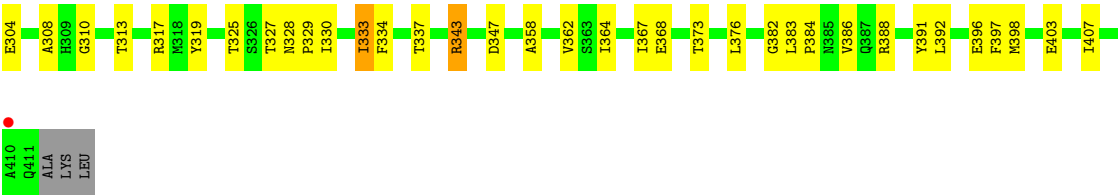


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

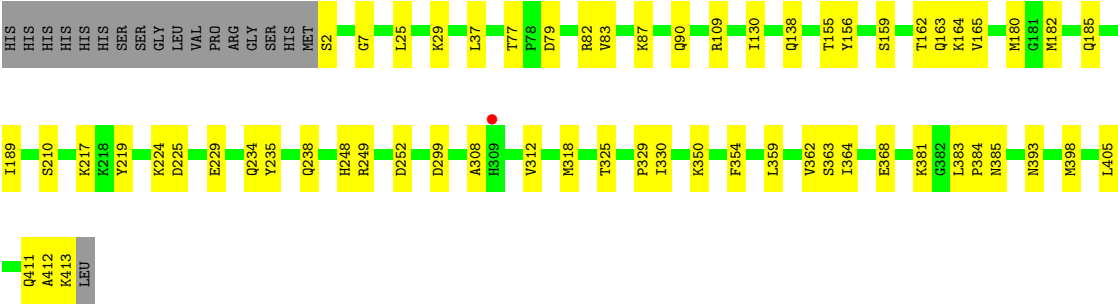
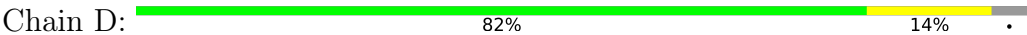


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic





● Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.82Å 104.86Å 107.71Å 90.00° 98.19° 90.00°	Depositor
Resolution (Å)	39.15 – 2.28 39.15 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.15-2.28) 98.3 (39.15-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.167 , 0.222 0.168 , 0.222	Depositor DCC
R_{free} test set	4053 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13870	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, NO3, CA, NDP, GOL, EE1

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	0.37	0/3355	0.54	0/4524
1	B	0.39	0/3330	0.53	1/4490 (0.0%)
1	C	0.33	0/3335	0.47	0/4500
1	D	0.39	0/3328	0.53	0/4488
All	All	0.37	0/13348	0.52	1/18002 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ASP	CB-CA-C	-5.17	110.60	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3245	47	0
1	B	3262	0	3227	45	0
1	C	3266	0	3211	86	0
1	D	3260	0	3221	47	0
2	A	58	28	0	0	0
2	C	58	28	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	40	19	19	1	0
5	D	40	19	19	3	0
6	B	10	4	4	1	0
7	D	6	8	8	1	0
8	A	107	0	0	3	0
8	B	130	0	0	2	0
8	C	71	0	0	1	0
8	D	154	0	0	2	0
All	All	13764	106	12954	212	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 8.

