



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 3MES / pdb_00003mes
Title : Crystal structure of choline kinase from *Cryptosporidium parvum* Iowa II, cgd3_2030
Authors : Qiu, W.; Wernimont, A.; Hills, T.; Lew, J.; Artz, J.D.; Xiao, T.; Allali-Hassani, A.; Vedadi, M.; Kozieradzki, I.; Cossar, D.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Hui, R.; Ma, D.; Structural Genomics Consortium (SGC)
Deposited on : 2010-03-31
Resolution : 2.35 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)

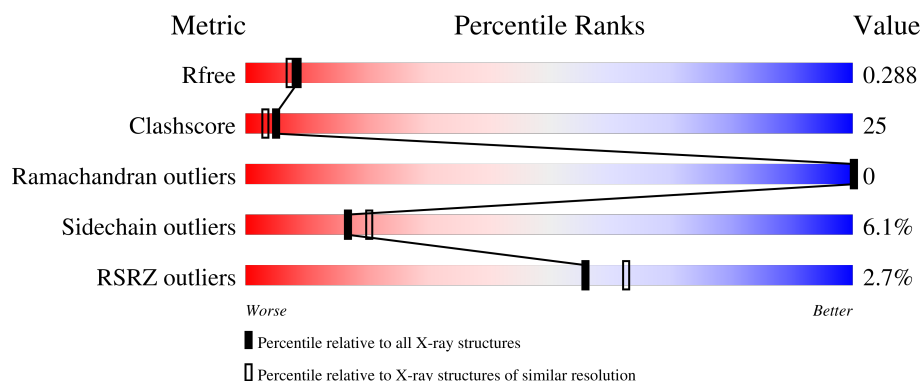
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	424	2% 53% 28% • 16%
1	B	424	3% 55% 25% • 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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
5	PT3	A	428	-	-	X	-
5	PT3	B	428	-	-	X	-
6	GOL	A	429	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6326 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 Choline kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2973	1935	480	547	11			
1	B	358	Total	C	N	O	S	0	0	0
			2979	1937	481	550	11			

There are 38 discrepancies between the modelled and reference sequences:

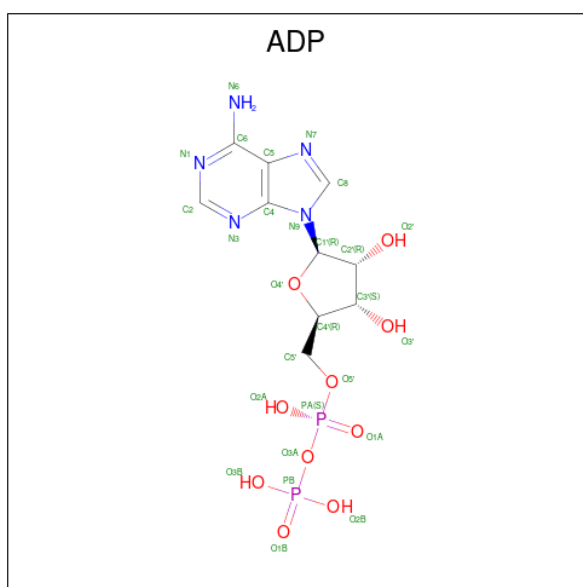
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5CUP2
A	2	GLY	-	expression tag	UNP Q5CUP2
A	3	SER	-	expression tag	UNP Q5CUP2
A	4	SER	-	expression tag	UNP Q5CUP2
A	5	HIS	-	expression tag	UNP Q5CUP2
A	6	HIS	-	expression tag	UNP Q5CUP2
A	7	HIS	-	expression tag	UNP Q5CUP2
A	8	HIS	-	expression tag	UNP Q5CUP2
A	9	HIS	-	expression tag	UNP Q5CUP2
A	10	HIS	-	expression tag	UNP Q5CUP2
A	11	SER	-	expression tag	UNP Q5CUP2
A	12	SER	-	expression tag	UNP Q5CUP2
A	13	GLY	-	expression tag	UNP Q5CUP2
A	14	LEU	-	expression tag	UNP Q5CUP2
A	15	VAL	-	expression tag	UNP Q5CUP2
A	16	PRO	-	expression tag	UNP Q5CUP2
A	17	ARG	-	expression tag	UNP Q5CUP2
A	18	GLY	-	expression tag	UNP Q5CUP2
A	19	SER	-	expression tag	UNP Q5CUP2
B	1	MET	-	expression tag	UNP Q5CUP2
B	2	GLY	-	expression tag	UNP Q5CUP2
B	3	SER	-	expression tag	UNP Q5CUP2
B	4	SER	-	expression tag	UNP Q5CUP2
B	5	HIS	-	expression tag	UNP Q5CUP2
B	6	HIS	-	expression tag	UNP Q5CUP2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q5CUP2
B	8	HIS	-	expression tag	UNP Q5CUP2
B	9	HIS	-	expression tag	UNP Q5CUP2
B	10	HIS	-	expression tag	UNP Q5CUP2
B	11	SER	-	expression tag	UNP Q5CUP2
B	12	SER	-	expression tag	UNP Q5CUP2
B	13	GLY	-	expression tag	UNP Q5CUP2
B	14	LEU	-	expression tag	UNP Q5CUP2
B	15	VAL	-	expression tag	UNP Q5CUP2
B	16	PRO	-	expression tag	UNP Q5CUP2
B	17	ARG	-	expression tag	UNP Q5CUP2
B	18	GLY	-	expression tag	UNP Q5CUP2
B	19	SER	-	expression tag	UNP Q5CUP2

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

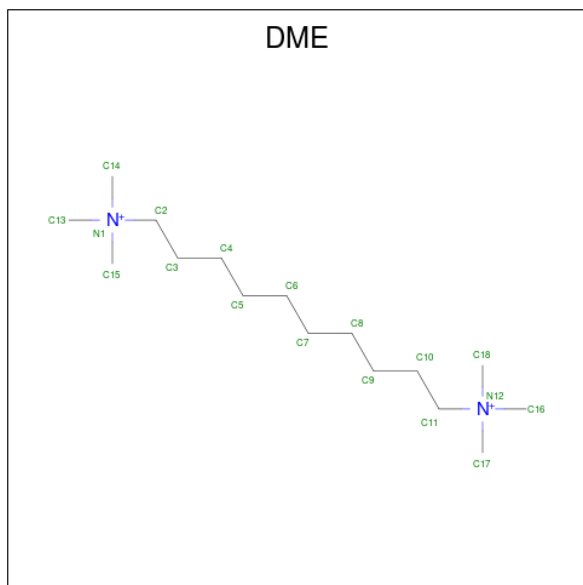


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

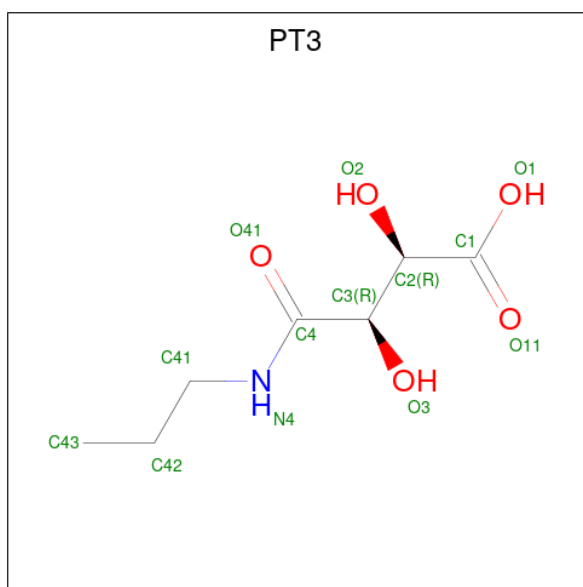
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is DECAMETHONIUM ION (CCD ID: DME) (formula: $C_{16}H_{38}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 18 16 2	0	0
4	B	1	Total C N 18 16 2	0	0

