



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:01 PM UTC

PDB ID : 1XJN / pdb_00001xjn
Title : Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dATP-CDP complex
Authors : Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.
Deposited on : 2004-09-23
Resolution : 2.25 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

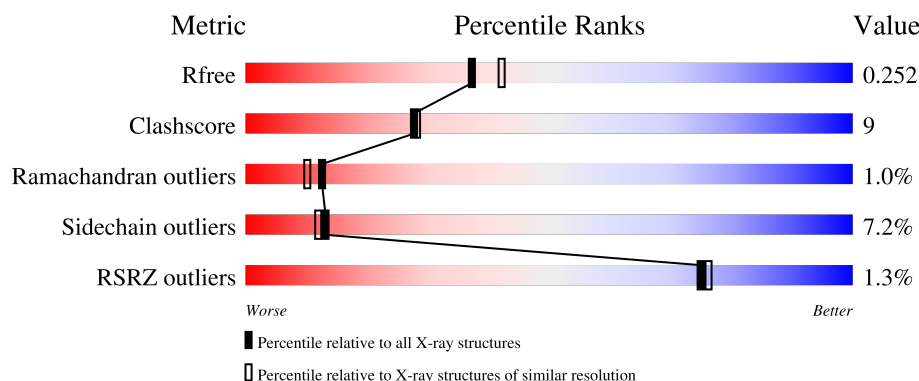
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	644	% 76% 15% • • •
1	B	644	2% 72% 18% • 5%
1	C	644	% 71% 20% • 5%
1	D	644	% 70% 20% • 6%

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
4	CL	B	1009	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20534 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.

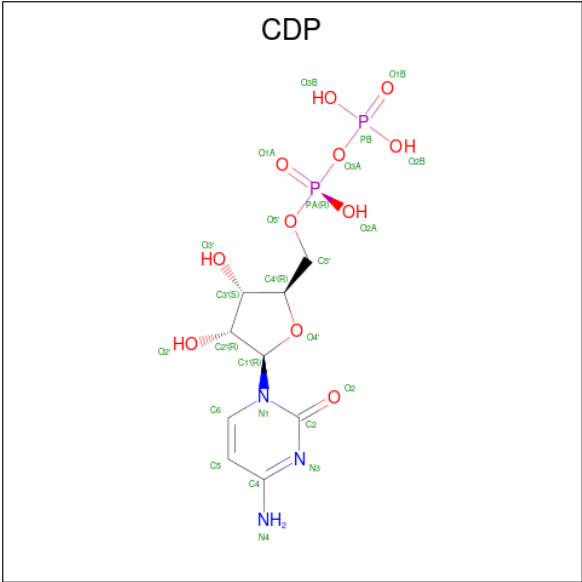
- Molecule 1 is a protein called ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4958	3181	839	918	20			
1	B	610	Total	C	N	O	S	0	0	0
			4898	3139	834	905	20			
1	C	615	Total	C	N	O	S	0	0	0
			4934	3161	838	915	20			
1	D	607	Total	C	N	O	S	0	0	0
			4874	3129	824	901	20			

There are 4 discrepancies between the modelled and reference sequences:

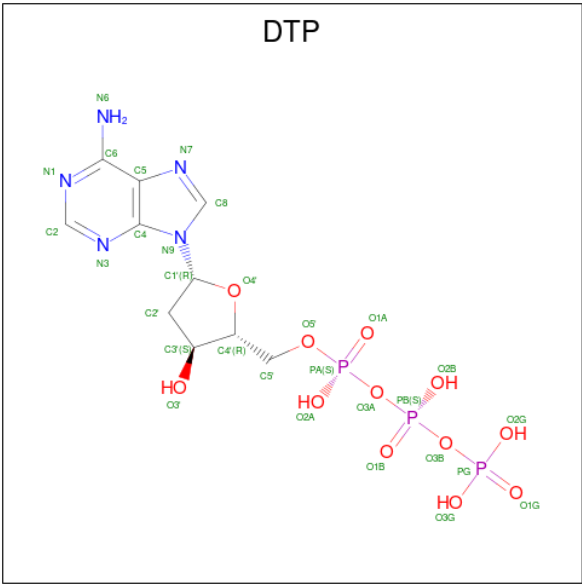
Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839
C	205	SER	TYR	SEE REMARK 999	UNP O33839
D	205	SER	TYR	SEE REMARK 999	UNP O33839

- Molecule 2 is CYTIDINE-5'-DIPHOSPHATE (CCD ID: CDP) (formula: C₉H₁₅N₃O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

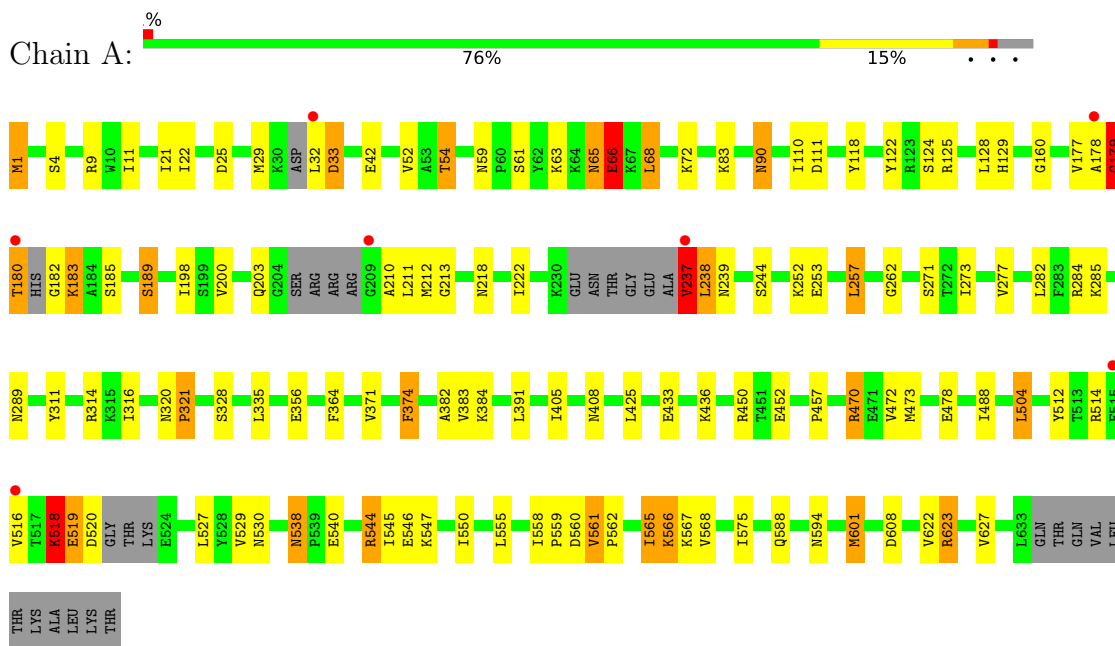
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total	O	0	0
			180	180		
5	B	197	Total	O	0	0
			197	197		
5	C	167	Total	O	0	0
			167	167		
5	D	105	Total	O	0	0
			105	105		

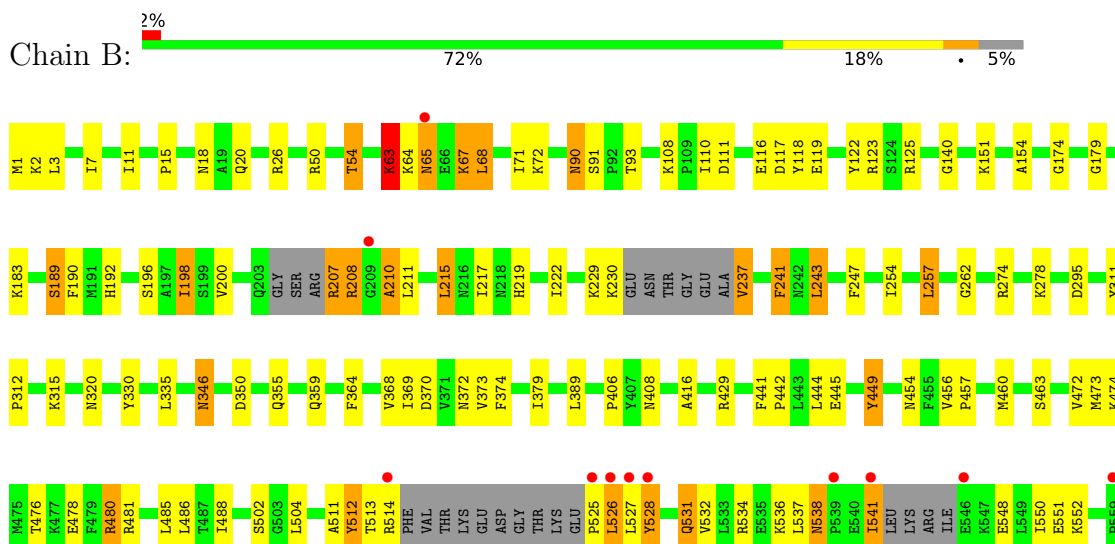
3 Residue-property plots

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

- Molecule 1: ribonucleotide reductase, B12-dependent



- Molecule 1: ribonucleotide reductase, B12-dependent



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.97Å 123.83Å 117.41Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	19.54 – 2.25 19.54 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.54-2.25) 99.3 (19.54-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.26Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.254 0.190 , 0.252	Depositor DCC
R_{free} test set	6927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtrriage
Anisotropy	0.575	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20534	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5686e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DTP, CL, CDP

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	1.18	6/5053 (0.1%)	1.20	24/6817 (0.4%)
1	B	1.22	8/4994 (0.2%)	1.24	22/6739 (0.3%)
1	C	1.11	7/5031 (0.1%)	1.16	16/6791 (0.2%)
1	D	1.11	8/4971 (0.2%)	1.19	11/6710 (0.2%)
All	All	1.16	29/20049 (0.1%)	1.20	73/27057 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	3
1	D	0	1
All	All	0	8

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	VAL	CA-CB	7.32	1.62	1.54
1	B	247	PHE	CA-C	-7.28	1.45	1.52
1	A	405	ILE	CA-CB	6.63	1.60	1.54
1	D	489	ALA	CA-CB	6.50	1.62	1.53
1	A	222	ILE	CA-CB	6.25	1.62	1.54
1	B	526	LEU	CA-C	6.25	1.59	1.53
1	D	245	VAL	CA-CB	6.08	1.61	1.54
1	B	373	VAL	CA-CB	5.98	1.61	1.54
1	D	412	ALA	N-CA	5.93	1.53	1.46
1	B	532	VAL	CA-CB	5.90	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	456	VAL	CA-C	5.88	1.56	1.52
1	A	200	VAL	CA-CB	5.83	1.61	1.54
1	C	624	GLY	N-CA	5.79	1.51	1.45
1	D	527	LEU	N-CA	5.74	1.53	1.46
1	A	316	ILE	CA-CB	5.55	1.60	1.54
1	D	527	LEU	CA-C	5.54	1.60	1.52
1	D	575	ILE	CA-CB	5.46	1.60	1.54
1	B	190	PHE	CA-C	5.41	1.59	1.52
1	C	513	THR	CA-CB	5.37	1.61	1.53
1	A	561	VAL	N-CA	5.32	1.51	1.46
1	D	22	ILE	CA-CB	5.30	1.60	1.54
1	C	507	ASN	CA-C	-5.28	1.46	1.52
1	B	575	ILE	CA-CB	5.26	1.60	1.54
1	C	180	THR	CA-CB	5.26	1.62	1.53
1	C	423	ILE	CA-CB	5.25	1.60	1.54
1	C	415	PHE	CA-C	5.20	1.59	1.52
1	B	449	TYR	N-CA	5.19	1.52	1.46
1	D	163	VAL	C-O	5.10	1.29	1.24
1	C	483	VAL	CA-CB	5.03	1.60	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	LEU	N-CA-C	10.30	126.48	111.96
1	C	527	LEU	N-CA-C	8.80	120.80	111.03
1	A	237	VAL	CA-C-N	8.69	137.35	121.70
1	A	237	VAL	C-N-CA	8.69	137.35	121.70
1	A	374	PHE	CA-C-N	-7.60	112.18	121.00
1	A	374	PHE	C-N-CA	-7.60	112.18	121.00
1	B	526	LEU	CA-C-N	7.59	135.37	121.70
1	B	526	LEU	C-N-CA	7.59	135.37	121.70
1	B	528	TYR	N-CA-C	7.42	121.54	109.59
1	C	377	ASP	N-CA-C	7.27	119.21	111.28
1	B	565	ILE	N-CA-C	-7.00	100.54	109.58
1	A	518	LYS	N-CA-C	6.80	122.09	109.24
1	B	478	GLU	N-CA-C	6.74	119.63	111.40
1	A	179	GLY	CA-C-N	6.72	133.79	121.70
1	A	179	GLY	C-N-CA	6.72	133.79	121.70
1	A	238	LEU	N-CA-C	6.65	129.62	111.00
1	C	561	VAL	N-CA-C	6.60	114.31	108.63
1	B	91	SER	CA-C-N	-6.47	112.96	119.56
1	B	91	SER	C-N-CA	-6.47	112.96	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	PRO	CA-C-N	6.45	133.31	121.70
1	D	525	PRO	C-N-CA	6.45	133.31	121.70
1	D	305	ASN	N-CA-C	6.43	118.37	111.36
1	D	534	ARG	N-CA-C	-6.33	100.91	110.28
1	A	565	ILE	N-CA-C	-6.27	100.68	109.21
1	B	623	ARG	NE-CZ-NH1	6.27	127.77	121.50
1	A	568	VAL	N-CA-C	6.20	116.25	110.42
1	C	418	ASN	N-CA-C	6.19	117.83	111.14
1	A	21	ILE	CB-CA-C	-6.12	103.88	112.14
1	C	67	LYS	N-CA-C	6.05	117.88	111.28
1	A	110	ILE	CA-C-N	6.01	128.61	120.38
1	A	110	ILE	C-N-CA	6.01	128.61	120.38
1	B	140	GLY	N-CA-C	6.00	118.93	112.33
1	C	183	LYS	N-CA-C	5.89	118.23	108.99
1	D	451	THR	N-CA-C	5.87	119.62	112.23
1	A	383	VAL	N-CA-C	5.86	116.04	110.53
1	B	623	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	210	ALA	N-CA-C	5.74	123.02	110.80
1	A	382	ALA	CA-C-N	5.71	127.86	120.56
1	A	382	ALA	C-N-CA	5.71	127.86	120.56
1	C	623	ARG	N-CA-C	-5.70	106.30	113.72
1	B	346	ASN	CB-CA-C	-5.66	104.28	111.86
1	D	253	GLU	N-CA-C	-5.61	105.16	112.23
1	B	346	ASN	N-CA-C	5.58	119.33	111.52
1	C	35	ASN	N-CA-C	5.52	118.69	110.14
1	B	623	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	D	385	GLU	N-CA-C	5.45	118.14	111.82
1	B	623	ARG	CD-NE-CZ	5.41	131.98	124.40
1	C	321	PRO	N-CA-C	5.39	121.79	113.75
1	A	111	ASP	CB-CA-C	-5.38	101.53	110.68
1	B	93	THR	N-CA-C	-5.34	105.54	111.36
1	B	210	ALA	N-CA-C	-5.33	103.36	110.55
1	D	527	LEU	N-CA-C	5.32	122.13	110.80
1	B	11	ILE	N-CA-C	5.29	117.66	111.05
1	D	67	LYS	N-CA-C	5.28	116.72	111.07
1	C	133	ALA	N-CA-C	5.17	119.65	113.23
1	C	219	HIS	CA-C-N	-5.16	114.29	119.56
1	C	219	HIS	C-N-CA	-5.16	114.29	119.56
1	A	252	LYS	CA-C-N	5.15	127.13	120.44
1	A	252	LYS	C-N-CA	5.15	127.13	120.44
1	B	623	ARG	N-CA-C	-5.14	107.03	113.72
1	A	321	PRO	N-CA-C	5.14	121.41	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	SER	N-CA-C	5.14	119.18	113.02
1	A	545	ILE	N-CA-C	5.13	117.46	111.05
1	C	623	ARG	CB-CG-CD	5.13	123.10	111.30
1	B	370	ASP	N-CA-C	5.13	117.61	111.71
1	B	463	SER	N-CA-C	5.12	116.85	108.76
1	B	67	LYS	N-CA-C	5.12	117.52	111.33
1	C	217	ILE	N-CA-C	5.06	118.15	111.17
1	C	538	ASN	CA-C-N	5.05	124.77	119.82
1	C	538	ASN	C-N-CA	5.05	124.77	119.82
1	A	328	SER	N-CA-C	-5.04	104.03	110.53
1	D	308	TYR	CA-C-N	5.02	125.29	119.47
1	D	308	TYR	C-N-CA	5.02	125.29	119.47