All (212) 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:30:LEU:HD21	1:C:398:MET:HE1	1.15	1.14
1:C:334:PHE:HA	1:C:337:THR:HG22	1.35	1.03
1:A:218:LYS:HE3	1:A:218:LYS:HA	1.46	0.97
1:D:225:ASP:O	1:D:229:GLU:HG3	1.75	0.86
1:A:119:ARG:HG3	1:A:285:TYR:HA	1.58	0.82
1:C:291:MET:HG2	1:C:308:ALA:HB2	1.63	0.80
1:C:102:ILE:HG22	1:C:103:LEU:HD12	1.64	0.79
1:B:317:ARG:O	1:B:321:LYS:HD2	1.82	0.78
1:C:26:ILE:HA	1:C:30:LEU:HD23	1.66	0.77
1:C:91:MET:HB3	1:D:217:LYS:HE2	1.64	0.77
1:C:30:LEU:HD21	1:C:398:MET:CE	2.07	0.76
1:C:35:VAL:HG12	1:C:37:LEU:CD2	2.15	0.76
1:C:81:LYS:HE3	1:D:224:LYS:HZ1	1.52	0.75
1:C:330:ILE:CD1	1:C:367:ILE:HD11	2.17	0.75
1:B:127:PRO:HG2	1:B:205:TRP:HH2	1.50	0.74
1:C:334:PHE:HA	1:C:337:THR:CG2	2.16	0.74
1:C:15:GLY:O	1:C:20:ARG:HD2	1.89	0.73
1:A:87:LYS:HE3	1:A:87:LYS:CA	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:OE2	1:C:14:GLN:HG3	1.90	0.71
1:A:87:LYS:HE3	1:A:87:LYS:HA	1.72	0.70
1:A:83:VAL:HA	1:A:88:LEU:HD12	1.74	0.69
1:B:49:ARG:HD2	8:B:608:HOH:O	1.92	0.69
1:A:180:MET:HE1	1:B:216:LEU:HD13	1.75	0.68
1:C:26:ILE:HA	1:C:30:LEU:CD2	2.23	0.68
1:C:291:MET:HG2	1:C:308:ALA:CB	2.23	0.68
1:D:180:MET:HE2	1:D:182:MET:HE2	1.76	0.67
1:B:29:LYS:HE3	1:B:399:ASP:OD1	1.97	0.65
1:C:334:PHE:CA	1:C:337:THR:HG22	2.19	0.64
1:C:35:VAL:HG12	1:C:37:LEU:HD22	1.81	0.63
1:A:112:ILE:HD12	1:A:334:PHE:CE2	2.35	0.62
1:B:30:LEU:HD11	1:B:398:MET:HE1	1.81	0.62
1:C:330:ILE:HD12	1:C:367:ILE:HD11	1.80	0.62
1:B:4:LYS:NZ	1:B:32:PHE:O	2.29	0.62
1:A:80:GLU:OE2	1:A:91:MET:HE1	2.00	0.62
1:C:23:TRP:CD2	1:C:73:CYS:HB2	2.35	0.61
1:C:403:GLU:O	1:C:407:ILE:HD13	2.00	0.61
1:C:81:LYS:HE3	1:D:224:LYS:NZ	2.15	0.61
1:C:392:LEU:HB3	1:C:396:GLU:HB2	1.82	0.61
1:D:77:THR:N	5:D:501:NDP:O2D	2.20	0.61
1:C:383:LEU:O	1:C:383:LEU:HD22	2.01	0.60
1:B:362:VAL:HG21	1:B:405:LEU:HA	1.84	0.59
1:C:46:ILE:HD11	1:C:78:PRO:HG3	1.84	0.59
1:C:81:LYS:HE2	1:C:81:LYS:H	1.68	0.58
1:C:79:ASP:O	1:C:83:VAL:HG23	2.03	0.58
1:C:35:VAL:HG12	1:C:37:LEU:HD21	1.82	0.58
1:A:282:ALA:HB2	1:A:291:MET:HG2	1.86	0.57
1:D:364:ILE:O	1:D:368:GLU:HG3	2.05	0.57
1:A:174:GLU:H	1:A:174:GLU:CD	2.12	0.56
1:C:319:TYR:HB2	1:C:325:THR:HG21	1.87	0.56
1:B:30:LEU:CD1	1:B:398:MET:HE1	2.35	0.56
1:A:312:VAL:HG12	1:A:315:HIS:HB2	1.87	0.56
1:A:218:LYS:HA	1:A:218:LYS:CE	2.24	0.56
1:C:30:LEU:CD2	1:C:398:MET:HE1	2.10	0.56
1:D:156:TYR:HB3	1:D:165:VAL:CG1	2.36	0.56
1:B:138:GLN:HG3	1:B:182:MET:HE1	1.86	0.56
1:D:138:GLN:HG3	1:D:182:MET:HE1	1.88	0.56
1:A:80:GLU:OE1	1:A:80:GLU:N	2.36	0.56
1:D:162:THR:HG22	1:D:163:GLN:N	2.21	0.55
1:B:80:GLU:O	1:B:83:VAL:HG22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ALA:HB2	1:C:291:MET:SD	2.47	0.55
1:B:257:GLN:HG2	8:B:607:HOH:O	2.05	0.55
1:C:313:THR:O	1:C:317:ARG:HG2	2.06	0.55
1:B:50:ASP:O	1:B:89:LYS:NZ	2.29	0.54
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.43	0.54
1:C:69:VAL:HG21	1:C:343:ARG:HG2	1.89	0.53
1:D:412:ALA:O	1:D:413:LYS:HB2	2.07	0.53
1:C:367:ILE:HD13	1:C:376:LEU:CD1	2.39	0.53
1:A:238:GLN:HG3	8:A:623:HOH:O	2.08	0.53
1:C:182:MET:HE3	1:D:182:MET:HE3	1.92	0.52
1:B:311:THR:C	1:B:312:VAL:HG23	2.35	0.52
1:C:21:ILE:O	1:C:25:LEU:HD12	2.09	0.52
1:C:182:MET:CE	1:D:182:MET:HE3	2.39	0.52
1:A:49:ARG:HD2	8:A:647:HOH:O	2.10	0.52
1:D:234:GLN:O	1:D:238:GLN:NE2	2.38	0.52
1:C:66:LYS:HA	1:C:66:LYS:HE2	1.92	0.51
1:D:383:LEU:HB3	1:D:384:PRO:HD3	1.91	0.51
1:C:26:ILE:HG23	1:C:30:LEU:HD23	1.92	0.51
1:A:312:VAL:HG12	1:A:312:VAL:O	2.09	0.51
1:D:235:TYR:HA	1:D:238:GLN:NE2	2.24	0.51
1:D:7:GLY:HA3	1:D:37:LEU:HD23	1.90	0.51
1:C:13:MET:CE	1:C:64:ILE:HD11	2.41	0.51
1:A:247:GLU:OE1	1:A:249:ARG:NH2	2.43	0.51
1:C:66:LYS:HA	1:C:66:LYS:CE	2.41	0.51
1:C:101:ASN:OD1	1:C:140:ARG:HD3	2.11	0.51
1:D:162:THR:CG2	1:D:163:GLN:N	2.74	0.51
1:A:53:ASN:HA	1:A:92:TRP:CH2	2.46	0.50
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.94	0.50
1:D:25:LEU:HD22	1:D:29:LYS:HE2	1.93	0.50
1:B:119:ARG:NH2	1:B:122:SER:O	2.40	0.50
1:C:5:ILE:HB	1:C:35:VAL:HG22	1.94	0.50
1:C:81:LYS:HD3	1:C:81:LYS:N	2.27	0.50
1:D:163:GLN:HG3	1:D:164:LYS:O	2.12	0.50
1:A:210:SER:HA	1:A:249:ARG:O	2.12	0.50
1:B:127:PRO:HG2	1:B:205:TRP:CH2	2.39	0.49
1:C:67:HIS:O	1:C:68:ASN:HB2	2.11	0.49
1:C:383:LEU:N	1:C:384:PRO:HD2	2.28	0.49
1:C:44:LEU:HD11	1:C:57:THR:HA	1.93	0.49
1:B:79:ASP:O	1:B:83:VAL:HG13	2.13	0.49
1:D:185:GLN:O	1:D:189:ILE:HG13	2.13	0.49
5:D:501:NDP:O2A	5:D:501:NDP:O2N	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HE2	1:B:219:TYR:CD2	2.47	0.49
1:D:362:VAL:HG21	1:D:405:LEU:HA	1.94	0.49
1:D:329:PRO:CB	1:D:398:MET:HE1	2.43	0.49
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.94	0.48
1:C:388:ARG:HH11	1:C:388:ARG:HG3	1.78	0.48
1:D:299:ASP:OD2	7:D:502:GOL:H12	2.14	0.48
1:C:30:LEU:HD22	1:C:30:LEU:N	2.28	0.48
1:B:22:ILE:HD11	1:B:394:THR:CG2	2.43	0.48
1:C:382:GLY:O	1:C:386:VAL:HG23	2.12	0.48
1:C:391:TYR:CD1	1:C:391:TYR:C	2.92	0.48
1:A:127:PRO:HD2	1:A:205:TRP:CH2	2.49	0.48
1:B:22:ILE:HD11	1:B:394:THR:HG21	1.94	0.48
1:D:412:ALA:O	1:D:413:LYS:CB	2.62	0.48
1:D:381:LYS:HE2	1:D:385:ASN:O	2.14	0.48
1:B:383:LEU:N	1:B:384:PRO:HD2	2.28	0.48
1:C:149:PRO:HB2	1:D:159:SER:OG	2.14	0.48
1:A:112:ILE:HD11	1:A:292:THR:HG21	1.96	0.47
1:C:123:GLY:O	1:C:262:GLU:HA	2.14	0.47
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.94	0.47
1:C:17:GLU:O	1:C:21:ILE:HG12	2.14	0.47
1:B:6:SER:O	1:B:349:ASN:ND2	2.47	0.47
1:C:388:ARG:HG3	1:C:388:ARG:NH1	2.29	0.47
1:B:210:SER:HA	1:B:249:ARG:O	2.15	0.47
1:B:23:TRP:CD2	1:B:73:CYS:HB2	2.50	0.46
1:C:22:ILE:HD11	1:C:327:THR:HB	1.97	0.46
1:B:16:ASP:HB2	1:B:311:THR:HG21	1.98	0.46
1:A:87:LYS:HA	1:A:87:LYS:CE	2.37	0.46
1:C:78:PRO:HD2	1:C:92:TRP:O	2.16	0.46
1:A:267:TRP:CD1	1:A:269:CYS:HG	2.34	0.46
1:A:200:ALA:HA	1:A:266:ILE:HG13	1.97	0.46
1:C:197:PHE:CZ	1:C:231:TYR:HB2	2.51	0.46
1:D:83:VAL:O	1:D:87:LYS:N	2.49	0.46
1:C:81:LYS:H	1:C:81:LYS:CE	2.28	0.45
1:C:91:MET:HB3	1:D:217:LYS:CE	2.42	0.45
1:C:347:ASP:HB3	8:C:666:HOH:O	2.16	0.45
1:C:392:LEU:HD22	1:C:397:PHE:HA	1.98	0.45
1:C:407:ILE:N	1:C:407:ILE:HD12	2.31	0.45
1:D:252:ASP:OD1	1:D:252:ASP:N	2.50	0.45
1:C:291:MET:HE3	1:C:291:MET:HB2	1.78	0.45
1:D:413:LYS:HD2	1:D:413:LYS:HA	1.65	0.45
1:D:354:PHE:CZ	1:D:412:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HG2	1:A:368:GLU:OE2	2.16	0.45
1:B:38:ASP:OD2	1:B:40:HIS:NE2	2.48	0.45
1:C:113:ILE:HD11	1:C:285:TYR:CD1	2.51	0.45
1:C:46:ILE:HD12	1:C:49:ARG:NH1	2.32	0.45
1:C:151:LYS:HE2	1:C:151:LYS:HB3	1.77	0.45
1:A:392:LEU:HD21	1:D:350:LYS:NZ	2.32	0.44
1:D:109:ARG:HH21	1:D:308:ALA:HB1	1.81	0.44
1:B:114:CYS:HB2	1:B:117:ILE:HG12	2.00	0.44
1:C:66:LYS:HE2	1:C:66:LYS:CA	2.46	0.44
1:A:330:ILE:CD1	1:A:363:SER:HB3	2.47	0.44
5:B:501:NDP:O1X	5:B:501:NDP:O3B	2.29	0.44
1:B:13:MET:CE	1:B:64:ILE:HD11	2.47	0.44
1:A:199:MET:HB2	1:A:199:MET:HE2	1.66	0.44
1:A:279:ASP:OD2	1:B:252:ASP:HB3	2.18	0.44
1:C:12:GLU:O	1:C:41:SER:HA	2.18	0.44
1:C:358:ALA:O	1:C:362:VAL:HG23	2.17	0.44
1:B:81:LYS:HE3	1:B:81:LYS:HB2	1.57	0.44
1:B:151:LYS:HB2	1:B:151:LYS:HE2	1.62	0.44
1:C:328:ASN:HA	1:C:373:THR:HG21	1.98	0.44
1:D:210:SER:HA	1:D:249:ARG:O	2.18	0.44
1:D:359:LEU:HD12	1:D:359:LEU:O	2.18	0.44
1:D:155:THR:HG22	8:D:641:HOH:O	2.16	0.44
1:B:155:THR:HG21	1:B:164:LYS:NZ	2.33	0.43
1:C:330:ILE:HD11	1:C:367:ILE:HD11	1.95	0.43
1:A:114:CYS:HB2	1:A:117:ILE:HG12	1.99	0.43
1:C:253:ASP:O	1:C:257:GLN:HG2	2.17	0.43
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.81	0.43
8:A:616:HOH:O	1:B:155:THR:HG22	2.18	0.43
1:C:270:LYS:O	1:C:271:ASN:C	2.62	0.43
1:A:13:MET:CE	1:A:64:ILE:HD11	2.48	0.43
1:C:19:THR:O	1:C:23:TRP:HB2	2.19	0.43
1:C:178:VAL:HG11	1:D:219:TYR:HA	2.00	0.43
1:A:18:MET:HB3	1:A:312:VAL:HB	2.00	0.43
1:A:72:LYS:HE3	1:A:96:ASN:OD1	2.18	0.43
1:A:174:GLU:CD	1:A:174:GLU:N	2.76	0.43
1:B:29:LYS:CE	1:B:399:ASP:OD1	2.65	0.42
1:B:140:ARG:HD2	1:B:140:ARG:HA	1.85	0.42
1:D:318:MET:HE2	1:D:325:THR:HG22	2.01	0.42
1:A:325:THR:O	1:A:393:ASN:HB2	2.19	0.42
1:B:96:ASN:HD22	6:B:503:AKG:H41	1.85	0.42
1:C:392:LEU:N	1:C:392:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:TYR:HB3	1:D:165:VAL:HG12	2.00	0.42
1:D:330:ILE:HD12	1:D:363:SER:HB3	2.01	0.42
1:B:372:MET:HE2	1:B:372:MET:HB3	1.92	0.42
1:C:330:ILE:CD1	1:C:367:ILE:CD1	2.95	0.42
1:C:32:PHE:N	1:C:33:PRO:HD2	2.35	0.42
1:C:329:PRO:O	1:C:333:ILE:HD12	2.20	0.42
1:B:139:TYR:CD1	1:B:139:TYR:N	2.87	0.42
1:A:69:VAL:HG22	1:A:342:HIS:HD2	1.83	0.42
1:C:11:VAL:O	1:C:70:GLY:HA2	2.20	0.42
1:C:364:ILE:HG22	1:C:368:GLU:OE1	2.20	0.42
1:C:70:GLY:O	1:C:304:GLU:HA	2.20	0.41
1:C:81:LYS:N	1:C:81:LYS:CD	2.83	0.41
1:C:391:TYR:C	1:C:392:LEU:HD12	2.45	0.41
1:A:252:ASP:OD1	1:A:252:ASP:N	2.49	0.41
1:A:392:LEU:HD21	1:D:350:LYS:HZ2	1.85	0.41
1:A:16:ASP:CB	1:A:76:ILE:HG13	2.51	0.41
1:B:17:GLU:HB2	1:B:311:THR:HB	2.02	0.41
1:B:155:THR:CG2	1:B:164:LYS:HE3	2.50	0.41
1:A:247:GLU:OE1	1:A:249:ARG:NH1	2.50	0.41
1:D:224:LYS:HD2	1:D:248:HIS:CE1	2.54	0.41
1:D:79:ASP:OD1	1:D:82:ARG:HG2	2.20	0.41
1:A:180:MET:HG2	1:B:182:MET:HG2	2.02	0.41
1:B:109:ARG:HA	1:B:292:THR:O	2.20	0.41
1:D:77:THR:HG22	5:D:501:NDP:O2D	2.21	0.41
1:C:310:GLY:HA2	2:C:502:EE1:C05	2.51	0.41
1:A:115:LYS:HG2	1:A:115:LYS:H	1.74	0.40
1:B:25:LEU:O	1:B:29:LYS:HB2	2.21	0.40
1:D:109:ARG:NH1	8:D:603:HOH:O	2.38	0.40
1:C:68:ASN:HA	1:C:302:THR:HG23	2.02	0.40
1:D:325:THR:O	1:D:393:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/430 (96%)	401 (97%)	11 (3%)	1 (0%)	43	53
1	B	410/430 (95%)	396 (97%)	14 (3%)	0	100	100
1	C	411/430 (96%)	392 (95%)	19 (5%)	0	100	100
1	D	410/430 (95%)	399 (97%)	11 (3%)	0	100	100
All	All	1644/1720 (96%)	1588 (97%)	55 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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	350/364 (96%)	349 (100%)	1 (0%)	86	92
1	B	348/364 (96%)	342 (98%)	6 (2%)	53	70
1	C	346/364 (95%)	341 (99%)	5 (1%)	59	74
1	D	347/364 (95%)	342 (99%)	5 (1%)	59	74
All	All	1391/1456 (96%)	1374 (99%)	17 (1%)	63	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	B	22	ILE
1	B	36	GLU
1	B	159	SER
1	B	173	GLU
1	B	237	SER
1	B	312	VAL