- Molecule 5 is N-PROPYL-TARTRAMIC ACID (CCD ID: PT3) (formula: $C_7H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	7	1	5		
5	B	1	Total	C	N	O	0	0
			13	7	1	5		

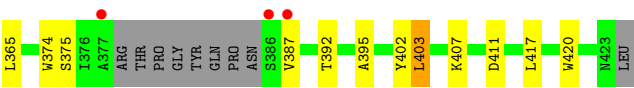
- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	143	Total 143	O 143	0	0
7	B	105	Total 105	O 105	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.09Å 67.96Å 92.11Å 90.00° 116.54° 90.00°	Depositor
Resolution (Å)	19.72 – 2.35 19.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.72-2.35) 99.6 (19.72-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.245 , 0.291 0.246 , 0.288	Depositor DCC
R_{free} test set	1964 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6326	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.38% 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, ADP, DME, PT3, MG

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	0.28	0/3040	0.66	0/4104
1	B	0.30	1/3046 (0.0%)	0.66	0/4113
All	All	0.29	1/6086 (0.0%)	0.66	0/8217

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	GLN	C-O	-5.11	1.17	1.24

There are no bond angle outliers.

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	2973	0	2949	147	0
1	B	2979	0	2949	134	1
2	A	27	0	12	4	0
2	B	27	0	12	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	18	0	38	7	0
4	B	18	0	38	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	13	0	11	8	0
5	B	13	0	12	12	0
6	A	6	0	8	8	0
7	A	143	0	0	20	0
7	B	105	0	0	10	0
All	All	6326	0	6029	302	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 25.