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	LYS	Peptide
1	B	241	PHE	Peptide
1	B	525	PRO	Peptide
1	B	63	LYS	Peptide
1	C	182	GLY	Peptide
1	C	241	PHE	Peptide
1	C	526	LEU	Peptide
1	D	540	GLU	Peptide

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	4958	0	5014	83	0
1	B	4898	0	4948	91	0
1	C	4934	0	4980	90	0
1	D	4874	0	4920	97	0
2	A	25	0	12	1	0
2	B	25	0	12	1	0
2	C	25	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	25	0	12	1	0
3	A	30	0	12	0	0
3	B	30	0	12	0	0
3	C	60	0	24	0	0
4	B	1	0	0	3	0
5	A	180	0	0	7	0
5	B	197	0	0	12	0
5	C	167	0	0	5	0
5	D	105	0	0	5	0
All	All	20534	0	19958	359	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 9.

All (359) 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:601:MET:HE1	1:B:610:VAL:HG22	1.18	1.16
1:A:565:ILE:O	1:A:566:LYS:HB2	1.45	1.12
1:D:212:MET:HE1	1:D:244:SER:HB2	1.23	1.12
1:B:565:ILE:O	1:B:566:LYS:CB	1.95	1.09
1:D:212:MET:CE	1:D:244:SER:HB2	1.83	1.07
1:B:565:ILE:O	1:B:566:LYS:HB2	1.49	1.05
1:C:32:LEU:HD12	1:C:32:LEU:H	1.22	1.04
1:A:565:ILE:O	1:A:566:LYS:CB	2.04	1.03
1:D:601:MET:HE1	1:D:610:VAL:HG22	1.06	1.03
1:D:257:LEU:HD22	1:D:262:GLY:HA3	1.41	1.02
1:D:212:MET:HE1	1:D:244:SER:CB	1.94	0.96
1:B:2:LYS:HE3	5:B:1182:HOH:O	1.67	0.94
1:B:63:LYS:HB3	1:B:64:LYS:O	1.66	0.93
1:B:601:MET:HE1	1:B:610:VAL:CG2	1.99	0.92
1:B:207:ARG:NH1	4:B:1009:CL:CL	2.41	0.90
1:D:601:MET:CE	1:D:610:VAL:HG22	1.98	0.89
1:A:65:ASN:H	1:A:65:ASN:HD22	1.21	0.88
1:B:601:MET:CE	1:B:610:VAL:HG22	2.02	0.87
1:C:512:TYR:O	1:C:527:LEU:O	1.93	0.86
1:D:601:MET:HE1	1:D:610:VAL:CG2	2.01	0.86
1:D:257:LEU:CD2	1:D:262:GLY:HA3	2.04	0.86
1:B:18:ASN:HD21	1:B:514:ARG:HH21	1.22	0.83
1:D:578:MET:HB3	5:D:1061:HOH:O	1.76	0.83
1:A:544:ARG:HH11	1:A:544:ARG:CB	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:LEU:HD22	1:C:262:GLY:HA3	1.60	0.82
1:A:538:ASN:HD21	1:A:540:GLU:HG2	1.44	0.82
1:A:519:GLU:H	1:A:520:ASP:HA	1.44	0.82
5:C:1166:HOH:O	1:D:181:HIS:HE1	1.63	0.81
1:B:514:ARG:C	1:B:526:LEU:CB	2.53	0.81
1:B:210:ALA:O	5:B:1176:HOH:O	1.99	0.80
1:D:514:ARG:O	1:D:526:LEU:HB2	1.79	0.80
1:B:514:ARG:C	1:B:526:LEU:HB2	2.08	0.78
1:A:601:MET:CE	1:A:627:VAL:HB	2.13	0.77
1:D:212:MET:HE3	1:D:214:ILE:HG12	1.63	0.77
1:C:63:LYS:HB2	1:C:66:GLU:HG3	1.66	0.77
1:D:450:ARG:NH1	1:D:477:LYS:O	2.17	0.77
1:B:50:ARG:NH2	1:B:108:LYS:O	2.18	0.76
1:C:31:ASP:OD2	1:C:33:ASP:HB2	1.85	0.76
1:C:338:ILE:HG12	1:C:357:LEU:HD13	1.68	0.76
1:A:180:THR:HG23	1:A:182:GLY:HA3	1.67	0.75
1:B:565:ILE:O	1:B:566:LYS:HB3	1.85	0.75
1:A:544:ARG:HB2	1:A:544:ARG:NH1	2.02	0.75
1:D:580:HIS:CE1	1:D:600:ASN:HD22	2.05	0.75
1:B:537:LEU:HD13	1:B:565:ILE:HD13	1.68	0.75
1:A:538:ASN:ND2	1:A:540:GLU:HG2	2.03	0.74
1:A:198:ILE:HG12	1:A:211:LEU:HD21	1.69	0.73
1:B:122:TYR:O	1:B:125:ARG:HD3	1.88	0.73
1:A:212:MET:HB2	1:A:321:PRO:HA	1.71	0.73
1:B:514:ARG:NE	5:B:1056:HOH:O	2.22	0.72
1:D:418:ASN:HD21	1:D:464:ASN:HD22	1.36	0.71
1:C:9:ARG:HH11	1:C:9:ARG:HB3	1.55	0.71
1:C:277:VAL:HG21	1:C:282:LEU:HD22	1.72	0.71
1:A:519:GLU:H	1:A:520:ASP:CA	2.05	0.70
1:D:531:GLN:O	1:D:534:ARG:O	2.10	0.70
1:D:487:THR:O	1:D:488:ILE:HD13	1.92	0.70
1:A:65:ASN:H	1:A:65:ASN:ND2	1.84	0.69
1:D:257:LEU:HD22	1:D:262:GLY:CA	2.22	0.69
1:A:601:MET:HE2	1:A:627:VAL:HB	1.72	0.69
1:D:212:MET:HE3	1:D:214:ILE:CG1	2.22	0.69
1:B:538:ASN:HD22	1:B:541:ILE:CD1	2.05	0.69
1:A:1:MET:HE2	5:A:1138:HOH:O	1.93	0.69
1:B:63:LYS:HB3	1:B:64:LYS:C	2.18	0.69
1:D:538:ASN:HD22	1:D:539:PRO:HD2	1.57	0.69
1:B:355:GLN:O	1:B:359:GLN:HG3	1.94	0.68
1:A:68:LEU:HD22	1:A:72:LYS:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:HD13	1:B:480:ARG:HG2	1.76	0.67
1:A:59:ASN:HD22	1:A:61:SER:H	1.42	0.67
1:A:544:ARG:HH11	1:A:544:ARG:HB3	1.59	0.67
1:B:538:ASN:HD22	1:B:541:ILE:HD12	1.58	0.67
1:B:514:ARG:C	1:B:526:LEU:HB3	2.18	0.67
1:B:616:GLU:O	1:B:620:THR:HG23	1.95	0.66
1:C:9:ARG:HH11	1:C:9:ARG:CB	2.07	0.66
1:C:278:LYS:HB2	1:C:281:GLU:HG3	1.77	0.66
1:A:544:ARG:CB	1:A:544:ARG:NH1	2.58	0.66
1:C:265:GLU:OE2	1:C:274:ARG:HD2	1.97	0.65
1:C:277:VAL:CG2	1:C:282:LEU:HD22	2.27	0.65
1:D:171:ARG:HD2	5:D:1071:HOH:O	1.97	0.65
1:C:284:ARG:NH2	1:C:608:ASP:OD1	2.30	0.64
1:C:456:VAL:HG22	1:C:473:MET:HG3	1.79	0.64
1:D:184:ALA:HB2	5:D:1071:HOH:O	1.96	0.64
1:D:381:LYS:O	1:D:385:GLU:HG3	1.97	0.64
1:C:601:MET:CE	1:C:627:VAL:HB	2.27	0.63
1:D:229:LYS:HG3	1:D:243:LEU:HD22	1.79	0.63
1:A:185:SER:HB3	1:A:189:SER:OG	1.99	0.63
1:D:534:ARG:O	1:D:535:GLU:CB	2.45	0.63
1:D:212:MET:HE3	1:D:244:SER:HB2	1.80	0.62
1:A:284:ARG:NH2	1:A:608:ASP:OD1	2.32	0.62
1:C:601:MET:HE2	1:C:627:VAL:HB	1.80	0.61
1:A:122:TYR:O	1:A:125:ARG:HD3	2.00	0.61
1:B:64:LYS:O	1:B:65:ASN:HB2	1.99	0.61
1:B:486:LEU:O	1:B:593:ASN:HB2	2.00	0.61
1:B:514:ARG:HG2	1:B:528:TYR:HB2	1.82	0.61
1:D:534:ARG:O	1:D:535:GLU:HB3	1.98	0.61
1:B:531:GLN:HE21	1:B:531:GLN:HA	1.65	0.61
1:C:202:LYS:C	1:C:203:GLN:HE21	2.08	0.61
1:B:237:VAL:O	1:B:237:VAL:CG1	2.49	0.61
1:C:63:LYS:HB2	1:C:66:GLU:CG	2.31	0.61
1:A:54:THR:HG22	1:A:118:TYR:HD2	1.66	0.60
1:D:476:THR:HB	1:D:480:ARG:HB3	1.83	0.60
1:B:119:GLU:O	1:B:123:ARG:HG3	2.02	0.60
1:D:542:LEU:HG	1:D:546:GLU:HB3	1.81	0.60
1:A:555:LEU:O	1:A:566:LYS:HE2	2.01	0.60
1:B:372:ASN:ND2	1:B:374:PHE:CZ	2.70	0.60
1:C:555:LEU:O	1:C:566:LYS:HE2	2.00	0.60
1:B:472:VAL:O	1:B:476:THR:HG23	2.02	0.59
1:D:192:HIS:CE1	5:D:1092:HOH:O	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLU:O	1:A:544:ARG:HG2	2.02	0.59
1:A:544:ARG:HH11	1:A:544:ARG:HB2	1.62	0.59
1:B:514:ARG:HD3	5:B:1056:HOH:O	2.02	0.59
1:C:408:ASN:HB3	1:C:575:ILE:HG23	1.84	0.59
1:C:453:ASP:O	1:C:454:ASN:HB2	2.01	0.59
1:A:538:ASN:HD22	1:A:540:GLU:H	1.50	0.59
1:D:18:ASN:HD22	1:D:526:LEU:HD22	1.68	0.58
1:B:207:ARG:O	1:B:208:ARG:HG2	2.03	0.58
1:A:320:ASN:ND2	2:A:1002:CDP:O3'	2.36	0.58
1:B:538:ASN:ND2	1:B:541:ILE:HD12	2.17	0.58
1:B:26:ARG:NH1	5:B:1136:HOH:O	2.33	0.58
1:B:274:ARG:HD2	5:B:1171:HOH:O	2.03	0.58
1:A:257:LEU:HD22	1:A:262:GLY:HA3	1.86	0.58
1:C:32:LEU:HD12	1:C:32:LEU:N	2.07	0.58
1:D:320:ASN:HB2	1:D:321:PRO:CD	2.34	0.58
1:D:408:ASN:HB3	1:D:575:ILE:HG23	1.85	0.58
1:B:18:ASN:ND2	1:B:514:ARG:HH21	1.98	0.57
1:D:445:GLU:HA	1:D:450:ARG:HG3	1.86	0.57
1:D:616:GLU:OE1	1:D:619:ARG:NH1	2.37	0.57
1:B:54:THR:HG22	1:B:118:TYR:HD2	1.69	0.57
1:B:198:ILE:HG12	1:B:211:LEU:HD21	1.87	0.57
1:C:80:ARG:HG2	1:C:80:ARG:HH11	1.69	0.57
1:C:559:PRO:O	1:C:560:ASP:CB	2.52	0.57
1:A:356:GLU:OE1	5:A:1142:HOH:O	2.18	0.57
1:A:425:LEU:HD12	1:A:472:VAL:HG21	1.87	0.57
1:A:408:ASN:HB3	1:A:575:ILE:HG23	1.87	0.57
1:B:1:MET:HG3	1:B:350:ASP:OD1	2.04	0.57
1:D:616:GLU:O	1:D:620:THR:HG23	2.05	0.57
1:D:64:LYS:C	1:D:66:GLU:H	2.13	0.57
1:A:65:ASN:ND2	1:A:65:ASN:N	2.53	0.57
1:C:198:ILE:HG12	1:C:211:LEU:HD11	1.86	0.57
1:D:212:MET:HB2	1:D:321:PRO:HA	1.86	0.57
1:B:364:PHE:CD1	1:B:364:PHE:C	2.83	0.56
1:D:538:ASN:HD22	1:D:539:PRO:CD	2.18	0.56
1:B:257:LEU:HD22	1:B:262:GLY:HA3	1.87	0.56
1:B:474:LYS:HE2	5:B:1187:HOH:O	2.05	0.56
1:A:601:MET:HE3	1:A:627:VAL:HB	1.87	0.56
1:D:237:VAL:HG12	1:D:237:VAL:O	2.05	0.56
1:B:514:ARG:CD	5:B:1056:HOH:O	2.53	0.55
1:C:25:ASP:OD1	5:C:1151:HOH:O	2.18	0.55
1:B:311:TYR:CD1	1:B:312:PRO:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:VAL:HB	1:C:566:LYS:HE3	1.88	0.55
1:D:32:LEU:HD22	1:D:32:LEU:H	1.72	0.55
1:C:601:MET:HE1	1:C:610:VAL:HG22	1.88	0.55
1:B:3:LEU:O	1:B:7:ILE:HG13	2.06	0.55
1:C:603:GLN:OE1	1:C:631:GLY:HA3	2.06	0.55
1:D:32:LEU:O	1:D:33:ASP:HB2	2.06	0.55
1:C:277:VAL:HG21	1:C:282:LEU:CD2	2.37	0.54
1:D:50:ARG:O	1:D:54:THR:HG23	2.08	0.54
1:D:64:LYS:O	1:D:65:ASN:ND2	2.40	0.54
1:C:128:LEU:HD13	1:D:179:GLY:HA3	1.90	0.54
1:C:177:VAL:O	1:C:178:ALA:HB3	2.07	0.54
1:D:50:ARG:O	1:D:54:THR:CG2	2.56	0.54
1:D:170:LEU:HD12	1:D:187:PRO:HA	1.90	0.54
1:A:488:ILE:HG21	1:A:504:LEU:HG	1.88	0.54
1:B:603:GLN:HG3	1:B:630:ASP:O	2.08	0.54
1:D:321:PRO:HD2	2:D:1003:CDP:O2'	2.07	0.54
1:C:22:ILE:CD1	1:C:496:ASN:HB3	2.38	0.54
1:C:177:VAL:O	1:C:178:ALA:CB	2.56	0.54
1:D:330:TYR:O	1:D:379:ILE:HA	2.08	0.54
1:D:454:ASN:HD22	1:D:474:LYS:NZ	2.06	0.54
1:A:277:VAL:HG21	1:A:282:LEU:HD22	1.90	0.53
1:C:250:ASP:OD1	1:C:252:LYS:HG2	2.07	0.53
1:A:177:VAL:HG12	1:A:179:GLY:H	1.73	0.53
1:C:555:LEU:HA	1:C:558:ILE:HD12	1.89	0.53
1:A:59:ASN:ND2	1:A:61:SER:H	2.05	0.53
1:B:111:ASP:O	5:B:1073:HOH:O	2.19	0.53
1:B:50:ARG:O	1:B:54:THR:HG23	2.09	0.53