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Mol	Chain	Res	Type
1	C	0	HIS
1	C	2	SER
1	C	12	GLU
1	C	333	ILE
1	C	343	ARG
1	D	2	SER
1	D	90	GLN
1	D	130	ILE
1	D	312	VAL
1	D	411	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	283	GLN
1	A	320	GLN
1	A	323	GLN
1	B	68	ASN
1	B	96	ASN
1	B	171	ASN
1	B	185	GLN
1	B	198	GLN
1	B	257	GLN
1	C	14	GLN
1	C	48	ASN
1	C	53	ASN
1	C	213	ASN
1	C	357	ASN
1	C	385	ASN
1	D	283	GLN
1	D	385	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](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	EE1	C	502	4	60,62,62	1.87	11 (18%)	81,95,95	1.61	16 (19%)
2	EE1	A	501	-	60,62,62	2.37	17 (28%)	81,95,95	1.64	18 (22%)
5	NDP	D	501	-	42,43,52	2.70	13 (30%)	62,67,80	1.70	16 (25%)
5	NDP	B	501	-	42,43,52	2.95	12 (28%)	62,67,80	1.69	15 (24%)
7	GOL	D	502	-	5,5,5	0.59	0	5,5,5	0.92	0
6	AKG	B	503	4	9,9,9	0.77	0	11,11,11	0.49	0
3	NO3	B	502	-	1,3,3	0.84	0	0,3,3	-	-
3	NO3	A	502	-	1,3,3	1.22	0	0,3,3	-	-
3	NO3	C	501	-	1,3,3	1.12	0	0,3,3	-	-