All (302) 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:220:ILE:HD13	1:B:221:ASP:N	1.29	1.46
2:B:425:ADP:H8	2:B:425:ADP:H5'2	1.04	1.09
1:B:220:ILE:CD1	1:B:221:ASP:N	2.22	1.03
2:B:425:ADP:H5'2	2:B:425:ADP:C8	1.96	1.00
1:B:100:LEU:HA	7:B:514:HOH:O	1.64	0.98
1:A:93:ASN:C	1:A:93:ASN:HD22	1.73	0.97
1:A:220:ILE:C	1:A:220:ILE:HD12	1.89	0.96
1:A:100:LEU:HA	7:A:557:HOH:O	1.65	0.96
1:A:270:GLN:NE2	1:A:272:ASN:HB2	1.81	0.93
5:A:428:PT3:O3	5:A:428:PT3:C41	2.16	0.93
1:A:254:LYS:HE2	1:A:261:SER:HA	1.51	0.92
1:B:358:LYS:HG3	1:B:420:TRP:CH2	2.06	0.90
1:A:50:ASP:OD2	1:A:52:GLU:HG2	1.72	0.89
1:B:240:MET:HE1	1:B:293:PHE:CZ	2.07	0.88
1:B:270:GLN:NE2	1:B:272:ASN:HD22	1.70	0.88
1:B:238:LEU:HD22	1:B:239:ILE:HD12	1.54	0.88
1:B:195:GLU:HG2	1:B:247:MET:CE	2.04	0.88
1:A:351:GLN:HE21	1:A:351:GLN:HA	1.36	0.88
1:B:270:GLN:NE2	1:B:272:ASN:HB2	1.90	0.87
1:B:220:ILE:HD13	1:B:221:ASP:H	1.09	0.87
1:B:249:ARG:O	1:B:249:ARG:HD3	1.73	0.87
1:A:106:LEU:HD22	2:A:425:ADP:C5	2.09	0.86
1:A:93:ASN:HD22	1:A:94:GLU:N	1.72	0.86
4:B:427:DME:C15	5:B:428:PT3:H431	2.06	0.85
1:A:270:GLN:HE22	1:A:272:ASN:HB2	1.40	0.85
1:A:270:GLN:NE2	1:A:272:ASN:HD22	1.75	0.85
1:A:272:ASN:HB3	6:A:429:GOL:H32	1.58	0.85
1:A:238:LEU:HD23	1:A:239:ILE:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:CD2	1:A:239:ILE:HD12	2.09	0.83
1:B:81:GLY:HA3	7:B:462:HOH:O	1.79	0.83
1:A:189:PRO:HG2	1:A:192:PHE:CE2	2.13	0.83
1:A:270:GLN:HE21	1:A:272:ASN:HD22	1.27	0.82
2:B:425:ADP:H8	2:B:425:ADP:C5'	1.91	0.82
1:B:93:ASN:HD22	1:B:94:GLU:N	1.79	0.81
1:A:277:THR:HB	7:A:532:HOH:O	1.81	0.81
1:B:172:ALA:HB2	1:B:333:PHE:CD1	2.16	0.81
1:B:240:MET:HE1	1:B:293:PHE:HZ	1.45	0.80
1:A:270:GLN:HG2	1:A:271:GLU:N	1.97	0.79
5:A:428:PT3:O3	5:A:428:PT3:H411	1.82	0.79
1:A:199:PHE:HB2	7:A:449:HOH:O	1.82	0.78
1:B:82:LEU:HD22	5:B:428:PT3:O2	1.84	0.77
4:B:427:DME:H153	5:B:428:PT3:H431	1.67	0.77
1:B:270:GLN:HG2	1:B:271:GLU:N	1.99	0.76
1:B:195:GLU:HG2	1:B:247:MET:HE3	1.66	0.76
1:B:168:CYS:O	1:B:171:VAL:HG13	1.85	0.76
1:A:243:GLU:OE2	1:A:249:ARG:HG2	1.87	0.75
1:B:267:ASN:HA	7:B:509:HOH:O	1.86	0.75
1:B:362:VAL:HG21	1:B:417:LEU:HD21	1.67	0.75
1:B:270:GLN:HE22	1:B:272:ASN:HB2	1.50	0.75
1:A:272:ASN:HB3	6:A:429:GOL:C3	2.18	0.74
1:A:81:GLY:HA3	7:A:518:HOH:O	1.86	0.74
1:A:128:ARG:HD3	1:A:142:ASP:OD2	1.87	0.74
1:A:246:SER:OG	1:A:249:ARG:HB2	1.88	0.74
1:B:220:ILE:HD13	1:B:221:ASP:CA	2.17	0.73
1:B:93:ASN:HD22	1:B:93:ASN:C	1.97	0.73
1:B:189:PRO:HG2	1:B:192:PHE:CE2	2.24	0.72
1:A:117:PHE:HB2	1:A:204:LEU:HD21	1.70	0.72
1:B:220:ILE:HD13	1:B:220:ILE:C	2.11	0.72
1:B:74:GLU:O	1:B:74:GLU:HG3	1.91	0.71
1:A:220:ILE:HD12	1:A:220:ILE:O	1.91	0.70
1:B:70:GLU:OE2	1:B:70:GLU:N	2.15	0.70
2:B:425:ADP:C8	2:B:425:ADP:C5'	2.72	0.70
1:A:249:ARG:O	1:A:249:ARG:HD3	1.91	0.70
1:A:356:MET:O	1:A:360:VAL:HG23	1.93	0.69
1:A:117:PHE:CB	1:A:204:LEU:HD21	2.23	0.69
1:A:212:GLN:HE22	1:A:215:LYS:NZ	1.91	0.68
1:B:219:GLN:O	1:B:392:THR:HG21	1.93	0.68
1:B:238:LEU:HD23	1:B:238:LEU:C	2.18	0.68
1:B:105:ILE:HD12	1:B:105:ILE:C	2.17	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:HB2	1:B:333:PHE:CE1	2.27	0.68
1:A:93:ASN:C	1:A:93:ASN:ND2	2.47	0.68
1:A:334:ILE:HD11	1:A:353:VAL:HG13	1.74	0.68
1:B:238:LEU:CD2	1:B:239:ILE:HD12	2.23	0.68
1:A:238:LEU:HD22	1:A:239:ILE:CD1	2.24	0.67
1:B:195:GLU:HG2	1:B:247:MET:HE1	1.75	0.67
1:B:270:GLN:HE21	1:B:272:ASN:HD22	1.42	0.67
1:B:290:ALA:HB2	7:B:501:HOH:O	1.95	0.67
5:A:428:PT3:O3	5:A:428:PT3:H412	1.95	0.66
1:A:254:LYS:CE	1:A:261:SER:HA	2.23	0.66
1:B:270:GLN:NE2	1:B:272:ASN:ND2	2.43	0.66
1:B:249:ARG:HD3	1:B:249:ARG:C	2.17	0.66
1:B:76:LYS:HG3	1:B:76:LYS:O	1.94	0.66
1:A:238:LEU:CD2	1:A:239:ILE:CD1	2.73	0.65
1:A:158:THR:OG1	1:A:161:GLN:HG3	1.97	0.65
1:A:185:ARG:HD2	7:A:542:HOH:O	1.95	0.65
1:A:270:GLN:HB2	1:A:304:GLU:HG3	1.79	0.65
1:A:134:ASN:HA	7:A:464:HOH:O	1.97	0.65
1:B:76:LYS:HE2	1:B:78:ILE:HG22	1.78	0.64
1:A:172:ALA:HB2	1:A:333:PHE:CD1	2.32	0.64
1:A:105:ILE:C	1:A:105:ILE:HD12	2.23	0.64
1:A:178:LEU:CD1	1:A:264:PHE:O	2.47	0.63
1:A:106:LEU:HD22	2:A:425:ADP:N7	2.13	0.63
1:A:182:ASN:H	1:A:182:ASN:HD22	1.46	0.63
1:B:82:LEU:HD22	5:B:428:PT3:HO2	1.64	0.62
1:B:128:ARG:HD3	1:B:142:ASP:OD2	1.99	0.62
1:B:178:LEU:HD13	1:B:264:PHE:O	2.00	0.62
1:B:182:ASN:HD22	1:B:182:ASN:H	1.47	0.62
4:B:427:DME:H152	5:B:428:PT3:H431	1.82	0.62
1:B:55:ILE:O	1:B:59:ARG:HG2	2.00	0.62
1:A:322:GLU:CD	1:A:322:GLU:H	2.08	0.61
1:A:334:ILE:HD11	1:A:353:VAL:HA	1.81	0.61
1:A:172:ALA:HB2	1:A:333:PHE:CE1	2.36	0.60
1:A:316:TYR:CZ	1:A:388:GLU:HG3	2.36	0.60
1:A:220:ILE:HD11	1:A:222:LYS:HG2	1.83	0.60
1:A:261:SER:HB2	7:A:444:HOH:O	2.02	0.60
1:B:125:ASP:HA	7:B:476:HOH:O	2.01	0.60
1:B:55:ILE:O	1:B:59:ARG:CG	2.51	0.59
1:B:249:ARG:HB2	7:B:470:HOH:O	2.02	0.59
1:B:270:GLN:HE21	1:B:272:ASN:ND2	2.01	0.59
1:B:272:ASN:ND2	5:B:428:PT3:H433	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HG3	1:A:74:GLU:O	2.02	0.59
1:B:237:GLU:OE1	1:B:237:GLU:N	2.30	0.59
1:A:178:LEU:HD13	1:A:264:PHE:O	2.03	0.58
1:B:215:LYS:HE2	1:B:217:ASN:ND2	2.19	0.58
1:A:189:PRO:HG2	1:A:192:PHE:HE2	1.68	0.58
1:B:249:ARG:CD	1:B:253:LEU:HD13	2.33	0.58
1:B:358:LYS:HG3	1:B:420:TRP:CZ2	2.37	0.58
1:B:272:ASN:HD22	5:B:428:PT3:H433	1.68	0.58
1:A:220:ILE:C	1:A:220:ILE:CD1	2.61	0.58
1:A:238:LEU:HD23	1:A:238:LEU:C	2.28	0.58
1:A:334:ILE:CD1	1:A:353:VAL:HG13	2.33	0.58
1:A:168:CYS:O	1:A:171:VAL:HG13	2.04	0.58
1:B:179:HIS:ND1	1:B:263:VAL:HG21	2.19	0.58
1:A:205:TRP:CZ3	1:A:374:TRP:HB2	2.40	0.57
1:B:143:PHE:HB2	1:B:144:PRO:HD2	1.85	0.57
1:B:358:LYS:CG	1:B:420:TRP:CH2	2.85	0.57
1:A:110:TYR:OH	1:A:147:ARG:HG3	2.05	0.57
1:B:134:ASN:HA	7:B:455:HOH:O	2.04	0.57
1:A:143:PHE:HB2	1:A:144:PRO:CD	2.35	0.56
1:B:101:LYS:HE3	1:B:102:HIS:CE1	2.40	0.56
1:B:254:LYS:HE2	1:B:261:SER:HA	1.88	0.56
1:A:330:ARG:O	1:A:334:ILE:HG23	2.04	0.56
1:A:270:GLN:NE2	1:A:272:ASN:CB	2.65	0.56
1:B:173:LYS:CE	1:B:174:ASN:ND2	2.69	0.56
1:A:106:LEU:HD22	2:A:425:ADP:C6	2.41	0.56
1:A:270:GLN:HE21	1:A:272:ASN:ND2	2.00	0.56
1:A:143:PHE:HB2	1:A:144:PRO:HD2	1.87	0.56
1:A:334:ILE:CG1	1:A:353:VAL:HG13	2.36	0.56
1:B:285:ASP:OD1	5:B:428:PT3:O1	2.24	0.55
1:A:205:TRP:CE3	1:A:374:TRP:HB2	2.42	0.55
1:B:270:GLN:NE2	1:B:272:ASN:CB	2.69	0.55
1:B:189:PRO:HB2	1:B:192:PHE:CD2	2.41	0.55
1:B:158:THR:OG1	1:B:161:GLN:HG3	2.07	0.54
1:B:238:LEU:HD22	1:B:239:ILE:CD1	2.31	0.54
1:A:167:ILE:O	1:A:171:VAL:HG12	2.07	0.54
1:B:76:LYS:HE2	1:B:78:ILE:CG2	2.37	0.54
1:A:106:LEU:CD2	2:A:425:ADP:N7	2.69	0.54
1:B:270:GLN:HG2	1:B:271:GLU:H	1.71	0.54
1:A:266:HIS:O	1:A:267:ASN:HB2	2.08	0.54
1:A:280:ASN:HA	7:A:491:HOH:O	2.08	0.53
1:B:270:GLN:HE22	1:B:272:ASN:HD22	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:MET:HE1	7:A:476:HOH:O	2.08	0.53