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.90	0.53
1:A:179:GLY:HA3	1:A:180:THR:HG22	1.90	0.52
1:C:22:ILE:HD12	1:C:496:ASN:HB3	1.91	0.52
1:B:408:ASN:HB3	1:B:575:ILE:HG23	1.90	0.52
1:B:592:ASP:O	1:B:623:ARG:NH2	2.42	0.52
1:C:17:LYS:O	1:C:21:ILE:HG13	2.09	0.52
1:D:429:ARG:O	1:D:433:GLU:HG2	2.09	0.52
1:B:108:LYS:HE2	1:B:117:ASP:OD2	2.09	0.52
1:D:187:PRO:O	1:D:191:MET:HG3	2.10	0.52
1:D:237:VAL:O	1:D:237:VAL:CG1	2.57	0.52
1:B:551:GLU:HG3	1:B:552:LYS:H	1.75	0.52
1:C:212:MET:HE3	1:C:212:MET:HA	1.91	0.52
1:D:272:THR:O	1:D:274:ARG:HG3	2.10	0.52
1:D:441:PHE:HB3	1:D:481:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ALA:HB1	1:D:462:MET:O	2.11	0.51
1:B:372:ASN:ND2	1:B:374:PHE:CE1	2.79	0.51
1:D:277:VAL:HG21	1:D:282:LEU:HD22	1.93	0.51
1:D:480:ARG:HD3	1:D:482:ASN:O	2.10	0.51
1:A:588:GLN:HE22	1:A:594:ASN:HA	1.76	0.51
1:C:50:ARG:O	1:C:54:THR:HG23	2.11	0.51
1:C:559:PRO:O	1:C:560:ASP:CG	2.54	0.51
1:D:407:TYR:CZ	1:D:506:PRO:HD3	2.46	0.51
1:A:623:ARG:HD2	5:A:1049:HOH:O	2.11	0.50
1:B:207:ARG:NH2	4:B:1009:CL:CL	2.80	0.50
1:B:237:VAL:O	1:B:237:VAL:HG12	2.10	0.50
1:B:511:ALA:HA	1:B:528:TYR:O	2.10	0.50
1:C:20:GLN:NE2	5:C:1128:HOH:O	2.43	0.50
1:A:457:PRO:HD2	1:A:473:MET:HE3	1.94	0.50
1:C:212:MET:CE	1:C:242:ASN:O	2.59	0.50
1:D:18:ASN:ND2	1:D:526:LEU:HD22	2.26	0.50
1:C:212:MET:HE3	1:C:242:ASN:O	2.12	0.50
1:C:32:LEU:H	1:C:32:LEU:CD1	1.95	0.50
1:B:15:PRO:O	1:B:20:GLN:NE2	2.45	0.49
1:C:134:CYS:HB3	1:C:320:ASN:HB3	1.94	0.49
1:B:18:ASN:ND2	5:B:1095:HOH:O	2.44	0.49
1:A:212:MET:HE3	1:A:213:GLY:H	1.77	0.49
1:C:84:ALA:CB	1:C:86:LEU:HD22	2.43	0.49
1:D:62:TYR:CE1	1:D:70:ARG:HG3	2.48	0.49
1:A:277:VAL:CG2	1:A:282:LEU:HD22	2.43	0.48
1:A:452:GLU:HG3	5:A:1147:HOH:O	2.12	0.48
1:B:454:ASN:HD22	1:B:474:LYS:NZ	2.11	0.48
1:D:126:ASN:OD1	1:D:126:ASN:C	2.53	0.48
1:B:72:LYS:O	1:B:110:ILE:HD11	2.13	0.48
1:A:1:MET:HE1	1:A:9:ARG:NE	2.28	0.48
1:D:378:LYS:HG3	5:D:1105:HOH:O	2.13	0.48
1:D:546:GLU:O	1:D:550:ILE:HD12	2.14	0.48
1:A:601:MET:CE	1:A:627:VAL:CB	2.89	0.48
1:A:512:TYR:HE1	1:A:514:ARG:HD3	1.79	0.48
1:C:122:TYR:O	1:C:125:ARG:HD3	2.14	0.48
1:B:548:GLU:O	1:B:552:LYS:HB3	2.14	0.48
1:C:559:PRO:O	1:C:560:ASP:HB2	2.14	0.48
1:A:212:MET:HE3	1:A:213:GLY:N	2.28	0.47
1:A:518:LYS:HE3	1:A:518:LYS:C	2.39	0.47
1:C:11:ILE:HG13	1:C:83:LYS:HD3	1.96	0.47
1:B:54:THR:HG22	1:B:118:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:GLN:CD	1:C:623:ARG:HD3	2.39	0.47
1:B:68:LEU:HD22	1:B:72:LYS:HD2	1.96	0.47
1:A:212:MET:HE1	1:A:244:SER:N	2.29	0.47
1:B:207:ARG:CZ	4:B:1009:CL:CL	2.97	0.47
1:C:623:ARG:HD2	5:C:1069:HOH:O	2.15	0.47
1:C:42:GLU:HB3	1:C:83:LYS:HE3	1.97	0.47
1:C:460:MET:HG2	1:C:590:TYR:CE1	2.49	0.47
1:B:151:LYS:O	1:B:154:ALA:HB3	2.15	0.47
1:D:343:PHE:CE2	1:D:354:LEU:HA	2.49	0.47
1:A:90:ASN:HB3	1:A:335:LEU:HB2	1.97	0.47
1:A:271:SER:OG	1:A:273:ILE:HG13	2.15	0.47
1:A:470:ARG:HG2	5:A:1084:HOH:O	2.15	0.47
1:D:474:LYS:HB2	1:D:474:LYS:HE2	1.73	0.47
1:B:174:GLY:HA2	1:B:183:LYS:HB3	1.96	0.46
1:C:460:MET:HE1	1:C:470:ARG:HD3	1.96	0.46
1:A:52:VAL:HG21	1:A:364:PHE:CZ	2.51	0.46
1:A:59:ASN:HD22	1:A:59:ASN:C	2.24	0.46
1:B:67:LYS:O	1:B:71:ILE:HG13	2.15	0.46
1:C:237:VAL:HG13	1:C:237:VAL:O	2.15	0.46
1:D:220:PRO:HD3	1:D:267:SER:O	2.15	0.46
1:D:308:TYR:HD1	1:D:309:PRO:HD2	1.81	0.46
1:D:472:VAL:O	1:D:476:THR:HG23	2.14	0.46
1:A:311:TYR:HA	1:A:314:ARG:O	2.15	0.46
1:A:538:ASN:HD22	1:A:538:ASN:C	2.23	0.46
1:D:268:HIS:CG	1:D:269:PRO:HD2	2.51	0.46
1:C:237:VAL:HG22	1:C:239:ASN:OD1	2.16	0.46
1:C:541:ILE:O	1:C:545:ILE:HG12	2.16	0.46
1:B:189:SER:O	1:B:192:HIS:HB2	2.16	0.46
1:D:450:ARG:NH1	1:D:478:GLU:HA	2.31	0.46
1:D:563:GLU:OE1	1:D:567:LYS:NZ	2.46	0.46
1:A:273:ILE:HA	5:A:1040:HOH:O	2.16	0.46
1:B:389:LEU:HD12	1:B:485:LEU:HD23	1.98	0.46
1:B:406:PRO:HB3	1:B:567:LYS:O	2.16	0.46
1:D:212:MET:HE1	1:D:244:SER:OG	2.14	0.46
1:B:217:ILE:HA	1:B:222:ILE:HG12	1.98	0.45
1:A:237:VAL:HA	1:A:239:ASN:N	2.31	0.45
1:B:441:PHE:HB3	1:B:481:ARG:O	2.16	0.45
1:C:47:ARG:HD2	1:C:97:ALA:O	2.16	0.45
1:D:486:LEU:O	1:D:593:ASN:HB2	2.16	0.45
1:C:1:MET:HE1	1:C:9:ARG:CZ	2.46	0.45
1:D:476:THR:HA	1:D:479:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HG22	5:B:1024:HOH:O	2.16	0.45
1:D:35:ASN:HB3	1:D:36:TYR:H	1.61	0.45
1:A:65:ASN:O	1:A:66:GLU:CB	2.64	0.45
1:D:11:ILE:O	1:D:83:LYS:NZ	2.47	0.45
1:A:512:TYR:CE1	1:A:514:ARG:HD3	2.52	0.45
1:A:561:VAL:HB	1:A:566:LYS:HE3	1.99	0.45
1:B:449:TYR:OH	1:B:457:PRO:HG3	2.17	0.44
1:D:166:ASN:HB2	1:D:317:ASN:O	2.17	0.44
1:B:457:PRO:HD2	1:B:473:MET:HE3	2.00	0.44
1:C:218:ASN:HA	1:C:266:LEU:HD22	1.99	0.44
1:B:229:LYS:CG	1:B:243:LEU:HD22	2.48	0.44
1:C:56:GLU:HB2	1:C:71:ILE:HG12	1.99	0.44
1:D:327:LEU:HD22	1:D:331:GLU:HB3	1.99	0.44
1:C:138:PRO:HD3	1:C:329:ASP:HB3	2.00	0.44
1:D:67:LYS:O	1:D:71:ILE:HG13	2.18	0.44
1:D:90:ASN:C	1:D:90:ASN:HD22	2.24	0.44
1:D:456:VAL:HG22	1:D:473:MET:HG3	2.00	0.44
1:A:177:VAL:O	1:A:179:GLY:N	2.51	0.43
1:B:320:ASN:ND2	2:B:1001:CDP:O3'	2.51	0.43
1:B:564:LYS:HA	1:B:564:LYS:HD3	1.77	0.43
1:C:311:TYR:CD1	1:C:312:PRO:HA	2.54	0.43
1:D:64:LYS:O	1:D:66:GLU:N	2.52	0.43
1:A:63:LYS:O	1:A:65:ASN:O	2.36	0.43
1:B:512:TYR:N	1:B:512:TYR:CD2	2.85	0.43
1:C:429:ARG:O	1:C:432:TYR:HB3	2.17	0.43
1:C:453:ASP:O	1:C:454:ASN:CB	2.67	0.43
1:C:592:ASP:O	1:C:623:ARG:NH2	2.52	0.43
1:D:358:VAL:O	1:D:362:VAL:HG23	2.19	0.43
1:A:11:ILE:O	1:A:83:LYS:HE2	2.18	0.43
1:A:182:GLY:O	1:A:183:LYS:HB2	2.18	0.43
1:B:90:ASN:HB3	1:B:335:LEU:HB2	2.01	0.43
1:C:84:ALA:HB3	1:C:86:LEU:HD22	2.01	0.43
1:C:567:LYS:HA	1:C:567:LYS:HD3	1.73	0.43
1:B:429:ARG:HG2	5:B:1199:HOH:O	2.19	0.42
1:C:62:TYR:HB3	1:C:67:LYS:HG3	2.00	0.42
1:C:164:GLY:HA2	1:C:212:MET:O	2.19	0.42
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.55	0.42
1:B:585:ASP:O	1:B:589:ARG:HG3	2.18	0.42
1:C:80:ARG:HG2	1:C:80:ARG:NH1	2.33	0.42
1:C:172:PRO:HD2	1:C:271:SER:HB2	2.01	0.42
1:C:399:LEU:HG	1:C:403:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:PRO:O	1:A:565:ILE:O	2.38	0.42
1:C:90:ASN:HD22	1:C:90:ASN:C	2.25	0.42
1:A:129:HIS:ND1	1:A:371:VAL:O	2.52	0.42
1:A:527:LEU:CD1	1:A:550:ILE:HD11	2.50	0.42
1:B:368:VAL:O	1:B:369:ILE:C	2.61	0.42
1:C:542:LEU:C	1:C:542:LEU:HD23	2.44	0.42
1:B:215:LEU:HD13	1:B:219:HIS:HB3	2.02	0.42
1:D:32:LEU:H	1:D:32:LEU:CD2	2.32	0.42
1:A:374:PHE:HE1	5:A:1168:HOH:O	2.02	0.42
1:B:611:LEU:O	1:B:614:TYR:HB2	2.19	0.42
1:C:181:HIS:HA	1:C:182:GLY:HA2	1.75	0.42
1:A:519:GLU:N	1:A:520:ASP:HA	2.23	0.42
1:C:254:ILE:HD13	1:C:254:ILE:HA	1.93	0.42
1:D:328:SER:O	1:D:331:GLU:HB2	2.20	0.42
1:D:450:ARG:HH12	1:D:478:GLU:HA	1.85	0.42
1:A:529:VAL:O	1:A:530:ASN:C	2.62	0.41
1:A:128:LEU:HD13	1:B:179:GLY:HA3	2.02	0.41
1:A:558:ILE:HA	1:A:559:PRO:HD3	1.85	0.41
1:C:157:THR:HG22	1:C:201:VAL:CG1	2.50	0.41
1:D:62:TYR:CD1	1:D:70:ARG:HG3	2.55	0.41
1:D:432:TYR:HB2	1:D:476:THR:HG22	2.01	0.41
1:D:349:VAL:HG22	1:D:399:LEU:HD11	2.02	0.41
1:C:38:GLU:HG2	1:C:43:ASP:HB3	2.01	0.41
1:A:567:LYS:HD3	1:A:567:LYS:HA	1.55	0.41
1:B:330:TYR:O	1:B:379:ILE:HA	2.20	0.41
1:C:344:TYR:CD1	1:C:403:LEU:HD13	2.56	0.41
1:C:615:LEU:HD23	1:C:615:LEU:HA	1.88	0.41
1:D:303:GLU:CG	1:D:623:ARG:HG3	2.51	0.41
1:D:542:LEU:HG	1:D:546:GLU:CB	2.50	0.41
1:A:546:GLU:O	1:A:550:ILE:HD12	2.21	0.41
1:C:158:LYS:NZ	5:C:1087:HOH:O	2.46	0.41
1:C:130:MET:HE2	1:C:159:VAL:HG23	2.02	0.41
1:B:241:PHE:HB3	1:B:243:LEU:HD13	2.02	0.41
1:C:542:LEU:O	1:C:546:GLU:HG3	2.21	0.41
1:D:401:TYR:CE1	1:D:569:PHE:HA	2.55	0.41
1:D:460:MET:HA	1:D:590:TYR:CZ	2.56	0.41
1:C:212:MET:HE2	1:C:213:GLY:H	1.86	0.41
1:A:32:LEU:HA	1:A:33:ASP:HA	1.80	0.40
1:A:544:ARG:HG2	1:A:544:ARG:H	1.69	0.40
1:D:254:ILE:HD13	1:D:254:ILE:HA	1.91	0.40
1:C:476:THR:HB	1:C:480:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:O	1:A:66:GLU:HB3	2.20	0.40
1:C:320:ASN:HB2	1:C:321:PRO:CD	2.51	0.40
1:D:339:ASP:OD2	1:D:342:LYS:NZ	2.37	0.40
1:D:538:ASN:ND2	1:D:539:PRO:HD2	2.31	0.40
1:A:160:GLY:HA2	1:A:203:GLN:OE1	2.21	0.40
1:C:1:MET:HE1	1:C:9:ARG:NH2	2.36	0.40
1:C:486:LEU:O	1:C:593:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	606/644 (94%)	577 (95%)	21 (4%)	8 (1%)	9	6
1	B	600/644 (93%)	572 (95%)	22 (4%)	6 (1%)	12	10
1	C	607/644 (94%)	576 (95%)	25 (4%)	6 (1%)	12	10
1	D	597/644 (93%)	555 (93%)	37 (6%)	5 (1%)	16	14
All	All	2410/2576 (94%)	2280 (95%)	105 (4%)	25 (1%)	12	10