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	EE1	C	502	4	-	16/49/96/96	0/5/5/5
5	NDP	D	501	-	-	10/27/59/77	0/4/4/5
7	GOL	D	502	-	-	3/4/4/4	-
6	AKG	B	503	4	-	3/9/9/9	-
5	NDP	B	501	-	-	6/27/59/77	0/4/4/5
2	EE1	A	501	-	-	13/49/96/96	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	NDP	P2B-O2B	13.06	1.82	1.59
5	D	501	NDP	P2B-O2B	12.12	1.80	1.59
2	A	501	EE1	P39-O38	11.57	1.79	1.59
2	C	502	EE1	P39-O38	8.43	1.74	1.59
5	B	501	NDP	PA-O3	6.76	1.66	1.59
2	A	501	EE1	C10-C15	6.60	1.60	1.51
5	B	501	NDP	O4B-C4B	5.49	1.57	1.45
5	B	501	NDP	PN-O5D	5.20	1.79	1.59
5	D	501	NDP	O4B-C4B	4.95	1.56	1.45
5	D	501	NDP	PN-O5D	4.64	1.77	1.59
2	C	502	EE1	O21-C22	-4.60	1.34	1.45
2	A	501	EE1	O21-C22	-4.02	1.36	1.45
5	D	501	NDP	C2B-C1B	3.77	1.62	1.53
2	A	501	EE1	C07-N06	3.60	1.46	1.37
2	C	502	EE1	P25-O28	-3.50	1.55	1.59
5	B	501	NDP	C2B-C1B	3.42	1.61	1.53
5	B	501	NDP	C3B-C2B	3.36	1.60	1.53
2	A	501	EE1	O24-C23	-3.31	1.32	1.44
2	A	501	EE1	C02-N01	3.29	1.42	1.33
2	A	501	EE1	P29-O32	3.27	1.72	1.59
2	A	501	EE1	O38-C37	-3.17	1.33	1.44
5	D	501	NDP	PA-O3	3.12	1.62	1.59
5	D	501	NDP	O5B-C5B	-3.11	1.32	1.44
5	D	501	NDP	O4B-C1B	3.10	1.49	1.42
5	D	501	NDP	C3B-C2B	3.04	1.59	1.53
2	C	502	EE1	P25-O24	2.99	1.71	1.59
2	C	502	EE1	C07-N06	2.85	1.44	1.37
5	B	501	NDP	O4B-C1B	2.78	1.48	1.42
5	D	501	NDP	C2D-C1D	2.76	1.62	1.53
5	B	501	NDP	C3D-C4D	2.67	1.59	1.53
2	C	502	EE1	O58-C57	-2.66	1.36	1.43
5	B	501	NDP	O5B-C5B	-2.58	1.34	1.44
2	A	501	EE1	C48-C54	2.54	1.43	1.39
5	D	501	NDP	O4D-C1D	2.49	1.47	1.42
5	D	501	NDP	C3D-C4D	2.42	1.59	1.53
5	B	501	NDP	C5A-C4A	2.41	1.43	1.39
2	A	501	EE1	C11-C12	2.39	1.57	1.51
5	B	501	NDP	O2B-C2B	-2.35	1.36	1.44
2	C	502	EE1	P29-O32	2.34	1.68	1.59
2	A	501	EE1	C49-N50	2.33	1.40	1.34
5	D	501	NDP	O2B-C2B	-2.32	1.36	1.44
2	A	501	EE1	C46-N47	2.32	1.36	1.31
5	D	501	NDP	C2D-C3D	2.28	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	EE1	C02-N01	2.20	1.39	1.33
2	A	501	EE1	P25-O24	2.15	1.67	1.59
2	C	502	EE1	O38-C37	-2.14	1.36	1.44
2	C	502	EE1	O18-C17	-2.11	1.24	1.30
2	A	501	EE1	C55-C22	2.10	1.58	1.53
2	A	501	EE1	C37-C36	2.08	1.58	1.53
2	C	502	EE1	O44-C43	-2.07	1.37	1.43
5	B	501	NDP	PN-O3	2.04	1.61	1.59
2	A	501	EE1	O14-C12	2.03	1.28	1.22
2	A	501	EE1	O32-C33	-2.02	1.37	1.44

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	EE1	C07-N06-C05	-4.93	114.04	119.32
2	C	502	EE1	O21-C22-C55	4.41	113.90	105.15
2	A	501	EE1	C07-N06-C05	-4.36	114.65	119.32
5	D	501	NDP	C5D-C4D-C3D	-4.18	100.18	115.21
2	C	502	EE1	O19-C17-C15	-4.13	116.89	122.15
5	D	501	NDP	O4B-C1B-C2B	-4.06	99.59	106.59
2	A	501	EE1	O19-C17-C15	-4.02	117.02	122.15
5	B	501	NDP	C5D-C4D-C3D	-4.01	100.79	115.21
5	B	501	NDP	O2N-PN-O3	3.95	117.96	107.27
2	C	502	EE1	O38-C37-C36	-3.92	96.25	110.05
2	A	501	EE1	C37-C36-N45	-3.89	107.35	113.75
5	D	501	NDP	O2B-P2B-O1X	-3.86	95.59	109.33
5	D	501	NDP	O2N-PN-O3	3.58	116.94	107.27
5	B	501	NDP	O4B-C1B-C2B	-3.44	100.67	106.59
5	D	501	NDP	C2A-N1A-C6A	-3.30	113.32	118.73
2	A	501	EE1	O38-C37-C36	-3.22	98.72	110.05
5	B	501	NDP	O4B-C1B-N9A	3.21	114.26	108.09
2	A	501	EE1	O03-C02-N01	-3.12	115.90	122.89
5	B	501	NDP	O3X-P2B-O2B	-3.10	93.78	105.85
5	B	501	NDP	O3-PA-O1A	-3.08	101.43	110.70
2	A	501	EE1	C04-C05-N06	3.04	126.19	122.84
5	D	501	NDP	P2B-O2B-C2B	-3.00	115.43	123.43
5	D	501	NDP	PA-O5B-C5B	-2.94	104.51	121.35
2	A	501	EE1	O16-C15-C17	-2.84	114.99	119.35
5	B	501	NDP	P2B-O2B-C2B	-2.80	115.95	123.43
2	C	502	EE1	O03-C02-N01	-2.79	116.64	122.89
2	A	501	EE1	C10-C15-C17	2.72	122.00	116.63
2	A	501	EE1	O21-C22-C55	2.71	110.53	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	NDP	O3X-P2B-O2X	2.69	117.87	107.80
5	B	501	NDP	PA-O5B-C5B	-2.66	106.12	121.35
2	A	501	EE1	C23-C22-C55	-2.64	105.70	115.21
5	B	501	NDP	C2A-N1A-C6A	-2.64	114.40	118.73
2	C	502	EE1	O38-P39-O42	-2.58	100.12	109.33
5	B	501	NDP	O2B-P2B-O1X	-2.55	100.23	109.33
5	B	501	NDP	N3A-C4A-N9A	2.55	131.50	127.17
2	C	502	EE1	C54-N45-C36	-2.52	120.74	126.63
2	A	501	EE1	O21-C20-N06	2.50	112.86	108.08
2	C	502	EE1	C57-C55-C22	-2.50	97.79	102.61
2	C	502	EE1	C54-N45-C46	2.49	108.36	105.74
2	A	501	EE1	O40-P39-O42	2.49	120.53	110.83
5	B	501	NDP	C5A-C4A-N3A	-2.48	123.30	126.72
2	A	501	EE1	C20-N06-C07	2.45	125.96	120.77
2	A	501	EE1	O27-P25-O26	2.44	123.79	112.44
2	C	502	EE1	O21-C20-N06	2.43	112.71	108.08
2	C	502	EE1	O30-P29-O31	2.40	123.63	112.44
2	A	501	EE1	O30-P29-O31	2.38	123.52	112.44
2	A	501	EE1	C43-C37-C36	-2.33	98.35	102.81
5	D	501	NDP	O3X-P2B-O2X	2.32	116.49	107.80
5	B	501	NDP	O2N-PN-O1N	2.29	123.11	112.44
5	D	501	NDP	O3-PA-O1A	-2.27	103.88	110.70
5	D	501	NDP	O4B-C1B-N9A	2.26	112.43	108.09
5	D	501	NDP	O4D-C1D-N1N	2.23	114.12	110.57
5	B	501	NDP	O3-PN-O1N	-2.21	104.06	110.70
5	D	501	NDP	O2N-PN-O1N	2.21	122.71	112.44
2	C	502	EE1	C37-C43-C34	-2.18	97.31	101.99
5	D	501	NDP	C5A-C6A-N6A	-2.15	117.97	123.29
2	A	501	EE1	O30-P29-O28	2.14	113.05	107.27
2	C	502	EE1	C10-C15-C17	2.13	120.84	116.63
5	D	501	NDP	C5A-C6A-N1A	2.07	122.76	117.51
2	A	501	EE1	O40-P39-O38	-2.05	97.86	105.85
2	C	502	EE1	O13-C12-C11	2.03	120.33	114.00
2	C	502	EE1	C20-N06-C07	2.03	125.06	120.77
2	C	502	EE1	O27-P25-O26	2.02	121.85	112.44
5	D	501	NDP	O2A-PA-O1A	2.02	121.85	112.44
5	D	501	NDP	N3A-C4A-N9A	2.00	130.57	127.17