1:B:93:ASN:C	1:B:93:ASN:ND2	2.58	0.53
1:A:212:GLN:HE22	1:A:215:LYS:HZ2	1.57	0.53
1:B:222:LYS:O	1:B:226:SER:HB2	2.09	0.53
1:A:249:ARG:HD3	1:A:249:ARG:C	2.34	0.53
4:A:427:DME:C18	6:A:429:GOL:H12	2.39	0.53
7:A:482:HOH:O	1:B:348:PRO:HG2	2.09	0.53
1:B:212:GLN:O	1:B:215:LYS:HB3	2.09	0.53
1:A:270:GLN:HG2	1:A:271:GLU:H	1.74	0.52
1:A:270:GLN:HB2	1:A:304:GLU:CG	2.39	0.52
1:B:167:ILE:O	1:B:171:VAL:HG12	2.09	0.52
1:B:117:PHE:HB2	1:B:204:LEU:HD21	1.90	0.52
1:A:270:GLN:NE2	1:A:272:ASN:ND2	2.50	0.52
1:B:143:PHE:HB2	1:B:144:PRO:CD	2.39	0.52
1:B:355:ILE:O	1:B:358:LYS:HG2	2.10	0.52
4:B:427:DME:H101	5:B:428:PT3:O3	2.09	0.52
1:B:220:ILE:CD1	1:B:221:ASP:H	2.01	0.52
1:A:117:PHE:CG	1:A:204:LEU:HD11	2.45	0.52
1:B:269:LEU:HD11	1:B:274:LEU:HD21	1.91	0.52
1:A:199:PHE:N	7:A:449:HOH:O	2.37	0.52
1:A:285:ASP:OD1	5:A:428:PT3:O2	2.27	0.52
1:A:175:MET:HE3	1:A:269:LEU:HD23	1.92	0.51
1:B:77:GLN:HB2	1:B:87:PHE:CE1	2.45	0.51
1:B:266:HIS:O	1:B:267:ASN:HB2	2.09	0.51
1:B:365:LEU:HB3	1:B:402:TYR:CE1	2.45	0.51
1:B:123:GLU:OE2	1:B:287:GLU:HB2	2.11	0.51
1:A:353:VAL:O	1:A:357:THR:HG22	2.11	0.50
1:B:178:LEU:HD22	1:B:178:LEU:O	2.09	0.50
1:B:51:THR:O	1:B:55:ILE:HG13	2.10	0.50
1:B:220:ILE:CD1	1:B:220:ILE:C	2.74	0.50
4:A:427:DME:C18	6:A:429:GOL:C1	2.90	0.50
1:B:245:PHE:CD2	1:B:245:PHE:C	2.90	0.49
1:A:106:LEU:HB3	1:A:149:GLU:HB2	1.93	0.49
1:A:216:ASN:HB2	7:A:513:HOH:O	2.13	0.49
1:B:173:LYS:HG2	1:B:340:GLN:HE21	1.78	0.49
1:B:240:MET:HE1	1:B:293:PHE:CE2	2.45	0.49
1:B:196:PRO:HB2	1:B:198:LEU:CD2	2.42	0.49
1:A:117:PHE:CD2	1:A:204:LEU:HG	2.48	0.49
4:A:427:DME:H182	6:A:429:GOL:C1	2.43	0.49
4:B:427:DME:H153	5:B:428:PT3:C43	2.40	0.49
1:A:189:PRO:CG	1:A:192:PHE:CE2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:HG2	1:B:192:PHE:HE2	1.78	0.48
1:A:418:ASN:HB2	7:A:549:HOH:O	2.12	0.48
1:A:249:ARG:HH21	1:A:252:GLU:CD	2.22	0.48
1:A:118:TYR:HE2	1:A:120:SER:HB3	1.77	0.48
1:B:315:PRO:O	1:B:316:TYR:HB2	2.14	0.47
1:A:334:ILE:HG12	1:A:353:VAL:HG13	1.95	0.47
1:B:70:GLU:H	1:B:70:GLU:CD	2.05	0.47
1:B:407:LYS:NZ	1:B:407:LYS:HB3	2.29	0.47
1:B:168:CYS:O	1:B:171:VAL:CG1	2.60	0.47
1:A:114:VAL:HG13	1:A:114:VAL:O	2.13	0.47
1:B:135:ILE:HD13	1:B:178:LEU:HD23	1.96	0.47
1:A:136:ALA:HB1	1:A:137:PRO:HD2	1.97	0.47
1:A:369:ILE:O	1:A:373:LEU:HG	2.14	0.47
1:B:249:ARG:HD3	1:B:253:LEU:HD13	1.96	0.47
1:A:101:LYS:HE3	1:A:102:HIS:CE1	2.50	0.46
1:A:209:ALA:O	1:A:213:VAL:HG23	2.15	0.46
1:A:228:ILE:O	1:A:232:ILE:HG13	2.15	0.46
1:A:125:ASP:HA	7:A:563:HOH:O	2.15	0.46
1:A:50:ASP:OD2	1:A:52:GLU:CG	2.53	0.46
1:A:195:GLU:HG2	1:A:247:MET:HE3	1.97	0.46
1:B:225:TYR:CE2	1:B:229:LEU:HD11	2.51	0.46
1:B:375:SER:HB3	1:B:395:ALA:HB2	1.97	0.46
4:B:427:DME:H32	5:B:428:PT3:H431	1.97	0.46
4:B:427:DME:H173	5:B:428:PT3:O3	2.16	0.46
1:A:93:ASN:ND2	1:A:94:GLU:N	2.52	0.46
1:B:215:LYS:HE2	1:B:217:ASN:HD21	1.81	0.46
1:B:327:GLU:O	1:B:331:LYS:HG3	2.15	0.46
1:A:224:LEU:HD21	1:A:399:PHE:HB2	1.98	0.46
1:A:342:LEU:O	1:A:343:GLN:HB2	2.16	0.45
1:B:270:GLN:HB2	1:B:304:GLU:HG3	1.98	0.45
1:A:121:LYS:HB2	1:A:121:LYS:NZ	2.31	0.45
1:A:135:ILE:HG21	1:A:178:LEU:HD23	1.99	0.45
1:A:418:ASN:CB	7:A:549:HOH:O	2.64	0.45
1:B:362:VAL:HG21	1:B:417:LEU:CD2	2.43	0.45
1:A:182:ASN:HD22	1:A:182:ASN:N	2.12	0.45
1:A:320:LYS:HA	7:A:443:HOH:O	2.16	0.45
1:B:356:MET:O	1:B:360:VAL:HG23	2.17	0.45
1:A:351:GLN:HA	1:A:351:GLN:NE2	2.19	0.45
1:B:117:PHE:HB2	1:B:204:LEU:CD2	2.46	0.44
1:A:131:SER:OG	1:A:139:ILE:HG13	2.16	0.44
1:A:212:GLN:O	1:A:215:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PHE:CE2	1:A:330:ARG:HG2	2.53	0.44
1:A:117:PHE:HB3	1:A:204:LEU:HD21	1.98	0.44
1:A:237:GLU:OE2	1:A:244:LYS:NZ	2.47	0.44
1:A:331:LYS:HE2	1:A:357:THR:HG21	1.99	0.44
1:A:279:ASN:ND2	7:A:519:HOH:O	2.51	0.44
1:B:129:TYR:CE1	1:B:189:PRO:HD3	2.53	0.44
1:B:238:LEU:O	1:B:417:LEU:HD23	2.18	0.44
1:A:268:ASP:OD2	5:A:428:PT3:O41	2.35	0.44
1:A:199:PHE:CB	7:A:449:HOH:O	2.53	0.44
1:A:289:SER:O	1:A:290:ALA:HB2	2.19	0.43
1:A:390:ASP:OD1	1:A:390:ASP:C	2.61	0.43
1:B:402:TYR:HD2	1:B:403:LEU:HD13	1.83	0.43
5:A:428:PT3:H411	5:A:428:PT3:HO3	1.80	0.43
1:B:205:TRP:CE3	1:B:374:TRP:HB2	2.52	0.43
1:A:207:GLU:O	1:A:211:ILE:HG12	2.18	0.43
1:A:142:ASP:C	1:A:142:ASP:OD1	2.61	0.43
1:B:220:ILE:CD1	1:B:221:ASP:C	2.91	0.43
1:B:325:PRO:HB3	1:B:329:LEU:HD23	2.01	0.43
1:A:334:ILE:HD11	1:A:353:VAL:CA	2.48	0.43
1:A:402:TYR:CD2	1:A:402:TYR:C	2.96	0.43
1:A:60:LYS:NZ	7:A:504:HOH:O	2.51	0.43
1:A:105:ILE:C	1:A:105:ILE:CD1	2.92	0.43
1:A:305:TYR:CG	1:A:325:PRO:HD3	2.54	0.43
1:A:50:ASP:OD2	1:A:53:ILE:HG13	2.19	0.42
4:A:427:DME:H61	5:A:428:PT3:H412	2.01	0.42
1:A:87:PHE:HB2	1:A:107:PHE:HB3	2.00	0.42
1:B:306:ILE:O	1:B:319:PHE:HA	2.18	0.42
1:A:110:TYR:OH	1:A:147:ARG:CG	2.66	0.42
1:A:209:ALA:O	1:A:210:LYS:C	2.63	0.42
1:B:55:ILE:O	1:B:59:ARG:HG3	2.18	0.42
1:B:145:GLU:CD	1:B:145:GLU:H	2.27	0.42
1:A:270:GLN:HB2	1:A:304:GLU:CD	2.44	0.42
1:A:220:ILE:HG22	1:A:392:THR:HG23	2.00	0.42
1:A:387:VAL:O	1:A:387:VAL:CG1	2.68	0.42
1:B:142:ASP:OD1	1:B:142:ASP:C	2.63	0.42
1:B:354:HIS:HB2	7:B:460:HOH:O	2.19	0.42
1:A:322:GLU:CD	1:A:322:GLU:N	2.76	0.42
1:B:238:LEU:HD23	1:B:238:LEU:O	2.20	0.41
1:B:228:ILE:O	1:B:232:ILE:HG13	2.20	0.41
1:A:188:PHE:HA	1:A:189:PRO:HD3	1.93	0.41
1:A:245:PHE:HZ	1:A:247:MET:HE1	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:N	7:B:514:HOH:O	2.42	0.41
1:B:106:LEU:C	1:B:106:LEU:HD13	2.46	0.41
1:A:237:GLU:HA	1:A:243:GLU:O	2.20	0.41
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.78	0.41
4:A:427:DME:H82	5:A:428:PT3:H432	2.01	0.41
1:B:104:ARG:HG3	7:B:500:HOH:O	2.20	0.41
1:B:122:VAL:HG13	1:B:123:GLU:N	2.35	0.41
1:A:178:LEU:HB2	7:A:476:HOH:O	2.20	0.41
4:A:427:DME:H181	6:A:429:GOL:C1	2.51	0.41
1:B:219:GLN:HE21	1:B:219:GLN:C	2.29	0.41
1:B:238:LEU:C	1:B:238:LEU:CD2	2.89	0.41
1:A:420:TRP:CG	1:A:421:LEU:N	2.89	0.41
4:A:427:DME:H182	6:A:429:GOL:H12	2.02	0.41
1:B:105:ILE:C	1:B:105:ILE:CD1	2.88	0.41
1:B:179:HIS:CE1	1:B:263:VAL:HG21	2.55	0.41
1:A:80:SER:OG	6:A:429:GOL:H11	2.21	0.41
1:A:316:TYR:CZ	1:A:388:GLU:CG	3.04	0.41
1:A:332:LEU:CD2	1:B:332:LEU:HD22	2.50	0.41
1:A:346:VAL:HA	1:A:350:GLN:OE1	2.21	0.41
1:B:189:PRO:HB3	1:B:191:ARG:NH1	2.35	0.41
1:A:143:PHE:HD1	1:A:145:GLU:HG2	1.86	0.41
1:A:192:PHE:O	1:A:193:ASP:C	2.64	0.41
1:B:305:TYR:CG	1:B:325:PRO:HD3	2.56	0.41
1:A:324:TYR:CD1	1:A:325:PRO:HD2	2.56	0.40
1:B:180:ILE:HD12	1:B:180:ILE:C	2.46	0.40
1:B:235:LEU:O	1:B:239:ILE:HD13	2.22	0.40
1:B:195:GLU:CG	1:B:247:MET:HE1	2.48	0.40
1:B:403:LEU:HD12	1:B:403:LEU:HA	1.89	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:B:351:GLN:CG	1:B:351:GLN:OE1[2_555]	2.14	0.06