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	ALA
1	A	179	GLY
1	A	238	LEU
1	A	566	LYS
1	B	566	LYS
1	C	178	ALA
1	A	519	GLU
1	B	536	LYS

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Mol	Chain	Res	Type
1	C	33	ASP
1	C	560	ASP
1	D	33	ASP
1	D	35	ASN
1	A	4	SER
1	A	66	GLU
1	C	528	TYR
1	B	63	LYS
1	B	65	ASN
1	B	208	ARG
1	D	527	LEU
1	D	620	THR
1	A	183	LYS
1	B	460	MET
1	D	539	PRO
1	C	538	ASN
1	C	179	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	544/566 (96%)	509 (94%)	35 (6%)	16	15
1	B	537/566 (95%)	500 (93%)	37 (7%)	14	13
1	C	541/566 (96%)	498 (92%)	43 (8%)	11	9
1	D	535/566 (94%)	495 (92%)	40 (8%)	12	11
All	All	2157/2264 (95%)	2002 (93%)	155 (7%)	13	12

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	ILE
1	A	25	ASP
1	A	29	MET

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Mol	Chain	Res	Type
1	A	33	ASP
1	A	42	GLU
1	A	54	THR
1	A	65	ASN
1	A	66	GLU
1	A	68	LEU
1	A	90	ASN
1	A	180	THR
1	A	189	SER
1	A	218	ASN
1	A	237	VAL
1	A	253	GLU
1	A	257	LEU
1	A	285	LYS
1	A	289	ASN
1	A	384	LYS
1	A	391	LEU
1	A	433	GLU
1	A	436	LYS
1	A	450	ARG
1	A	470	ARG
1	A	478	GLU
1	A	504	LEU
1	A	516	VAL
1	A	518	LYS
1	A	538	ASN
1	A	544	ARG
1	A	547	LYS
1	A	560	ASP
1	A	601	MET
1	A	623	ARG
1	B	54	THR
1	B	68	LEU
1	B	90	ASN
1	B	116	GLU
1	B	189	SER
1	B	196	SER
1	B	198	ILE
1	B	200	VAL
1	B	207	ARG
1	B	215	LEU
1	B	230	LYS

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Mol	Chain	Res	Type
1	B	237	VAL
1	B	243	LEU
1	B	254	ILE
1	B	257	LEU
1	B	278	LYS
1	B	295	ASP
1	B	315	LYS
1	B	346	ASN
1	B	442	PRO
1	B	445	GLU
1	B	480	ARG
1	B	488	ILE
1	B	502	SER
1	B	504	LEU
1	B	512	TYR
1	B	513	THR
1	B	527	LEU
1	B	531	GLN
1	B	534	ARG
1	B	538	ASN
1	B	541	ILE
1	B	550	ILE
1	B	565	ILE
1	B	598	THR
1	B	623	ARG
1	B	627	VAL
1	C	8	SER
1	C	9	ARG
1	C	17	LYS
1	C	32	LEU
1	C	54	THR
1	C	57	LEU
1	C	63	LYS
1	C	65	ASN
1	C	68	LEU
1	C	86	LEU
1	C	90	ASN
1	C	143	ILE
1	C	181	HIS
1	C	189	SER
1	C	196	SER
1	C	198	ILE

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Mol	Chain	Res	Type
1	C	212	MET
1	C	215	LEU
1	C	254	ILE
1	C	257	LEU
1	C	276	LYS
1	C	282	LEU
1	C	315	LYS
1	C	357	LEU
1	C	391	LEU
1	C	403	LEU
1	C	444	LEU
1	C	450	ARG
1	C	464	ASN
1	C	470	ARG
1	C	486	LEU
1	C	504	LEU
1	C	514	ARG
1	C	526	LEU
1	C	527	LEU
1	C	534	ARG
1	C	535	GLU
1	C	543	LYS
1	C	551	GLU
1	C	564	LYS
1	C	573	LEU
1	C	623	ARG
1	C	627	VAL
1	D	14	GLU
1	D	24	ARG
1	D	31	ASP
1	D	32	LEU
1	D	54	THR
1	D	66	GLU
1	D	68	LEU
1	D	81	VAL
1	D	86	LEU
1	D	90	ASN
1	D	116	GLU
1	D	196	SER
1	D	199	SER
1	D	202	LYS
1	D	215	LEU

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Mol	Chain	Res	Type
1	D	243	LEU
1	D	254	ILE
1	D	257	LEU
1	D	292	LYS
1	D	315	LYS
1	D	403	LEU
1	D	434	LEU
1	D	444	LEU
1	D	452	GLU
1	D	474	LYS
1	D	478	GLU
1	D	504	LEU
1	D	526	LEU
1	D	535	GLU
1	D	536	LYS
1	D	540	GLU
1	D	541	ILE
1	D	542	LEU
1	D	546	GLU
1	D	551	GLU
1	D	567	LYS
1	D	573	LEU
1	D	598	THR
1	D	623	ARG
1	D	627	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	59	ASN
1	A	65	ASN
1	A	127	HIS
1	A	320	ASN
1	A	345	ASN
1	A	496	ASN
1	A	531	GLN
1	A	538	ASN
1	A	588	GLN
1	A	603	GLN
1	B	18	ASN
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	313	HIS
1	B	317	ASN
1	B	355	GLN
1	B	359	GLN
1	B	454	ASN
1	B	496	ASN
1	B	531	GLN
1	B	538	ASN
1	B	584	GLN
1	B	603	GLN
1	B	621	ASN
1	C	20	GLN
1	C	181	HIS
1	C	203	GLN
1	C	317	ASN
1	C	418	ASN
1	C	464	ASN
1	C	496	ASN
1	C	531	GLN
1	D	18	ASN
1	D	65	ASN
1	D	96	ASN
1	D	103	HIS
1	D	112	GLN
1	D	181	HIS
1	D	313	HIS
1	D	346	ASN
1	D	454	ASN
1	D	464	ASN
1	D	496	ASN
1	D	538	ASN
1	D	584	GLN
1	D	600	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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	CDP	C	1004	-	25,26,26	2.04	4 (16%)	38,40,40	1.68	8 (21%)
2	CDP	A	1002	-	25,26,26	1.90	4 (16%)	38,40,40	1.30	7 (18%)
2	CDP	B	1001	-	25,26,26	1.25	3 (12%)	38,40,40	1.49	5 (13%)
3	DTP	C	1008	-	31,32,32	1.28	3 (9%)	46,50,50	1.82	9 (19%)
2	CDP	D	1003	-	25,26,26	2.02	7 (28%)	38,40,40	1.69	8 (21%)
3	DTP	C	1007	-	31,32,32	1.55	6 (19%)	46,50,50	1.72	8 (17%)
3	DTP	B	1006	-	31,32,32	1.70	5 (16%)	46,50,50	1.88	9 (19%)
3	DTP	A	1005	-	31,32,32	2.34	7 (22%)	46,50,50	1.89	10 (21%)