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EE1	C11-C10-C15-C17
2	A	501	EE1	C11-C10-C15-O16
2	A	501	EE1	O16-C15-C17-O18
2	A	501	EE1	C23-O24-P25-O27
2	C	502	EE1	C11-C10-C15-C17
2	C	502	EE1	C11-C10-C15-O16
2	C	502	EE1	C10-C15-C17-O19
2	C	502	EE1	O16-C15-C17-O19
2	C	502	EE1	N01-C02-C04-C05
2	C	502	EE1	C23-O24-P25-O26
2	C	502	EE1	C23-O24-P25-O27
2	C	502	EE1	C23-O24-P25-O28
5	B	501	NDP	C5D-O5D-PN-O3
5	D	501	NDP	C5B-O5B-PA-O1A
5	D	501	NDP	C5B-O5B-PA-O2A
5	D	501	NDP	PA-O3-PN-O5D
5	D	501	NDP	C5D-O5D-PN-O3
5	D	501	NDP	O4D-C4D-C5D-O5D
5	D	501	NDP	C3D-C4D-C5D-O5D
7	D	502	GOL	O2-C2-C3-O3
5	B	501	NDP	O4D-C4D-C5D-O5D
7	D	502	GOL	O1-C1-C2-C3
7	D	502	GOL	C1-C2-C3-O3
5	D	501	NDP	C3B-C4B-C5B-O5B
2	C	502	EE1	O32-C33-C34-O35
5	D	501	NDP	O4B-C4B-C5B-O5B
2	A	501	EE1	O32-C33-C34-C43
2	A	501	EE1	O32-C33-C34-O35
2	C	502	EE1	O32-C33-C34-C43
2	A	501	EE1	O16-C15-C17-O19
2	A	501	EE1	N01-C02-C04-C05
2	A	501	EE1	C10-C15-C17-O19
6	B	503	AKG	C1-C2-C3-C4
2	C	502	EE1	O03-C02-C04-C05
2	C	502	EE1	C57-C20-N06-C05
2	A	501	EE1	C23-O24-P25-O28
2	C	502	EE1	C33-O32-P29-O31
5	B	501	NDP	C5D-O5D-PN-O2N
5	D	501	NDP	C5B-O5B-PA-O3
5	D	501	NDP	C5D-O5D-PN-O1N
2	C	502	EE1	O21-C20-N06-C05
2	A	501	EE1	O21-C20-N06-C05
6	B	503	AKG	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
6	B	503	AKG	C3-C4-C5-O3
2	A	501	EE1	C57-C20-N06-C05
2	A	501	EE1	O03-C02-C04-C05
2	C	502	EE1	C57-C20-N06-C07
5	B	501	NDP	PN-O3-PA-O1A
5	B	501	NDP	PN-O3-PA-O2A
2	C	502	EE1	O21-C20-N06-C07
5	B	501	NDP	C3D-C4D-C5D-O5D

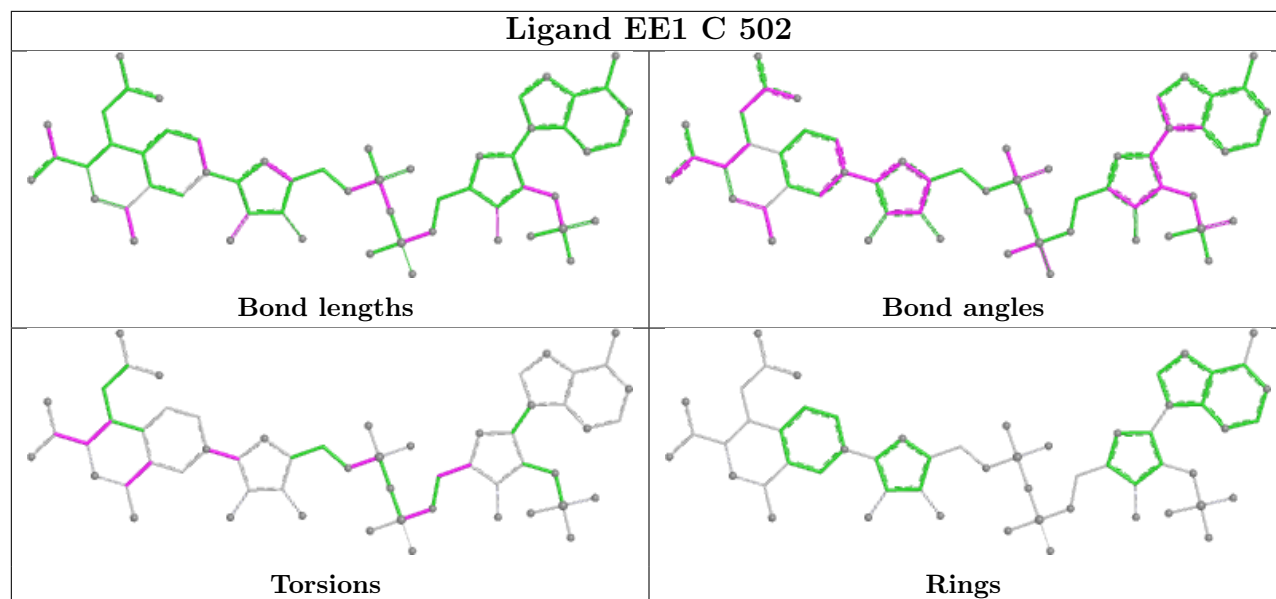
There are no ring outliers.

5 monomers are involved in 7 short contacts:

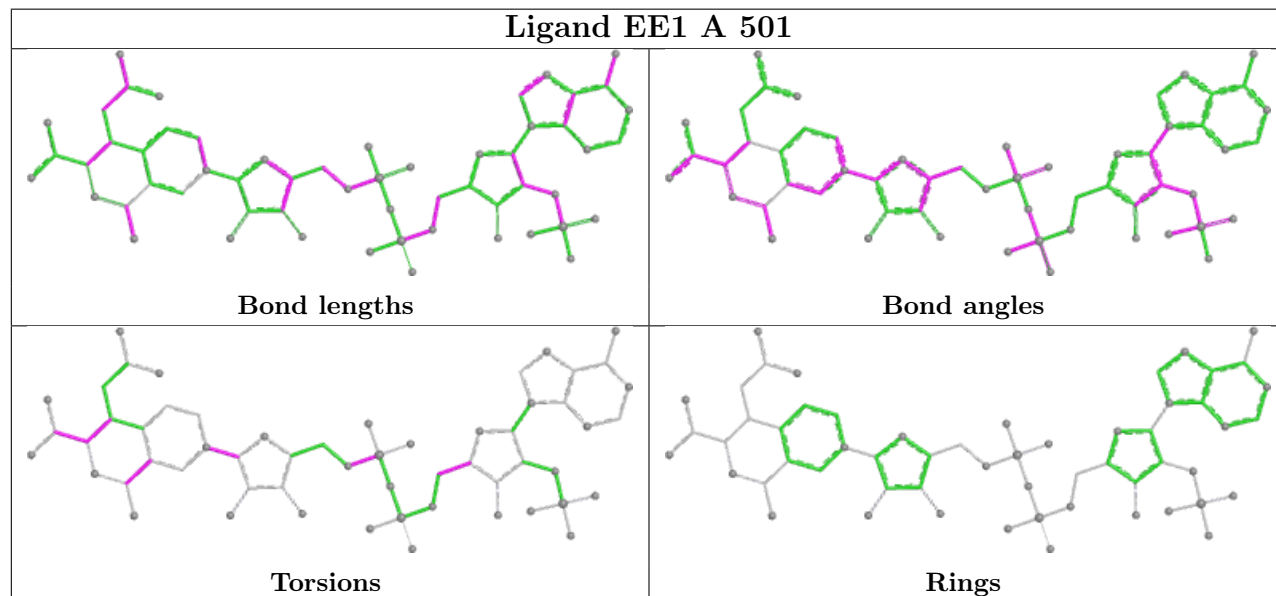
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	EE1	1	0
5	D	501	NDP	3	0
5	B	501	NDP	1	0
7	D	502	GOL	1	0
6	B	503	AKG	1	0