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	347/424 (82%)	331 (95%)	16 (5%)	0	100	100
1	B	348/424 (82%)	337 (97%)	11 (3%)	0	100	100
All	All	695/848 (82%)	668 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	329/391 (84%)	313 (95%)	16 (5%)	22	28
1	B	330/391 (84%)	306 (93%)	24 (7%)	13	14
All	All	659/782 (84%)	619 (94%)	40 (6%)	17	20

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	93	ASN
1	A	121	LYS
1	A	145	GLU
1	A	171	VAL
1	A	182	ASN
1	A	220	ILE
1	A	249	ARG

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	262	LEU
1	A	270	GLN
1	A	287	GLU
1	A	322	GLU
1	A	334	ILE
1	A	351	GLN
1	A	388	GLU
1	B	51	THR
1	B	59	ARG
1	B	70	GLU
1	B	74	GLU
1	B	76	LYS
1	B	93	ASN
1	B	121	LYS
1	B	145	GLU
1	B	171	VAL
1	B	178	LEU
1	B	182	ASN
1	B	210	LYS
1	B	219	GLN
1	B	220	ILE
1	B	240	MET
1	B	249	ARG
1	B	253	LEU
1	B	255	LEU
1	B	270	GLN
1	B	287	GLU
1	B	314	GLN
1	B	387	VAL
1	B	403	LEU
1	B	411	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	132	ASN
1	A	138	ASN
1	A	174	ASN
1	A	182	ASN
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	270	GLN
1	A	278	GLN
1	A	279	ASN
1	A	314	GLN
1	A	340	GLN
1	A	351	GLN
1	A	396	ASN
1	B	93	ASN
1	B	113	HIS
1	B	132	ASN
1	B	134	ASN
1	B	138	ASN
1	B	174	ASN
1	B	182	ASN
1	B	212	GLN
1	B	219	GLN
1	B	234	GLN
1	B	270	GLN
1	B	340	GLN
1	B	396	ASN