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	CDP	C	1004	-	-	3/16/32/32	0/2/2/2
2	CDP	A	1002	-	-	8/16/32/32	0/2/2/2
2	CDP	B	1001	-	-	1/16/32/32	0/2/2/2
3	DTP	C	1008	-	-	0/22/34/34	0/3/3/3
2	CDP	D	1003	-	-	1/16/32/32	0/2/2/2
3	DTP	C	1007	-	-	5/22/34/34	0/3/3/3
3	DTP	B	1006	-	-	0/22/34/34	0/3/3/3
3	DTP	A	1005	-	-	5/22/34/34	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005	DTP	PB-O3B	8.41	1.68	1.59
2	C	1004	CDP	PA-O3A	5.99	1.66	1.59
3	A	1005	DTP	PA-O3A	-5.97	1.53	1.59
3	B	1006	DTP	PA-O3A	-5.84	1.53	1.59
2	A	1002	CDP	PA-O3A	5.66	1.65	1.59
2	D	1003	CDP	PA-O3A	5.66	1.65	1.59
2	A	1002	CDP	O4'-C1'	5.51	1.54	1.42
2	C	1004	CDP	O4'-C1'	5.17	1.53	1.42
3	C	1007	DTP	PB-O3B	4.30	1.64	1.59
3	A	1005	DTP	PB-O3A	4.02	1.63	1.59
2	C	1004	CDP	C5'-C4'	-3.81	1.40	1.51
2	D	1003	CDP	PB-O3B	3.64	1.68	1.54
3	A	1005	DTP	C5-N7	-3.38	1.32	1.39
3	C	1007	DTP	PG-O3G	3.33	1.67	1.54
2	D	1003	CDP	O4'-C1'	3.32	1.49	1.42
3	C	1007	DTP	C1'-N9	3.17	1.52	1.46
3	B	1006	DTP	PB-O3B	-3.15	1.56	1.59
3	C	1008	DTP	C1'-N9	2.99	1.52	1.46
2	D	1003	CDP	C6-N1	2.96	1.45	1.38
3	C	1007	DTP	C5-N7	-2.90	1.33	1.39
3	C	1008	DTP	PG-O3G	2.83	1.65	1.54
2	D	1003	CDP	C6-C5	2.71	1.41	1.35
3	A	1005	DTP	PG-O3G	2.70	1.64	1.54
3	C	1008	DTP	O3'-C3'	2.65	1.48	1.43
3	B	1006	DTP	C1'-N9	2.58	1.51	1.46
3	A	1005	DTP	C8-N9	-2.50	1.33	1.37
2	C	1004	CDP	C6-C5	2.45	1.40	1.35
2	B	1001	CDP	PA-O3A	2.44	1.62	1.59
2	D	1003	CDP	C2-N1	2.41	1.45	1.40
3	B	1006	DTP	O3'-C3'	2.39	1.48	1.43
3	B	1006	DTP	PA-O5'	2.35	1.68	1.59
2	A	1002	CDP	C6-N1	2.32	1.43	1.38
2	B	1001	CDP	O4'-C1'	2.30	1.47	1.42
2	D	1003	CDP	C2'-C3'	2.19	1.59	1.53
3	C	1007	DTP	C8-N7	2.14	1.35	1.31
2	A	1002	CDP	PA-O2A	-2.11	1.45	1.55
3	A	1005	DTP	C1'-N9	2.09	1.50	1.46
2	B	1001	CDP	C6-C5	2.07	1.39	1.35
3	C	1007	DTP	C4-N9	-2.06	1.33	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1008	DTP	N3-C2-N1	-5.56	120.16	128.58
3	A	1005	DTP	C5-C4-N3	-5.31	119.40	126.72
3	B	1006	DTP	N3-C2-N1	-5.31	120.55	128.58
2	B	1001	CDP	O4'-C4'-C5'	-5.11	92.96	109.33
3	B	1006	DTP	C5-C4-N3	-5.10	119.69	126.72
3	A	1005	DTP	N3-C2-N1	-5.09	120.88	128.58
2	D	1003	CDP	C5'-C4'-C3'	-5.08	96.92	115.21
3	C	1007	DTP	N3-C2-N1	-4.77	121.36	128.58
2	C	1004	CDP	C4'-O4'-C1'	-4.71	99.07	109.47
3	B	1006	DTP	O3G-PG-O3B	-4.63	89.09	104.64
3	C	1008	DTP	N9-C8-N7	-4.40	107.69	113.94
3	C	1008	DTP	C5-C4-N3	-4.40	120.66	126.72
3	B	1006	DTP	C2-N3-C4	4.28	122.28	111.83
3	C	1007	DTP	C5-C4-N3	-4.26	120.85	126.72
2	C	1004	CDP	C2'-C1'-N1	4.00	124.39	113.25
3	C	1007	DTP	N9-C8-N7	-3.98	108.30	113.94
3	C	1008	DTP	C4-N9-C8	3.79	109.71	105.74
3	C	1008	DTP	C2-N3-C4	3.77	121.04	111.83
3	C	1008	DTP	N3-C4-N9	3.73	133.52	127.17
3	A	1005	DTP	N3-C4-N9	3.71	133.48	127.17
3	A	1005	DTP	C2-N3-C4	3.66	120.77	111.83
3	C	1007	DTP	C2-N3-C4	3.47	120.31	111.83
2	C	1004	CDP	O4'-C4'-C3'	-3.30	98.61	105.15
3	C	1007	DTP	C5-N7-C8	3.21	108.50	103.45
2	D	1003	CDP	O4'-C4'-C5'	3.21	119.61	109.33
2	D	1003	CDP	O3'-C3'-C2'	3.18	122.01	111.82
3	A	1005	DTP	N9-C8-N7	-3.08	109.57	113.94
3	B	1006	DTP	N9-C8-N7	-3.04	109.62	113.94
3	A	1005	DTP	C5-N7-C8	3.03	108.21	103.45
3	C	1007	DTP	C4-C5-N7	-3.02	107.12	110.58
2	D	1003	CDP	O2-C2-N3	-2.96	117.67	122.33
3	B	1006	DTP	N3-C4-N9	2.95	132.19	127.17
3	C	1008	DTP	C5-N7-C8	2.93	108.05	103.45
3	B	1006	DTP	C5-N7-C8	2.91	108.03	103.45
2	A	1002	CDP	C4'-O4'-C1'	-2.90	103.06	109.47
3	B	1006	DTP	C4-C5-N7	-2.82	107.36	110.58
3	C	1007	DTP	C5-C4-N9	2.80	108.86	105.81
2	D	1003	CDP	O4'-C1'-N1	-2.77	102.09	108.36
2	C	1004	CDP	C5'-C4'-C3'	-2.73	105.38	115.21
3	A	1005	DTP	C4-C5-N7	-2.69	107.51	110.58
2	A	1002	CDP	O4'-C1'-N1	2.68	114.43	108.36
3	A	1005	DTP	C2'-C1'-N9	-2.66	108.38	114.63
2	C	1004	CDP	O2A-PA-O3A	2.52	114.09	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	CDP	O3A-PB-O1B	-2.51	97.85	111.04
2	D	1003	CDP	C2'-C1'-N1	2.51	120.22	113.25
2	B	1001	CDP	C5'-C4'-C3'	2.50	124.22	115.21
3	C	1008	DTP	O2G-PG-O1G	2.43	120.30	110.83
2	A	1002	CDP	O4'-C4'-C3'	-2.40	100.40	105.15
2	C	1004	CDP	C5-C6-N1	-2.39	117.95	121.84
2	C	1004	CDP	O3A-PA-O1A	-2.35	103.63	110.70
2	A	1002	CDP	O3A-PA-O1A	-2.27	103.88	110.70
2	A	1002	CDP	O2B-PB-O3B	2.26	116.28	107.80
2	A	1002	CDP	O2B-PB-O1B	2.26	119.63	110.83
3	A	1005	DTP	O2G-PG-O3B	2.25	112.19	104.64
2	C	1004	CDP	O2A-PA-O1A	2.18	122.56	112.44
2	A	1002	CDP	O2A-PA-O1A	2.16	122.47	112.44
3	C	1007	DTP	O2G-PG-O1G	2.12	119.09	110.83
3	B	1006	DTP	C5-C4-N9	2.12	108.12	105.81
2	B	1001	CDP	C5-C6-N1	-2.08	118.47	121.84
2	D	1003	CDP	O2-C2-N1	2.06	122.93	118.90
3	C	1008	DTP	O2A-PA-O1A	2.05	121.96	112.44
3	A	1005	DTP	O2A-PA-O3A	2.04	112.78	107.27
2	D	1003	CDP	C1'-N1-C2	2.04	122.94	118.44
2	B	1001	CDP	O2B-PB-O3A	2.03	111.45	104.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	CDP	PA-O3A-PB-O3B
3	A	1005	DTP	PB-O3B-PG-O2G
3	A	1005	DTP	PB-O3B-PG-O3G
3	C	1007	DTP	C5'-O5'-PA-O3A
2	D	1003	CDP	PA-O3A-PB-O1B
2	A	1002	CDP	C2'-C1'-N1-C6
3	C	1007	DTP	PG-O3B-PB-O2B
2	A	1002	CDP	O4'-C1'-N1-C6
2	C	1004	CDP	O4'-C1'-N1-C6
3	C	1007	DTP	C5'-O5'-PA-O1A
2	C	1004	CDP	O4'-C1'-N1-C2
2	A	1002	CDP	O4'-C4'-C5'-O5'
2	A	1002	CDP	O4'-C1'-N1-C2
3	C	1007	DTP	PG-O3B-PB-O1B
2	A	1002	CDP	PA-O3A-PB-O1B
2	B	1001	CDP	PA-O3A-PB-O1B

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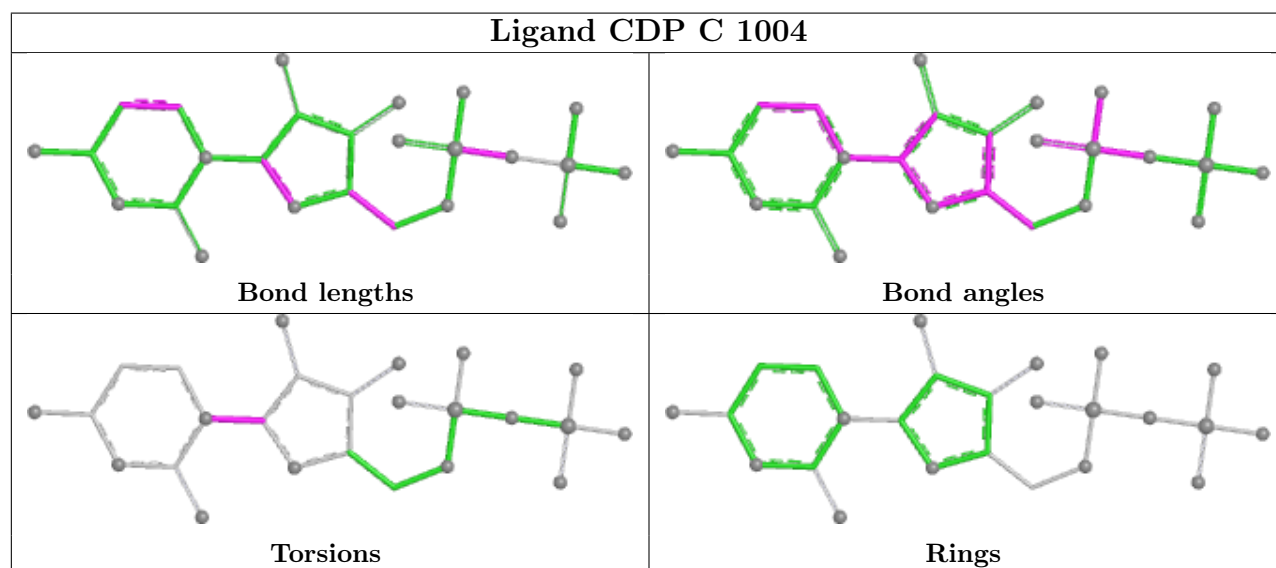
Mol	Chain	Res	Type	Atoms
2	A	1002	CDP	PA-O3A-PB-O2B
3	C	1007	DTP	PB-O3B-PG-O3G
2	C	1004	CDP	C2'-C1'-N1-C6
3	A	1005	DTP	PG-O3B-PB-O1B
3	A	1005	DTP	PG-O3B-PB-O2B
3	A	1005	DTP	PB-O3B-PG-O1G
2	A	1002	CDP	C2'-C1'-N1-C2

There are no ring outliers.