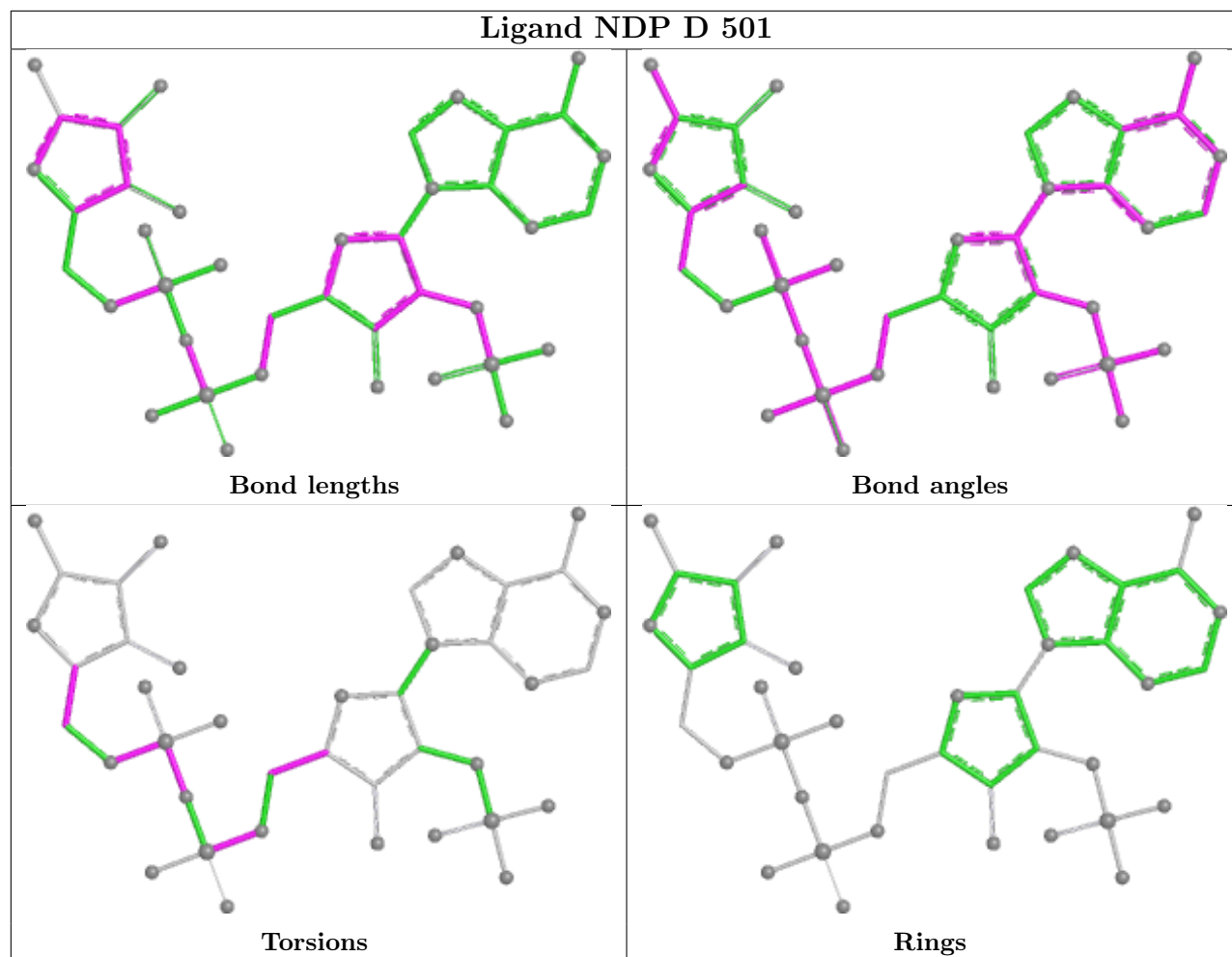
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