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	DME	A	427	-	17,17,17	0.71	0	22,22,22	0.61	0
2	ADP	B	425	3	28,29,29	1.44	4 (14%)	43,45,45	1.78	7 (16%)
5	PT3	A	428	3	12,12,12	0.73	0	15,15,15	0.73	0
2	ADP	A	425	3	28,29,29	1.42	4 (14%)	43,45,45	1.83	8 (18%)
5	PT3	B	428	3	12,12,12	0.69	0	15,15,15	0.85	0
6	GOL	A	429	-	5,5,5	0.39	0	5,5,5	0.24	0
4	DME	B	427	-	17,17,17	0.71	0	22,22,22	0.60	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
4	DME	A	427	-	-	9/15/15/15	-
2	ADP	B	425	3	-	4/16/32/32	0/3/3/3
5	PT3	A	428	3	-	2/16/16/16	-
2	ADP	A	425	3	-	0/16/32/32	0/3/3/3
5	PT3	B	428	3	-	9/16/16/16	-
6	GOL	A	429	-	-	4/4/4/4	-
4	DME	B	427	-	-	8/15/15/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	425	ADP	C5-C4	4.86	1.47	1.39
2	A	425	ADP	C5-C4	4.72	1.47	1.39
2	A	425	ADP	C5-C6	2.78	1.48	1.41
2	B	425	ADP	C5-C6	2.74	1.48	1.41
2	B	425	ADP	C8-N7	2.38	1.36	1.31
2	A	425	ADP	C8-N7	2.31	1.36	1.31
2	A	425	ADP	C5-N7	-2.23	1.35	1.39
2	B	425	ADP	C5-N7	-2.21	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	425	ADP	C5-C4-N3	-5.96	118.52	126.72
2	B	425	ADP	C5-C4-N3	-5.70	118.87	126.72
2	A	425	ADP	N3-C4-N9	4.67	135.12	127.17
2	B	425	ADP	N3-C4-N9	4.61	135.01	127.17
2	A	425	ADP	C2-N3-C4	3.77	121.03	111.83
2	B	425	ADP	C2-N3-C4	3.58	120.58	111.83
2	A	425	ADP	C4-C5-N7	-3.56	106.51	110.58
2	B	425	ADP	C4-C5-N7	-3.27	106.84	110.58
2	A	425	ADP	N3-C2-N1	-3.23	123.70	128.58
2	B	425	ADP	N3-C2-N1	-3.10	123.89	128.58
2	B	425	ADP	C4-N9-C8	2.67	108.54	105.74
2	A	425	ADP	C5-N7-C8	2.63	107.59	103.45
2	A	425	ADP	C4-N9-C8	2.54	108.41	105.74
2	B	425	ADP	C5-N7-C8	2.37	107.18	103.45
2	A	425	ADP	C6-C5-N7	2.07	136.09	132.09

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	425	ADP	C5'-O5'-PA-O3A
5	A	428	PT3	C3-C4-N4-C41
5	B	428	PT3	C1-C2-C3-O3
5	B	428	PT3	O2-C2-C3-O3
5	B	428	PT3	O2-C2-C3-C4
5	B	428	PT3	C2-C3-C4-O41
5	B	428	PT3	C2-C3-C4-N4
5	B	428	PT3	O3-C3-C4-O41
5	B	428	PT3	O3-C3-C4-N4
6	A	429	GOL	C1-C2-C3-O3
5	B	428	PT3	C1-C2-C3-C4
5	A	428	PT3	O41-C4-N4-C41
2	B	425	ADP	C3'-C4'-C5'-O5'
2	B	425	ADP	O4'-C4'-C5'-O5'
6	A	429	GOL	O1-C1-C2-C3
6	A	429	GOL	O2-C2-C3-O3
4	B	427	DME	C4-C5-C6-C7
4	A	427	DME	C6-C7-C8-C9
4	A	427	DME	C10-C11-N12-C17
4	B	427	DME	C5-C6-C7-C8
4	A	427	DME	C10-C11-N12-C18
5	B	428	PT3	N4-C41-C42-C43
4	A	427	DME	C2-C3-C4-C5

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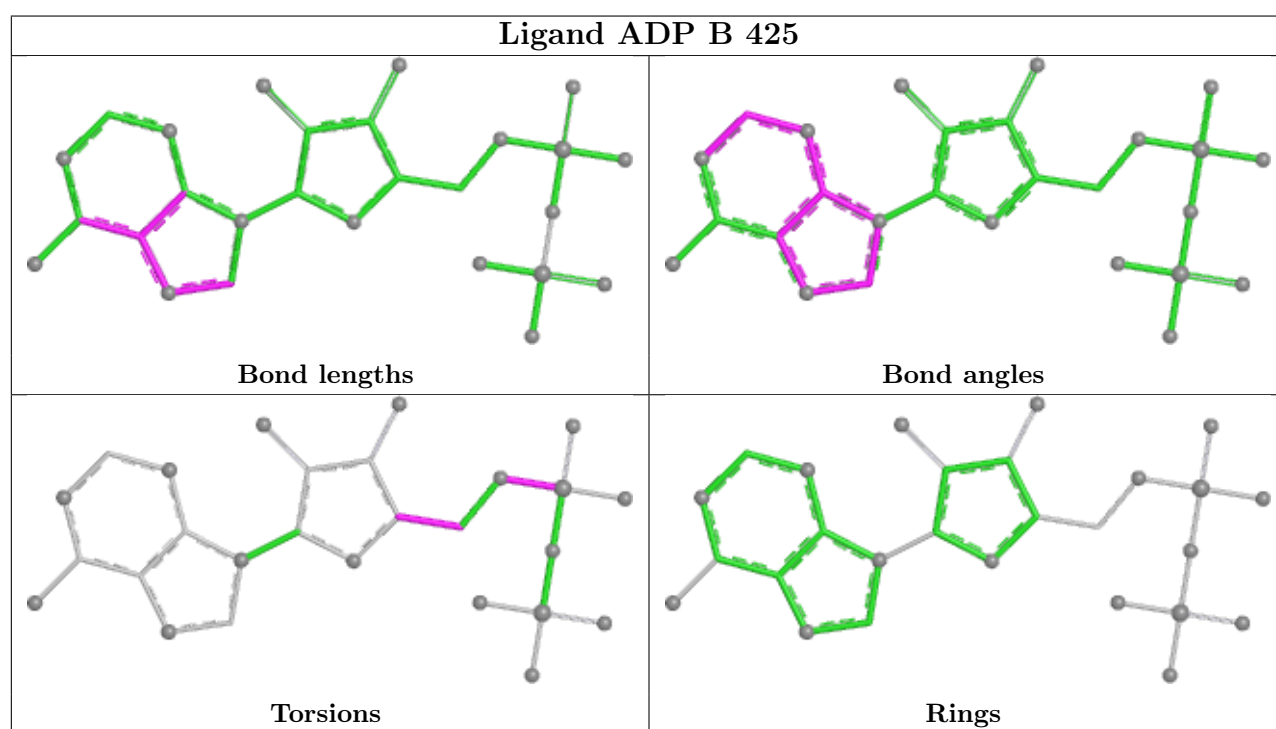
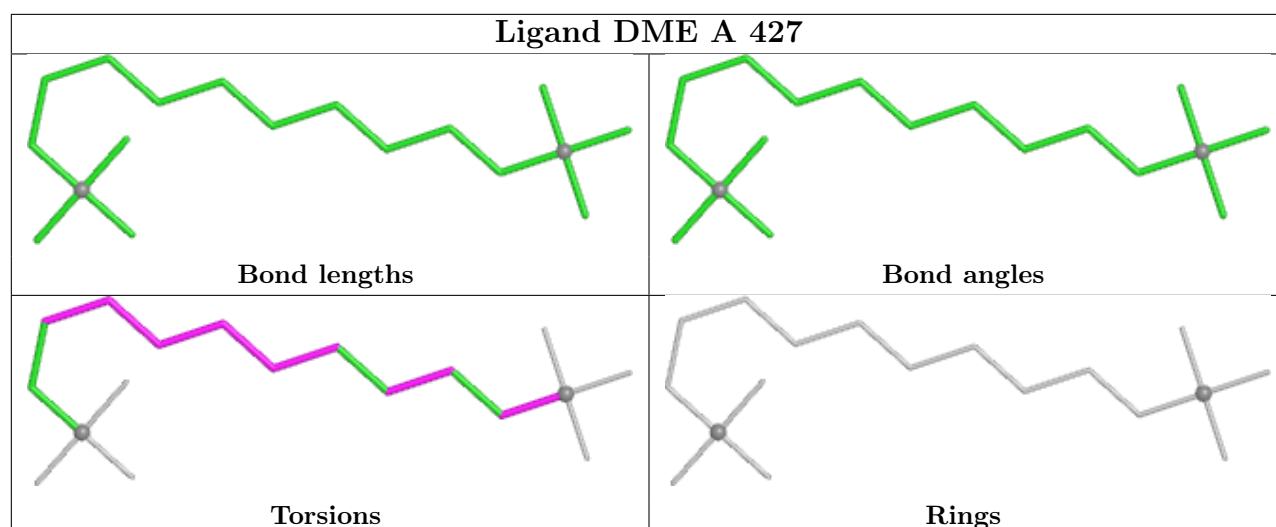
Mol	Chain	Res	Type	Atoms
6	A	429	GOL	O1-C1-C2-O2
4	A	427	DME	C10-C11-N12-C16
4	A	427	DME	C5-C6-C7-C8
4	B	427	DME	C6-C7-C8-C9
4	B	427	DME	C3-C2-N1-C13
4	B	427	DME	C7-C8-C9-C10
4	B	427	DME	C3-C2-N1-C15
4	B	427	DME	C3-C2-N1-C14
4	A	427	DME	C11-C10-C9-C8
4	A	427	DME	C4-C5-C6-C7
4	B	427	DME	C11-C10-C9-C8
2	B	425	ADP	C5'-O5'-PA-O1A
4	A	427	DME	C3-C4-C5-C6