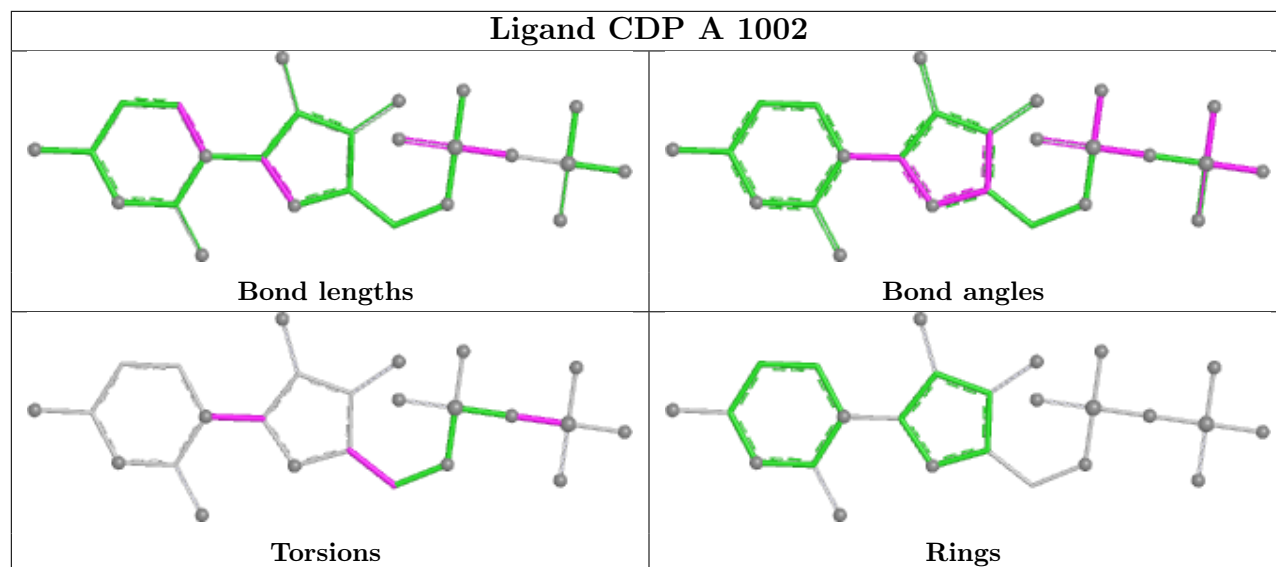
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	CDP	1	0
2	B	1001	CDP	1	0
2	D	1003	CDP	1	0

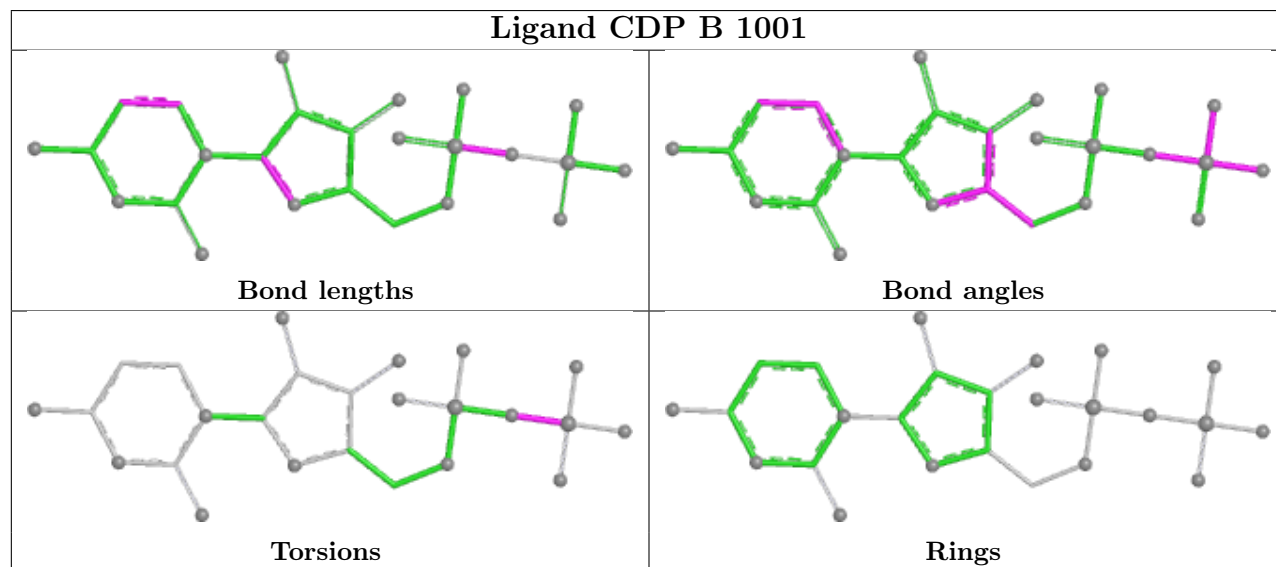
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



