Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 08:56 AM EDT

PDB ID	:	1XJN
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 (i) 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 (i)) were used in the production of this report:

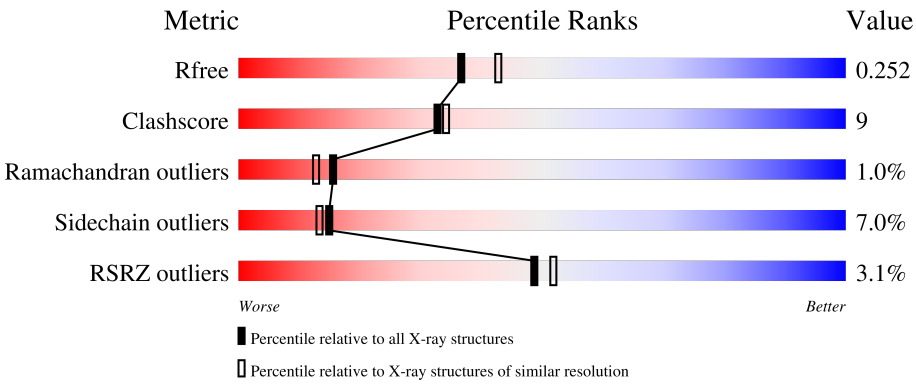
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 <=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	3% 80% 13% • •
1	B	644	3% 74% 17% • 5%
1	C	644	3% 73% 19% • 5%
1	D	644	3% 71% 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 (i)

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.

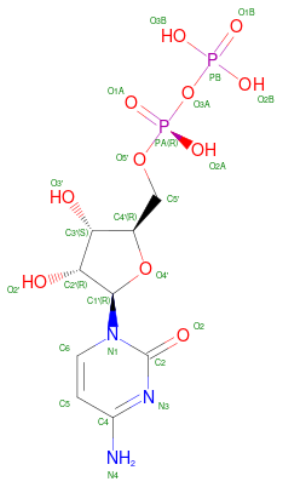
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	4958	3181	839	918	20	0	0	0
1	B	610	4898	3139	834	905	20	0	0	0
1	C	615	4934	3161	838	915	20	0	0	0
1	D	607	4874	3129	824	901	20	0	0	0

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 (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).

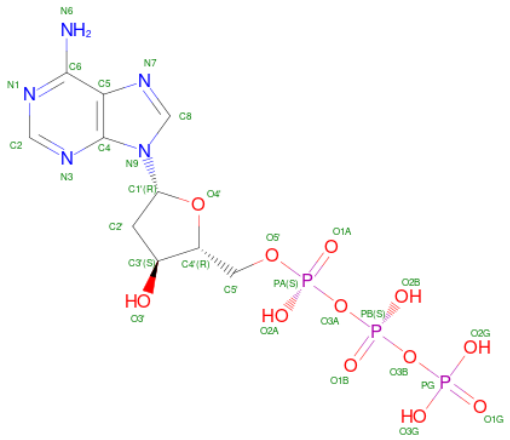
CDP



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 (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

DTP



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

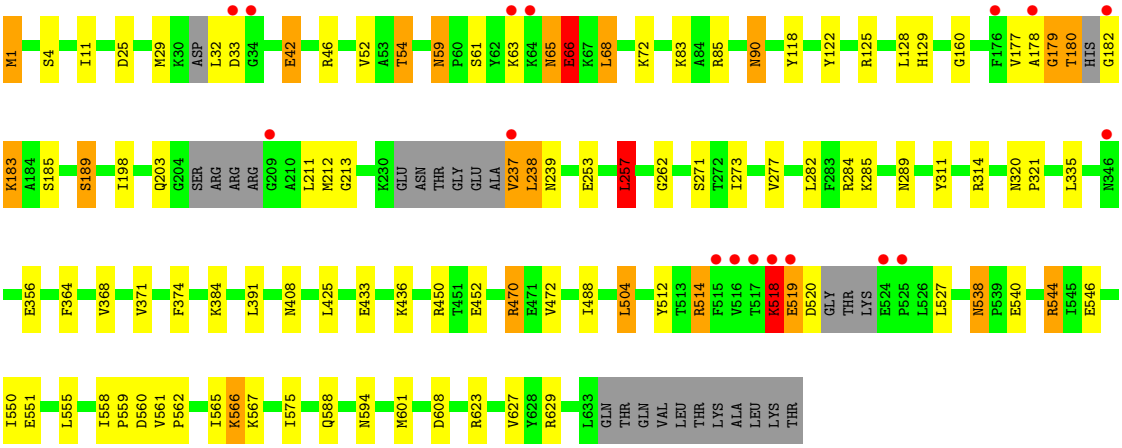
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	180	180	180	0	0
5	B	197	197	197	0	0
5	C	167	167	167	0	0
5	D	105	105	105	0	0