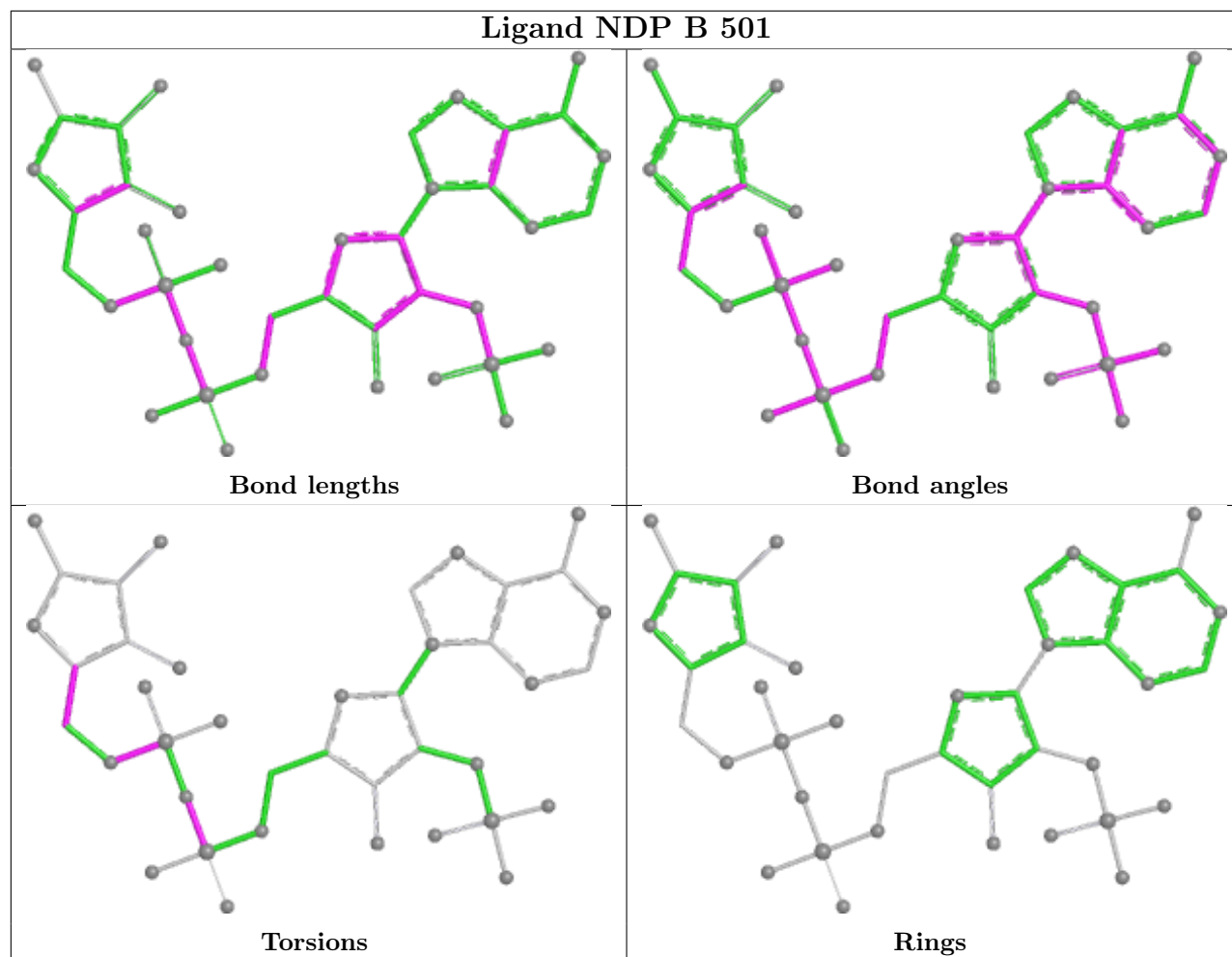
Ligand EE1 C 502

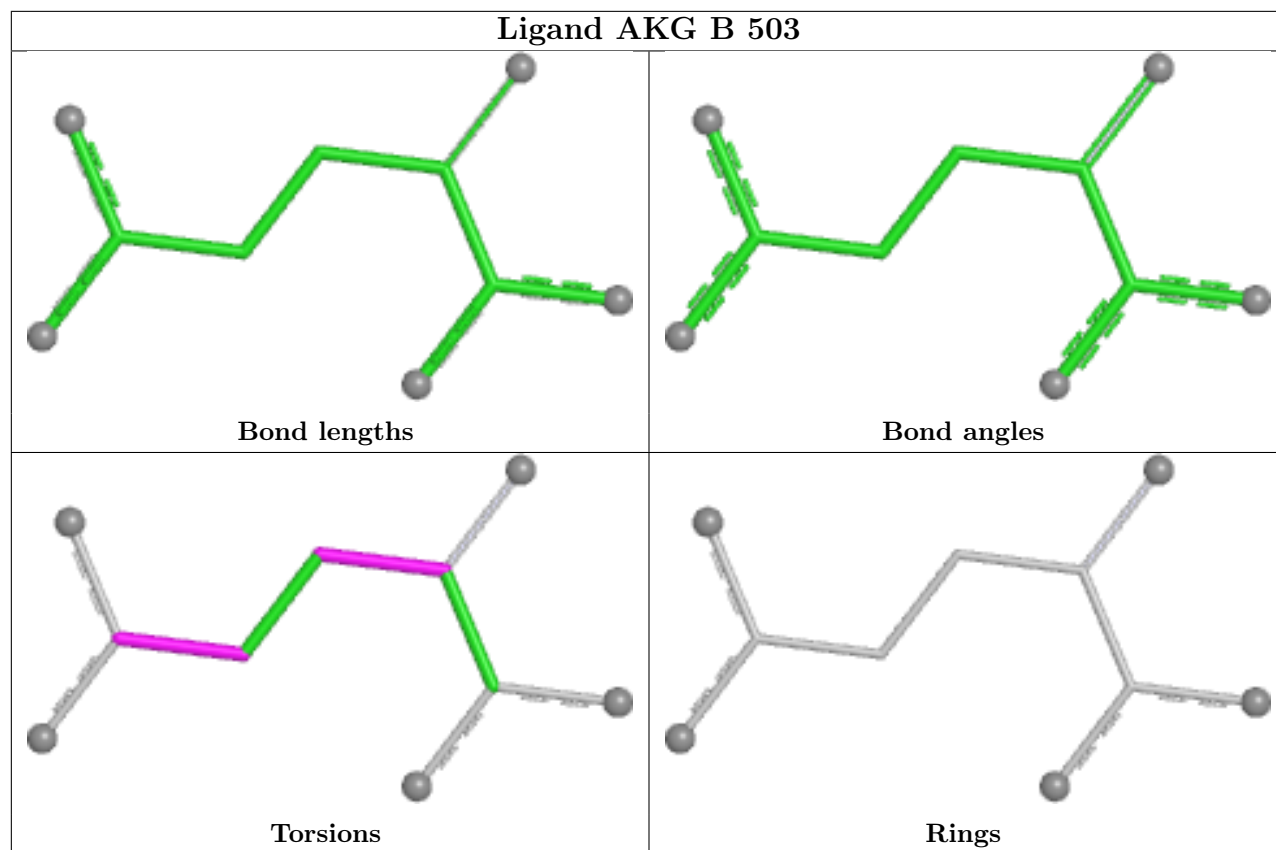


Ligand EE1 A 501









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	414/430 (96%)	-0.44	1 (0%) 91 91	17, 37, 63, 121	1 (0%)
1	B	411/430 (95%)	-0.51	1 (0%) 91 91	14, 37, 54, 75	1 (0%)
1	C	412/430 (95%)	0.13	5 (1%) 76 78	21, 56, 90, 106	1 (0%)
1	D	412/430 (95%)	-0.54	1 (0%) 91 91	25, 35, 51, 84	0
All	All	1649/1720 (95%)	-0.34	8 (0%) 87 88	14, 38, 77, 121	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	3.3
1	C	410	ALA	2.5
1	C	0	HIS	2.4
1	D	309	HIS	2.4
1	B	395	PHE	2.3
1	C	7	GLY	2.2
1	C	44	LEU	2.1
1	C	51	ALA	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

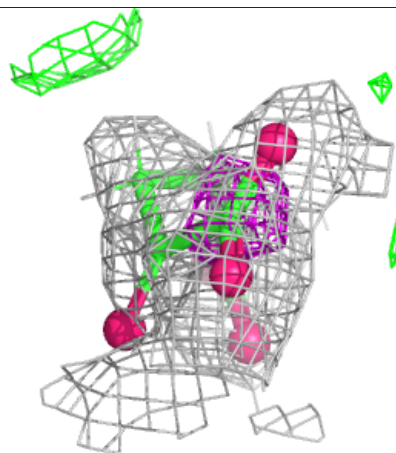
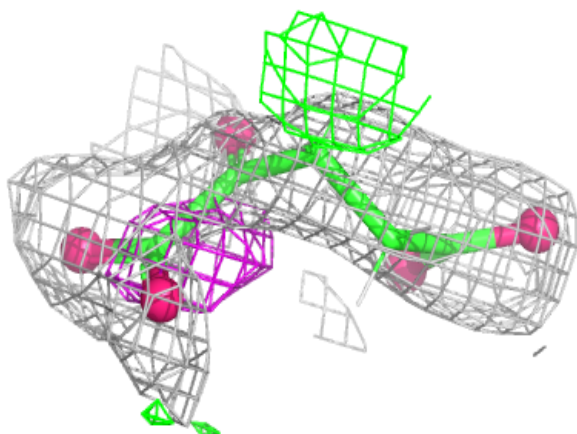
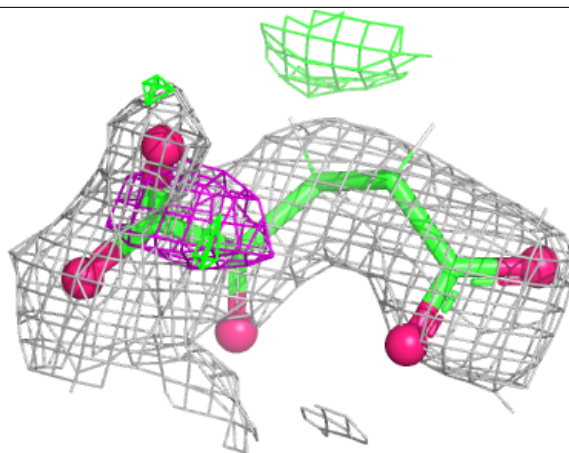
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AKG	B	503	10/10	0.66	0.14	56,67,78,78	0
3	NO3	A	502	4/4	0.87	0.13	34,35,52,56	0
2	EE1	C	502	58/58	0.87	0.11	45,61,79,82	0
3	NO3	C	501	4/4	0.89	0.13	44,49,49,63	0
3	NO3	B	502	4/4	0.90	0.09	49,50,54,59	0
7	GOL	D	502	6/6	0.90	0.14	44,53,68,68	0
5	NDP	B	501	40/48	0.93	0.08	30,43,73,77	0
5	NDP	D	501	40/48	0.93	0.09	29,43,67,76	0
2	EE1	A	501	58/58	0.95	0.07	37,46,59,75	0
4	CA	D	503	1/1	0.95	0.06	53,53,53,53	0
4	CA	C	503	1/1	0.96	0.05	59,59,59,59	0
4	CA	B	504	1/1	0.98	0.04	52,52,52,52	0
4	CA	A	503	1/1	0.99	0.05	38,38,38,38	0