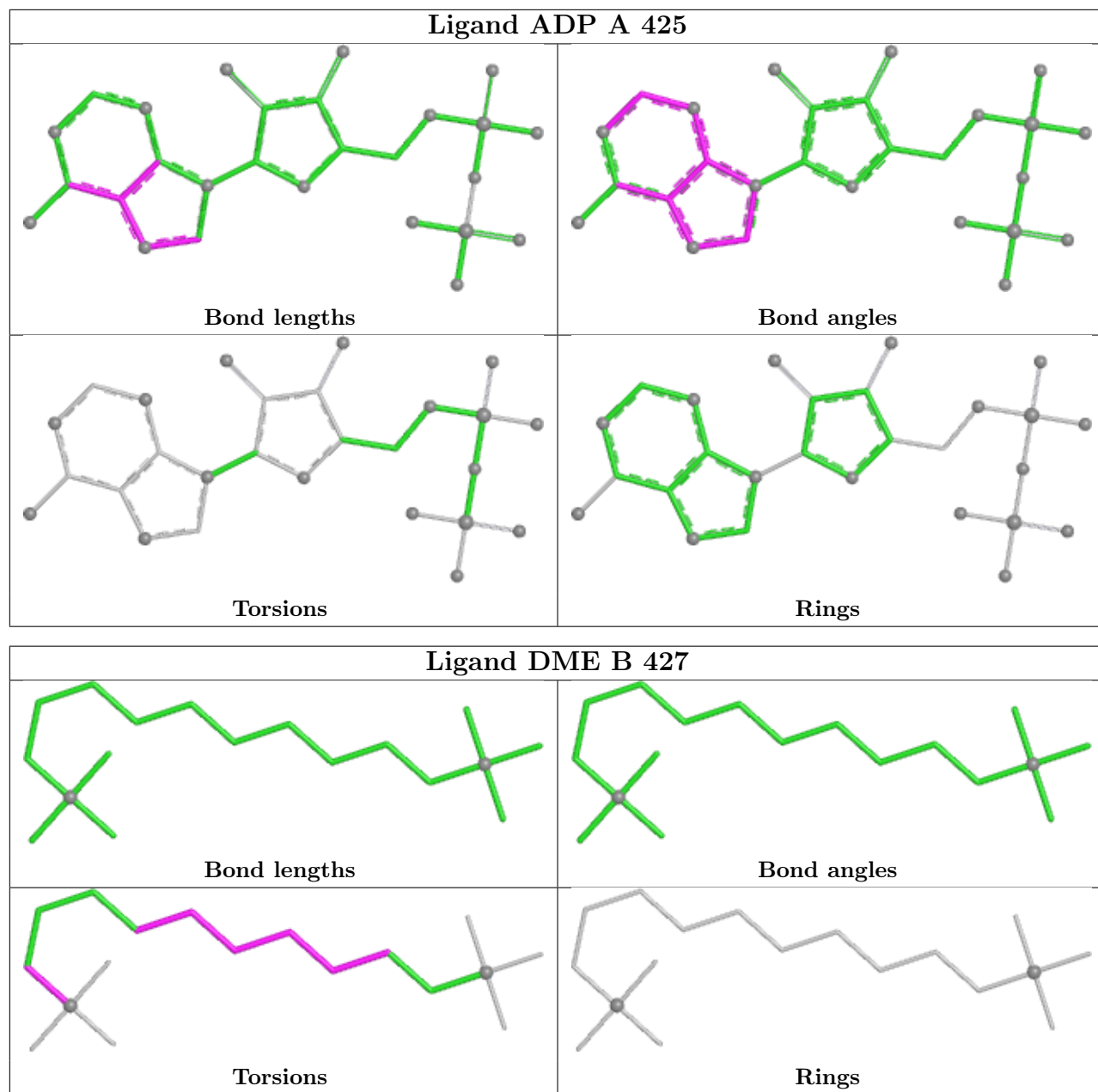
There are no ring outliers.