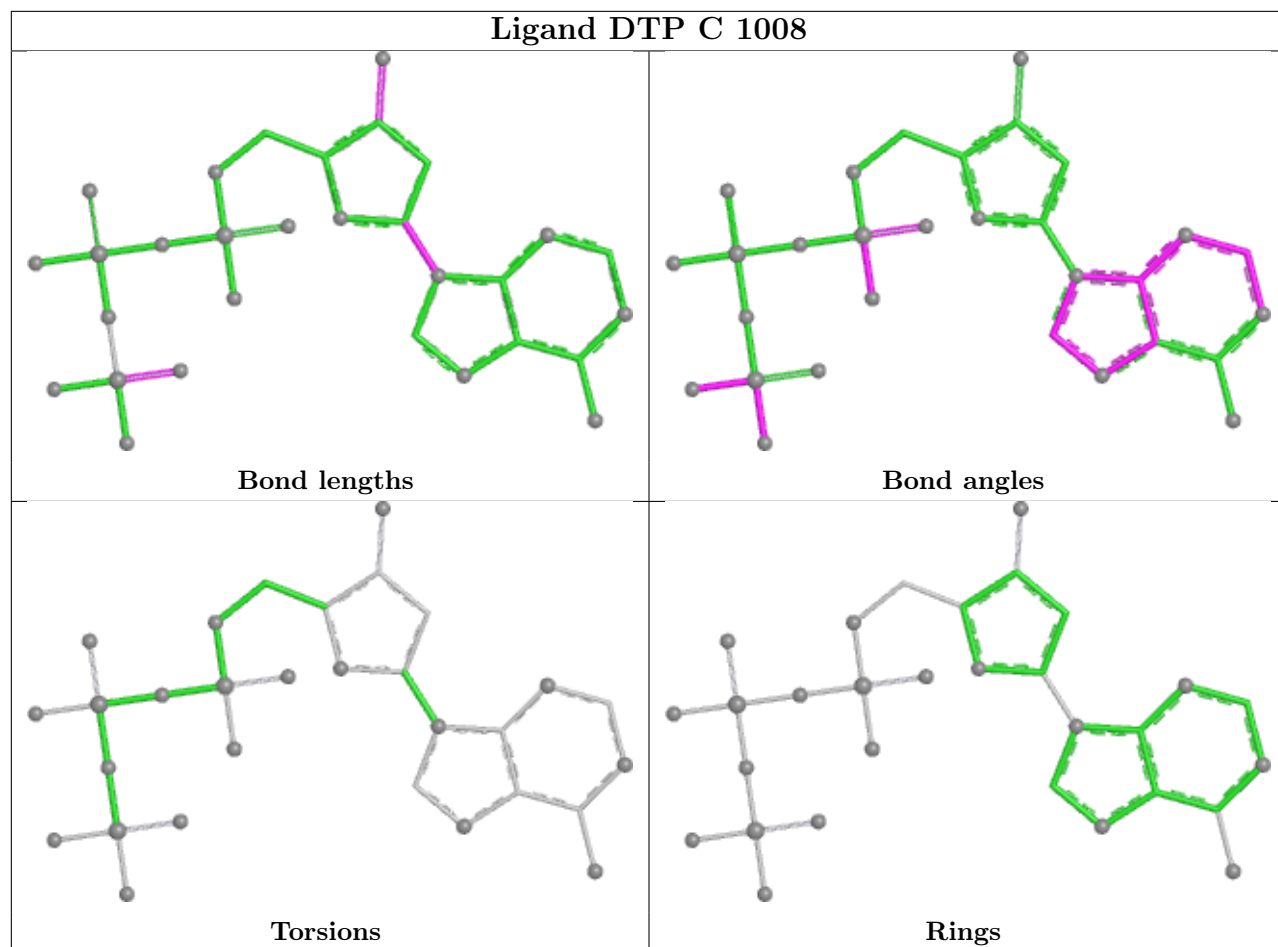
Ligand CDP A 1002



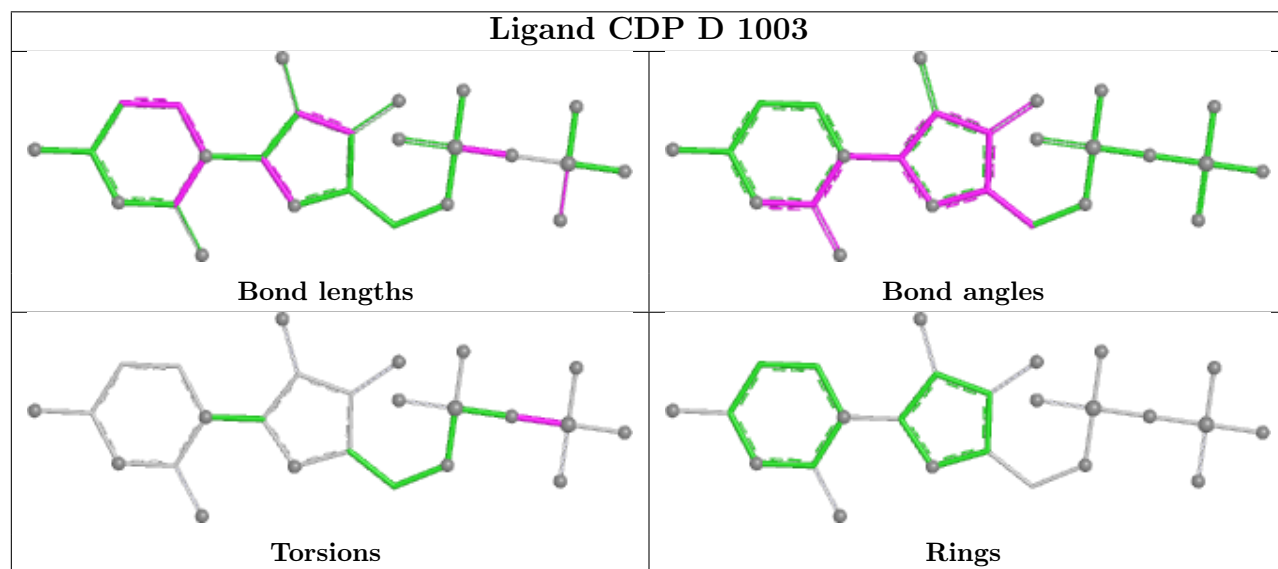
Ligand CDP B 1001

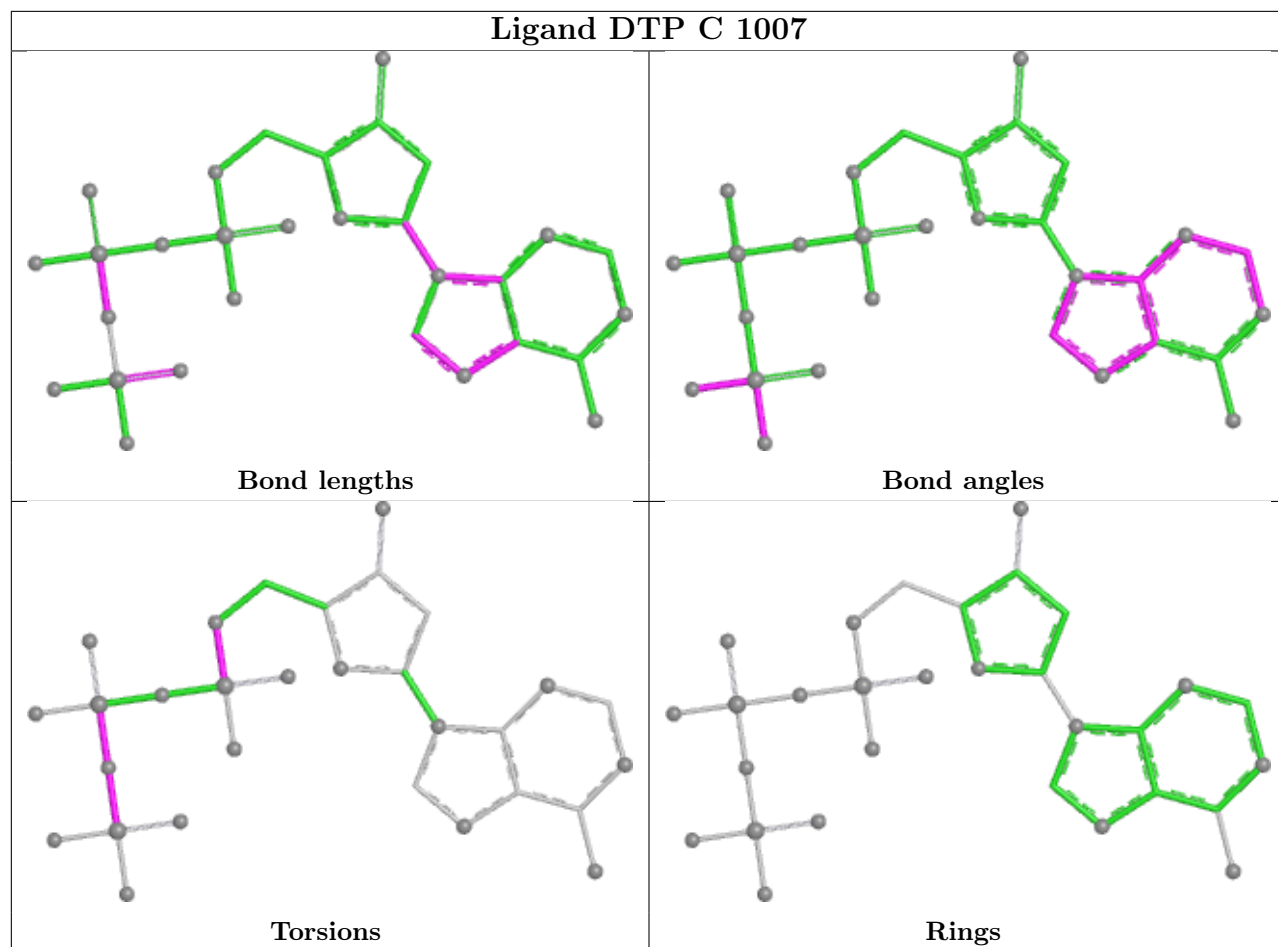


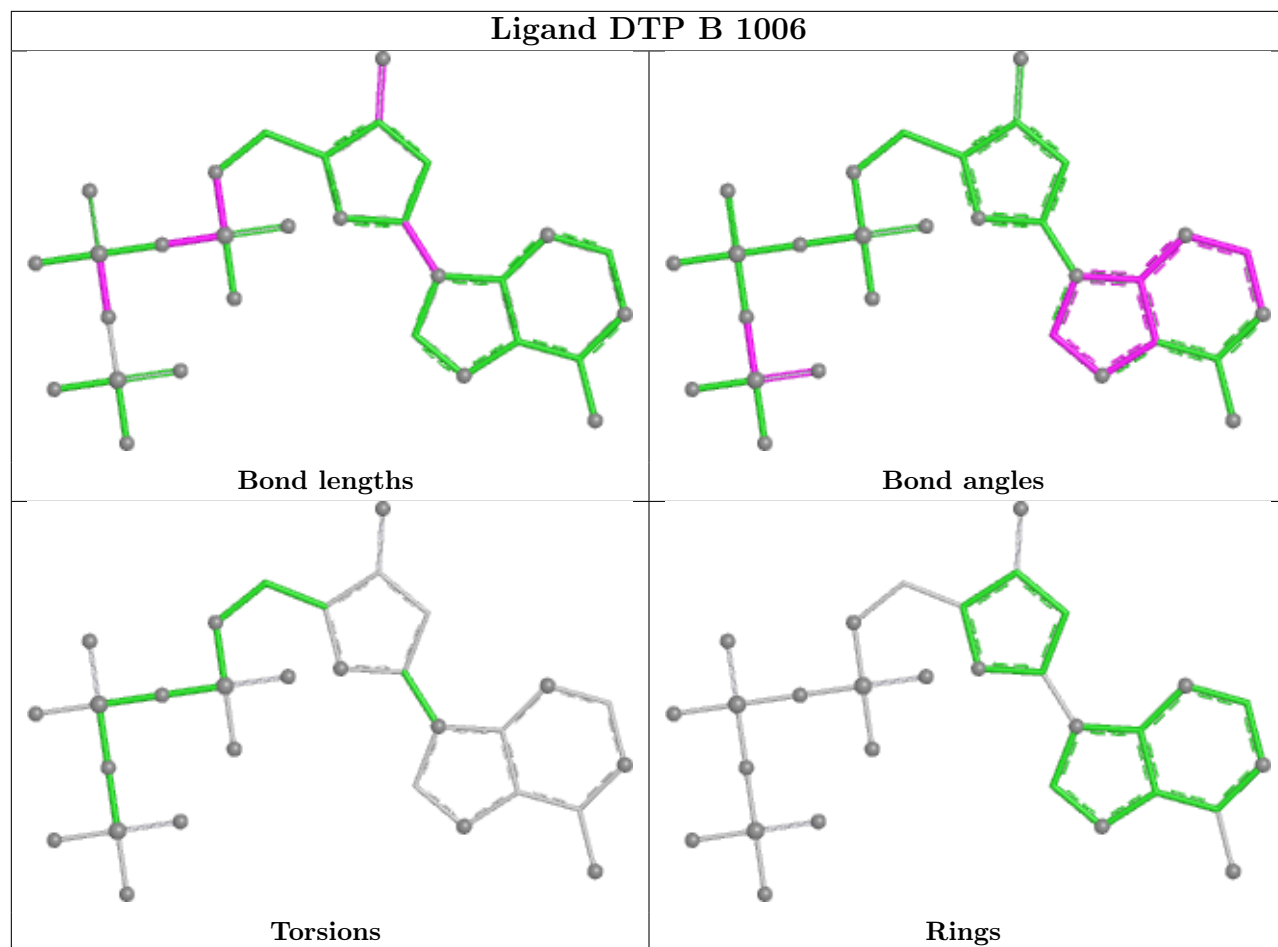
Ligand DTP C 1008

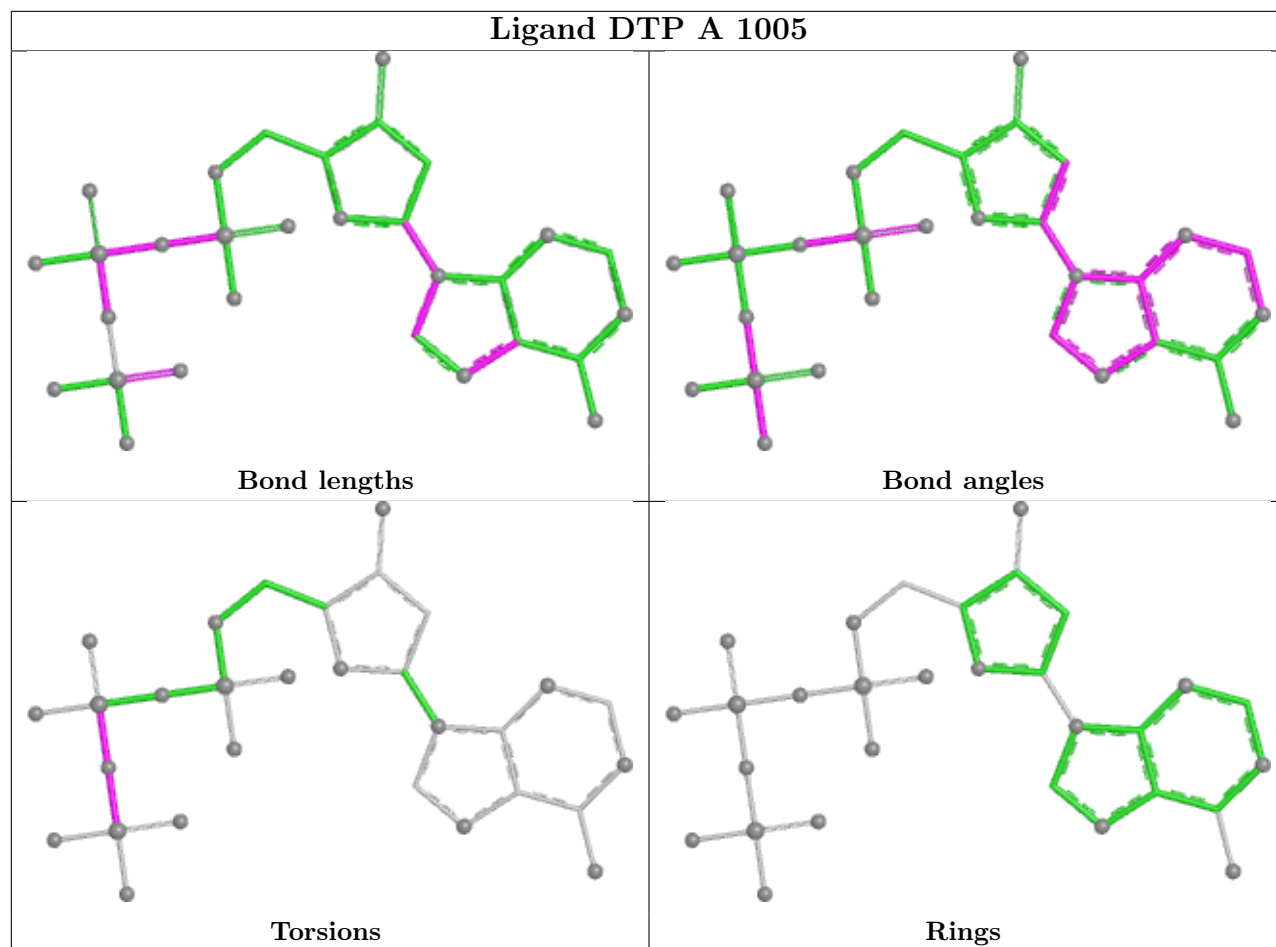


Ligand CDP D 1003









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	618/644 (95%)	-0.50	7 (1%) 78 79	13, 23, 49, 79	0
1	B	610/644 (94%)	-0.43	11 (1%) 67 68	12, 23, 54, 70	0
1	C	615/644 (95%)	-0.40	6 (0%) 79 81	16, 26, 52, 68	0
1	D	607/644 (94%)	-0.23	7 (1%) 76 77	19, 29, 56, 69	0
All	All	2450/2576 (95%)	-0.39	31 (1%) 75 76	12, 26, 53, 79	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	LEU	5.8
1	B	209	GLY	5.6
1	C	181	HIS	4.5
1	B	541	ILE	4.3
1	B	527	LEU	4.0
1	A	209	GLY	3.5
1	A	32	LEU	3.5
1	A	515	PHE	3.4
1	A	237	VAL	3.3
1	D	525	PRO	3.2
1	C	180	THR	3.2
1	A	516	VAL	3.1
1	C	32	LEU	3.1
1	D	237	VAL	3.0
1	D	34	GLY	3.0
1	D	542	LEU	2.9
1	C	237	VAL	2.8
1	A	178	ALA	2.7
1	B	559	PRO	2.6
1	C	525	PRO	2.6
1	B	65	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	514	ARG	2.4
1	D	541	ILE	2.4
1	C	34	GLY	2.3
1	A	180	THR	2.3
1	D	526	LEU	2.3
1	B	525	PRO	2.2
1	B	546	GLU	2.2
1	B	528	TYR	2.1
1	B	539	PRO	2.1
1	D	527	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

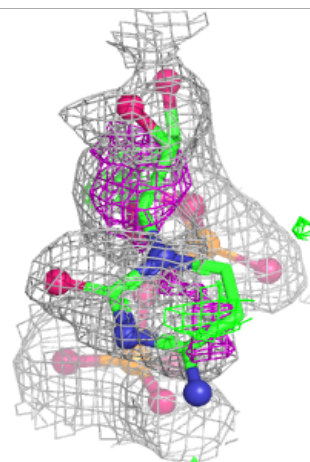
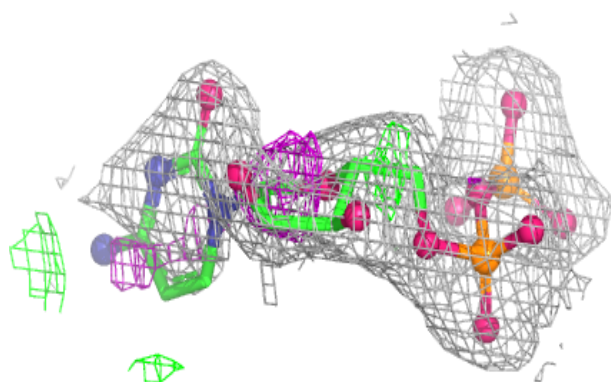
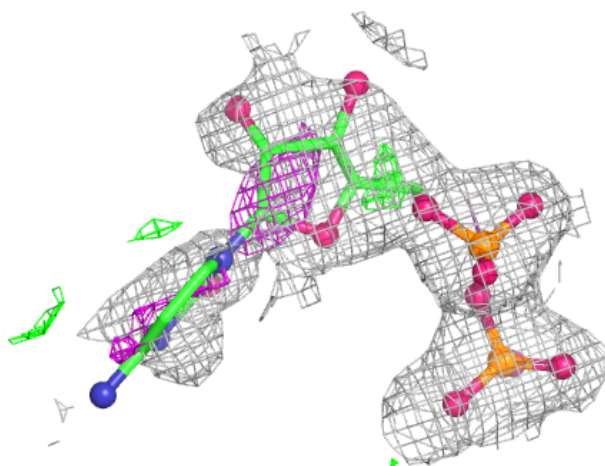
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1009	1/1	0.89	0.11	58,58,58,58	0
2	CDP	C	1004	25/25	0.93	0.11	23,50,64,64	0
2	CDP	D	1003	25/25	0.94	0.11	26,43,58,59	0
3	DTP	C	1007	30/30	0.94	0.07	25,30,56,59	0
2	CDP	A	1002	25/25	0.94	0.12	22,52,66,67	0
2	CDP	B	1001	25/25	0.96	0.08	22,32,41,41	0
3	DTP	B	1006	30/30	0.96	0.06	13,21,40,42	0
3	DTP	C	1008	30/30	0.97	0.05	14,21,40,41	0
3	DTP	A	1005	30/30	0.97	0.06	15,24,57,59	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.

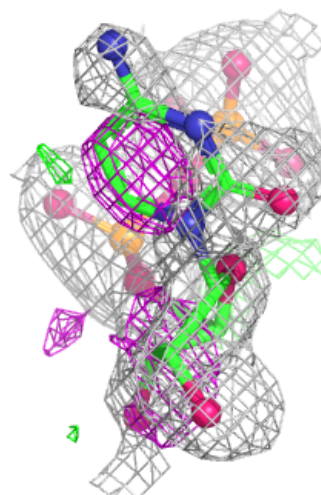
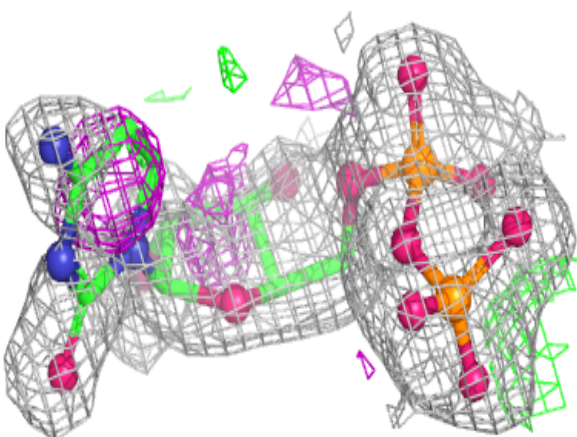
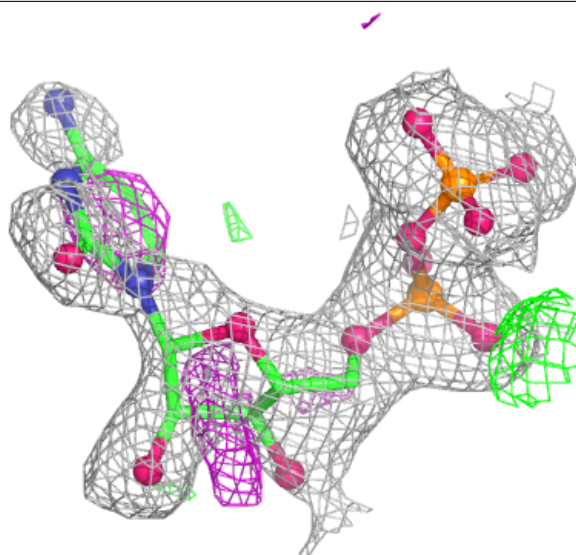
Electron density around CDP C 1004:

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



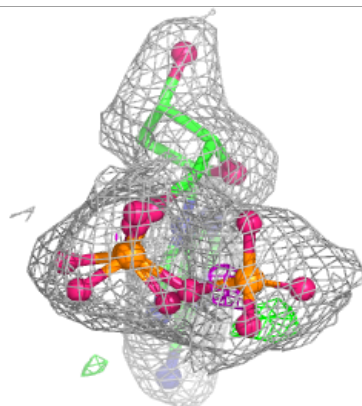
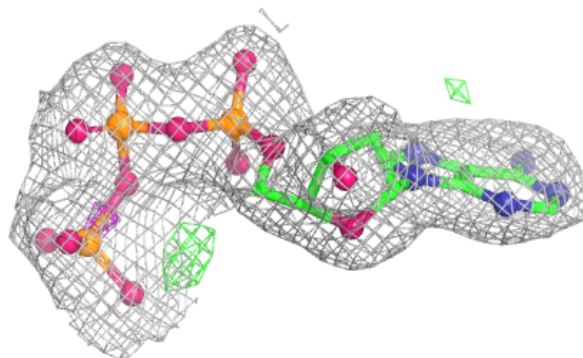
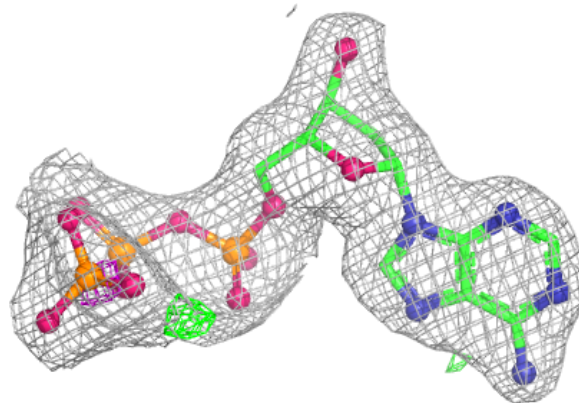
Electron density around CDP D 1003:

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

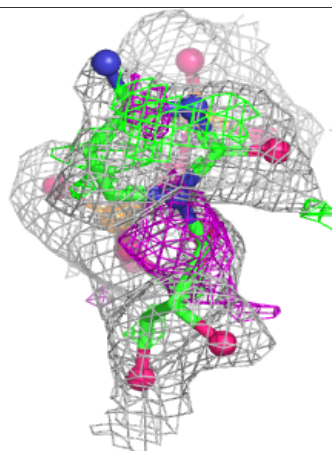
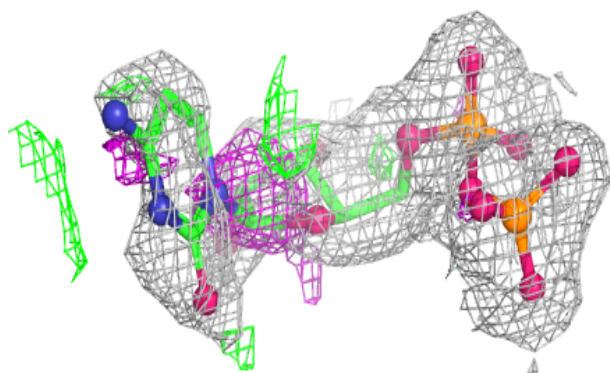
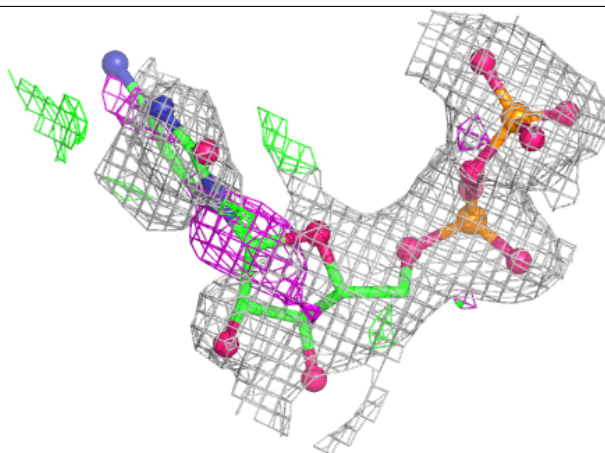


Electron density around DTP C 1007:

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

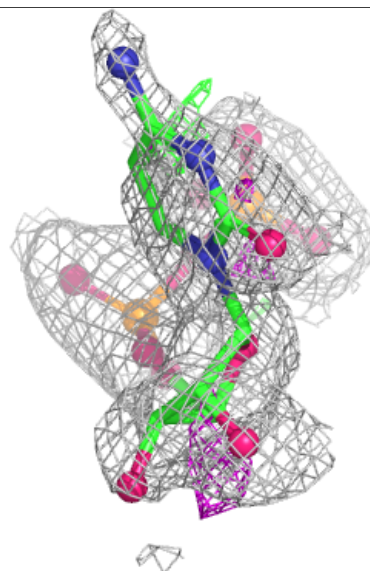
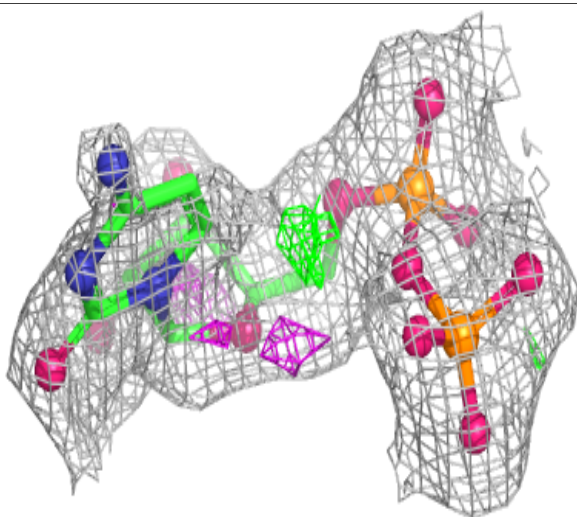
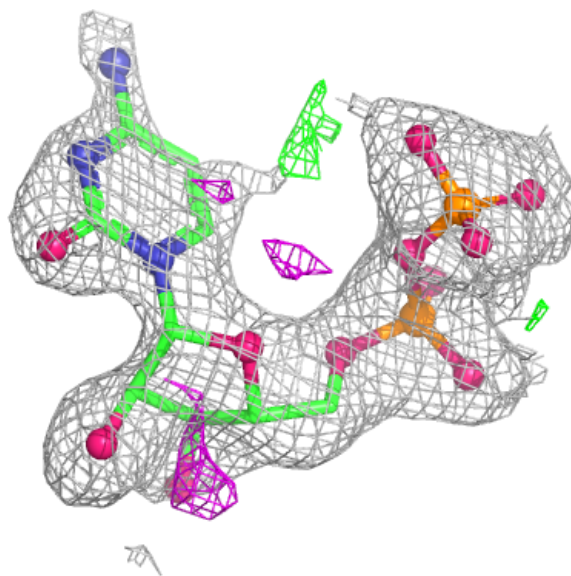
**Electron density around CDP A 1002:**

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



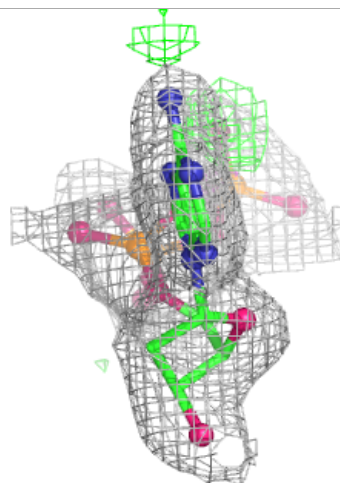
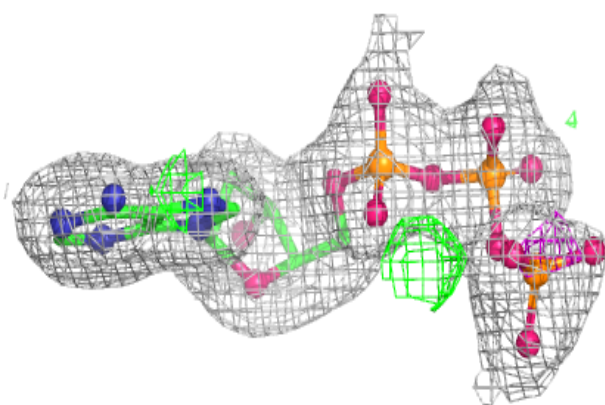
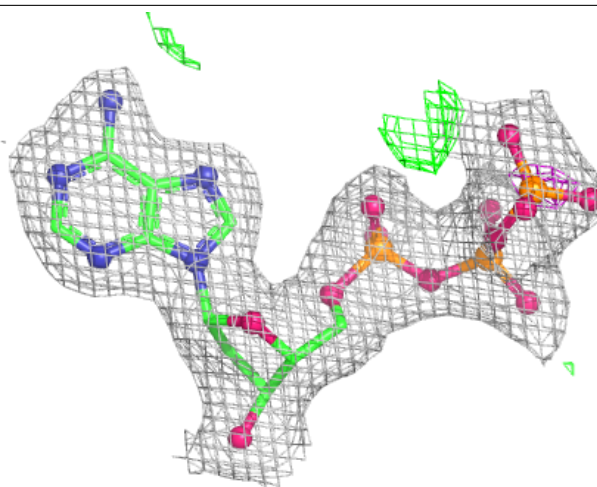
Electron density around CDP B 1001:

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



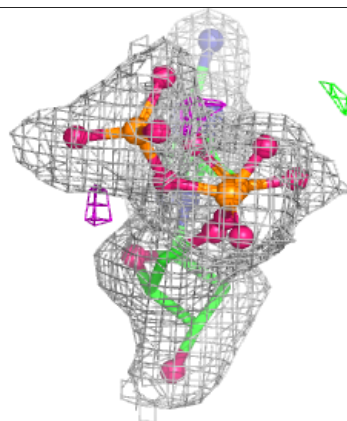
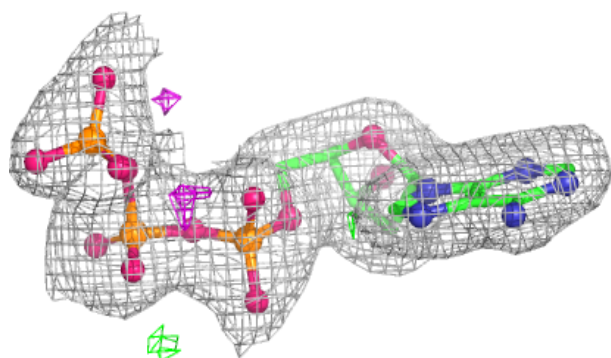
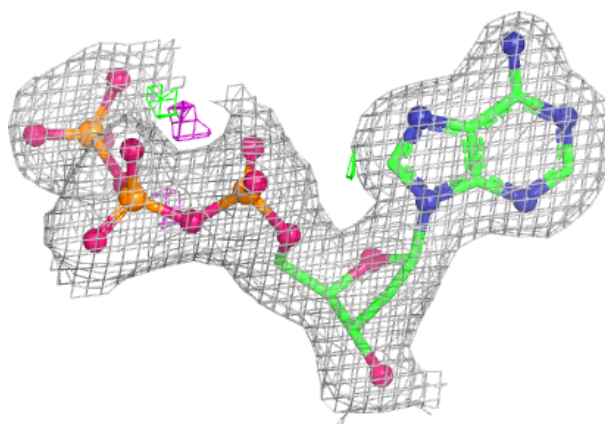
Electron density around DTP B 1006:

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

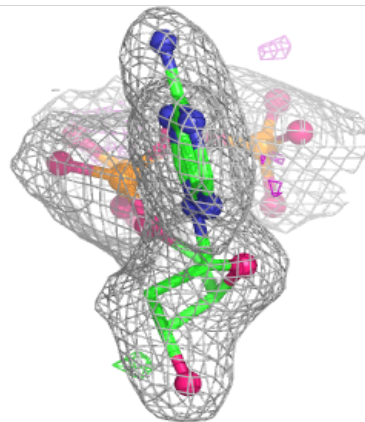
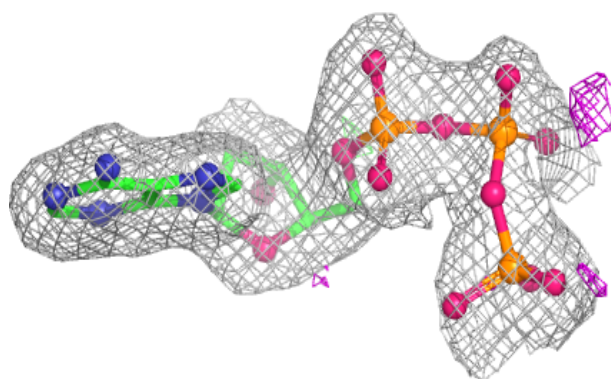
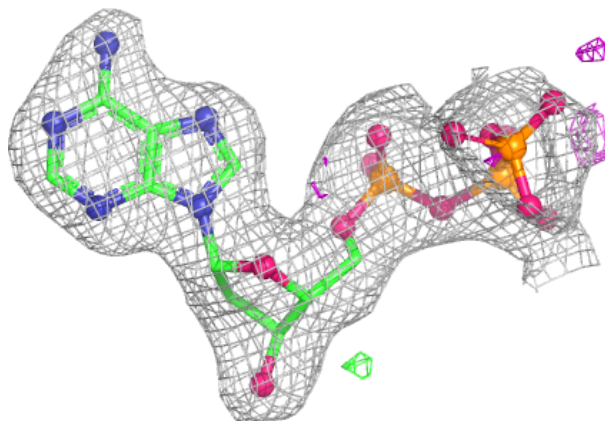


Electron density around DTP C 1008:

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

**Electron density around DTP A 1005:**

$2mF_o-DF_c$ (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.