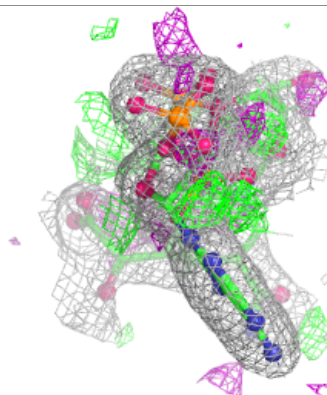
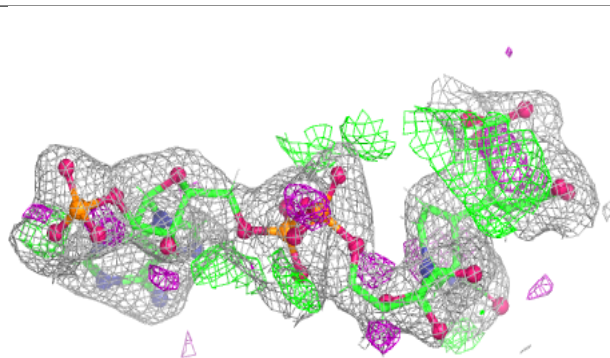
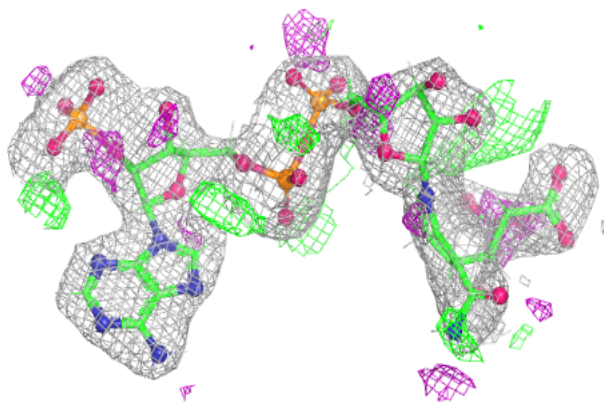
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AKG B 503:

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

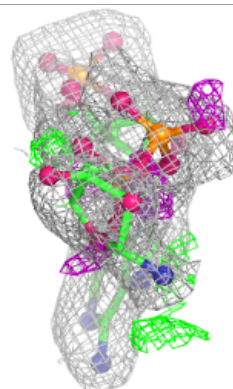
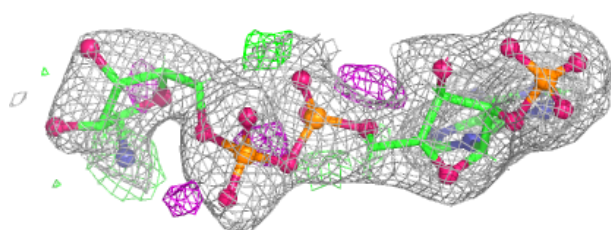
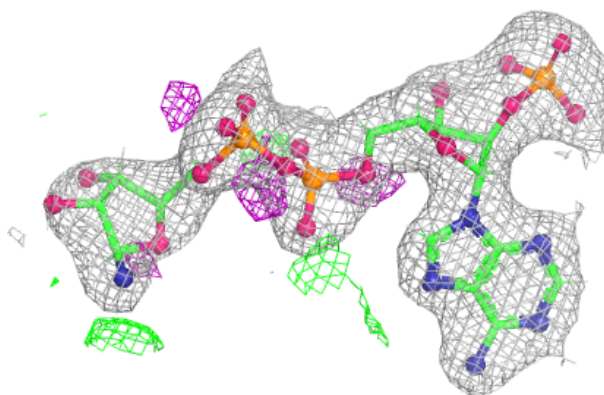
**Electron density around EE1 C 502:**

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

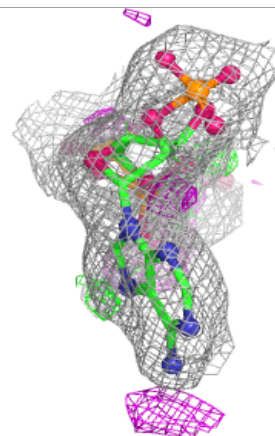
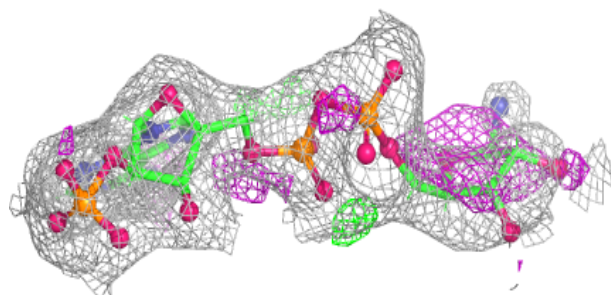
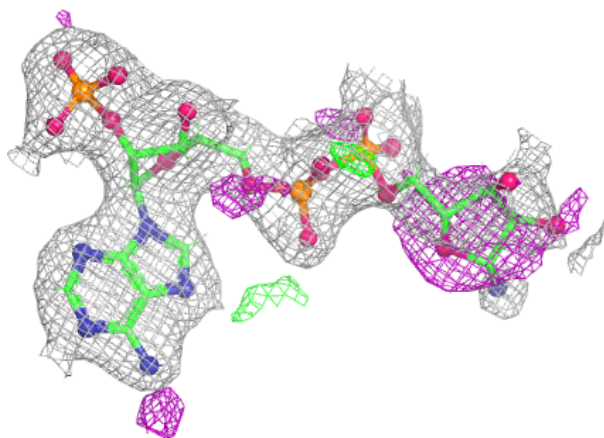


Electron density around NDP B 501:

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

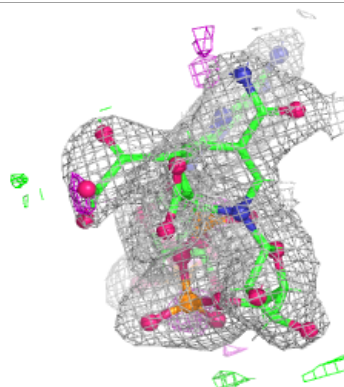
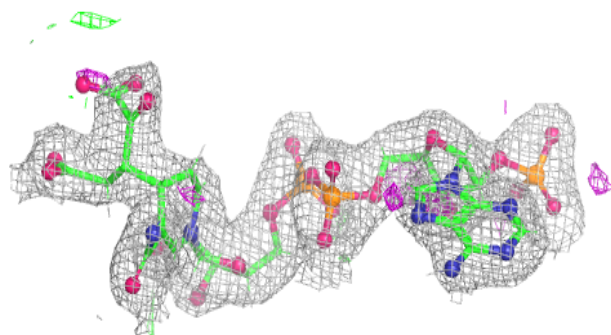
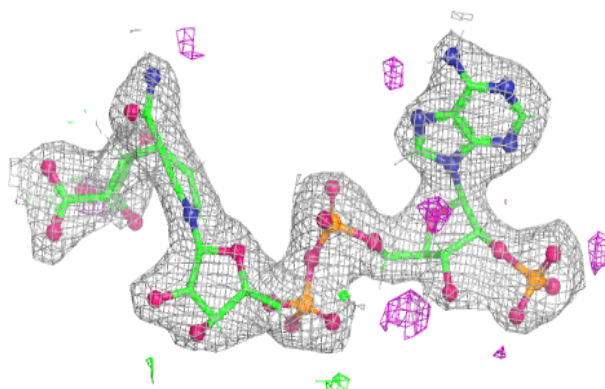
**Electron density around NDP D 501:**

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



Electron density around EE1 A 501:

$2mF_o-DF_c$ (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.