7 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	427	DME	7	0
2	B	425	ADP	4	0
5	A	428	PT3	8	0
2	A	425	ADP	4	0
5	B	428	PT3	12	0
6	A	429	GOL	8	0
4	B	427	DME	7	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 [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	357/424 (84%)	0.38	8 (2%) 62 67	15, 24, 37, 43	0
1	B	358/424 (84%)	0.38	11 (3%) 51 58	13, 24, 36, 46	1 (0%)
All	All	715/848 (84%)	0.38	19 (2%) 56 63	13, 24, 36, 46	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	SER	3.6
1	A	81	GLY	3.3
1	A	216	ASN	3.3
1	A	118	TYR	3.2
1	A	114	VAL	3.1
1	B	117	PHE	3.0
1	B	387	VAL	2.9
1	B	217	ASN	2.7
1	A	117	PHE	2.4
1	B	50	ASP	2.4
1	B	114	VAL	2.4
1	A	387	VAL	2.3
1	A	423	ASN	2.2
1	B	153	ASP	2.2
1	B	242	GLY	2.2
1	B	118	TYR	2.1
1	B	234	GLN	2.1
1	B	377	ALA	2.0
1	A	242	GLY	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](#)

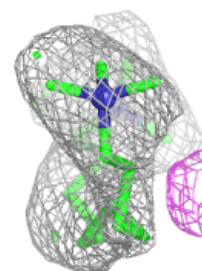
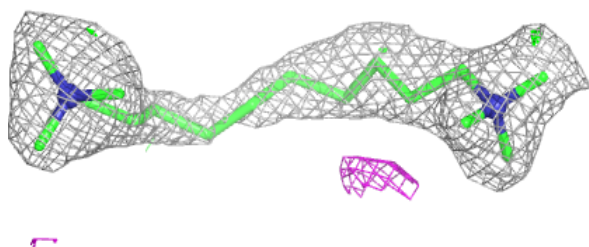
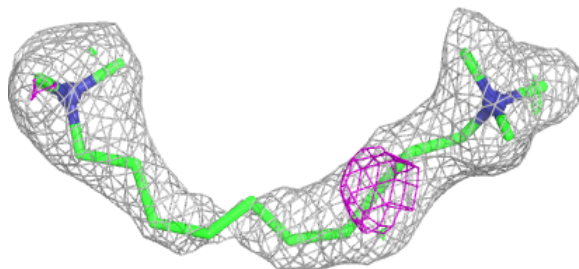
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PT3	B	428	13/13	0.79	0.15	32,32,33,33	0
4	DME	B	427	18/18	0.80	0.16	29,32,34,35	0
6	GOL	A	429	6/6	0.86	0.12	31,31,32,32	0
5	PT3	A	428	13/13	0.89	0.10	25,25,26,26	0
4	DME	A	427	18/18	0.90	0.11	17,21,23,23	0
2	ADP	B	425	27/27	0.94	0.08	23,24,25,25	0
3	MG	A	430	1/1	0.96	0.04	17,17,17,17	0
2	ADP	A	425	27/27	0.96	0.06	20,21,22,22	0
3	MG	B	429	1/1	0.98	0.04	18,18,18,18	0
3	MG	A	426	1/1	0.98	0.03	18,18,18,18	0
3	MG	B	426	1/1	0.98	0.03	16,16,16,16	0

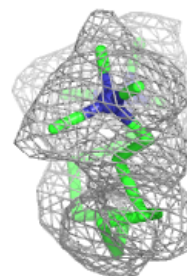
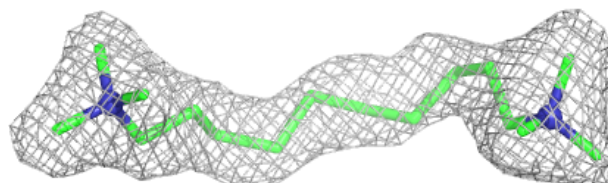
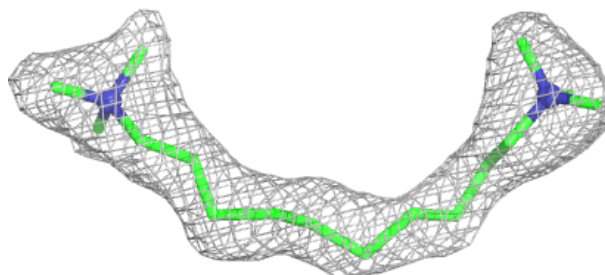
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DME B 427:

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

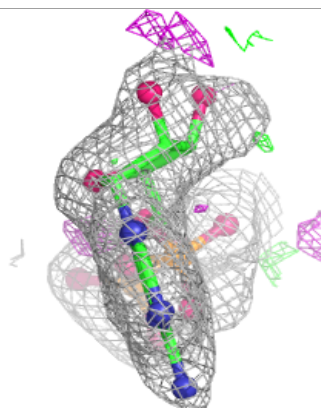
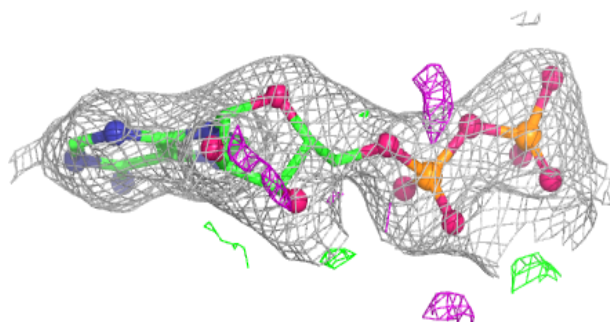
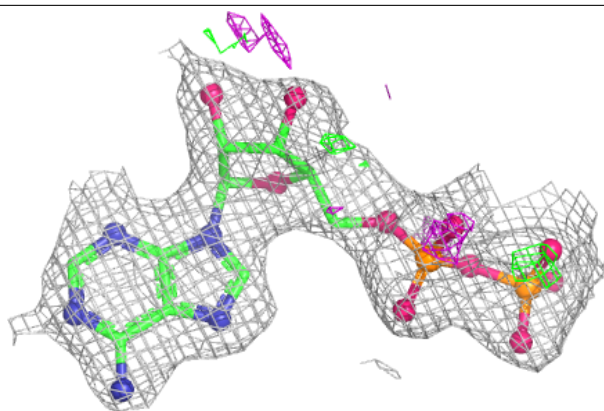
**Electron density around DME A 427:**

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

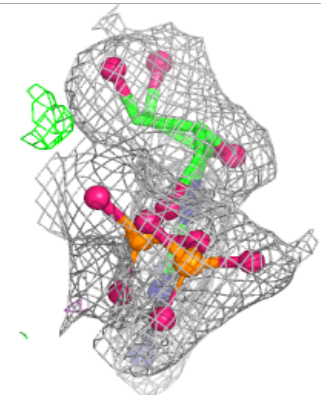
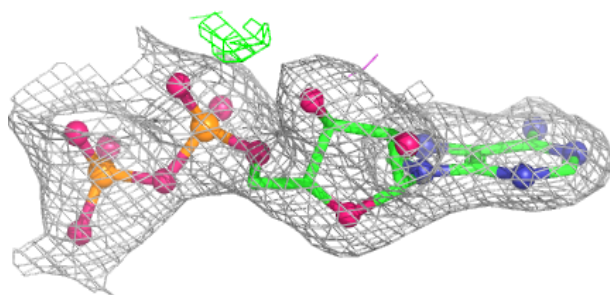
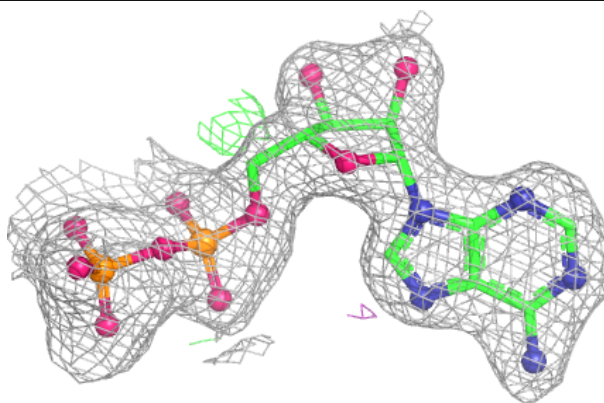


Electron density around ADP B 425:

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

**Electron density around ADP A 425:**

$2mF_o-DF_c$ (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.