3 Residue-property plots (i)

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

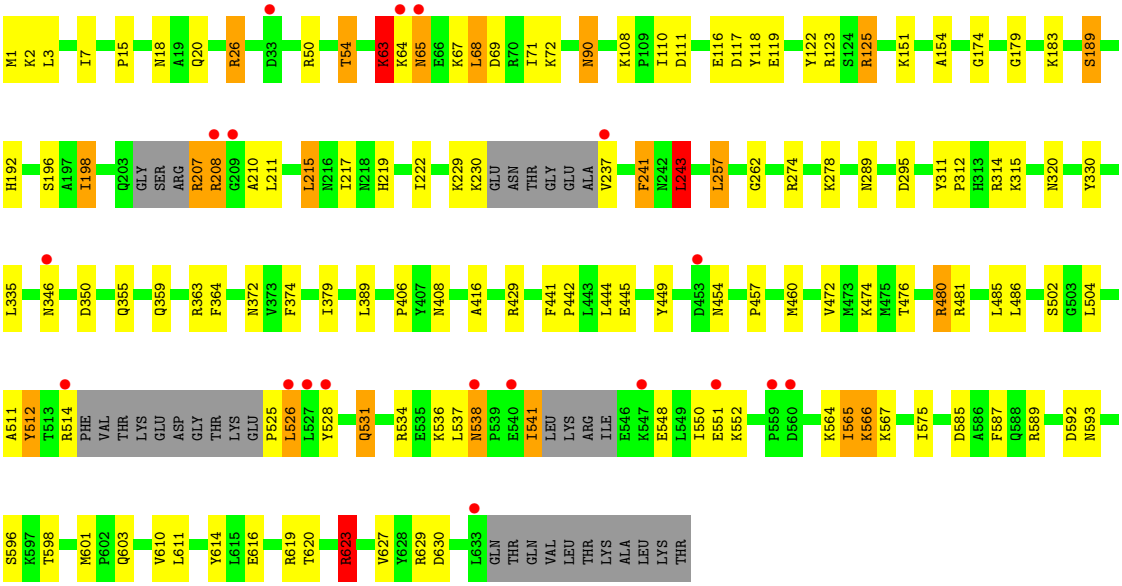
• Molecule 1: ribonucleotide reductase, B12-dependent

Chain A:



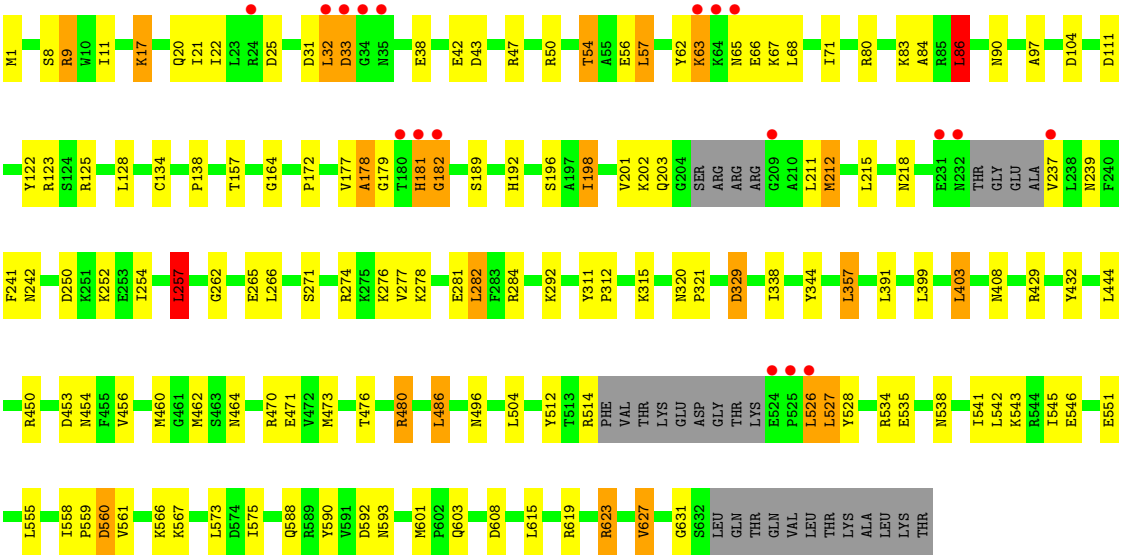
• Molecule 1: ribonucleotide reductase, B12-dependent

Chain B:



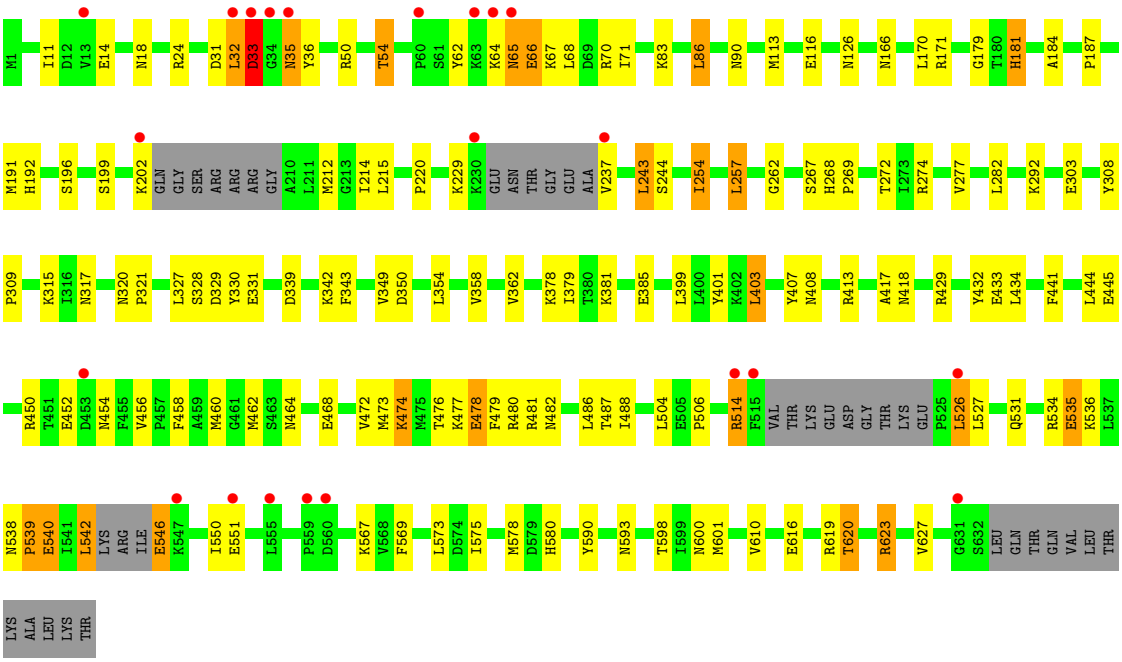
• Molecule 1: ribonucleotide reductase, B12-dependent

Chain C:



• Molecule 1: ribonucleotide reductase, B12-dependent

Chain D:



4 Data and refinement statistics (i)

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 19.53 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.54-2.25) 99.5 (19.53-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.26Å)	Xtriage
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	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, CDP, CL

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	0.96	2/5053 (0.0%)	0.93	6/6817 (0.1%)
1	B	1.00	1/4994 (0.0%)	0.98	15/6739 (0.2%)
1	C	0.90	1/5031 (0.0%)	0.90	7/6791 (0.1%)
1	D	0.91	1/4971 (0.0%)	0.91	9/6710 (0.1%)
All	All	0.94	5/20049 (0.0%)	0.93	37/27057 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	471	GLU	CG-CD	5.42	1.60	1.51
1	A	42	GLU	CB-CG	-5.34	1.42	1.52
1	A	368	VAL	CB-CG1	5.23	1.63	1.52
1	D	468	GLU	CB-CG	-5.16	1.42	1.52
1	B	116	GLU	CG-CD	5.13	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	623	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	B	623	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	C	623	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	C	623	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	B	629	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	D	623	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	B	125	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	619	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	629	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	238	LEU	N-CA-C	6.90	129.62	111.00
1	C	257	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	85	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	619	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	D	623	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	237	VAL	C-N-CA	6.26	137.35	121.70
1	C	57	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	623	ARG	CD-NE-CZ	5.98	131.98	123.60
1	D	329	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	B	526	LEU	N-CA-C	5.73	126.48	111.00
1	B	629	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	D	413	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	526	LEU	C-N-CA	5.47	135.37	121.70
1	D	329	ASP	CB-CG-OD2	5.45	123.21	118.30
1	D	113	MET	CG-SD-CE	-5.36	91.63	100.20
1	A	257	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	69	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	86	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	363	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	629	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	403	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	243	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	314	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	329	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	623	ARG	CB-CG-CD	5.03	124.69	111.60
1	D	86	LEU	CA-CB-CG	5.03	126.87	115.30
1	C	619	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	350	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	LYS	Peptide

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4958	0	5014	79	0
1	B	4898	0	4948	91	0
1	C	4934	0	4980	83	0
1	D	4874	0	4920	95	0
2	A	25	0	12	1	0
2	B	25	0	12	1	0
2	C	25	0	12	0	0
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	4	0
5	D	105	0	0	5	0
All	All	20534	0	19958	346	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 (346) 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:D:212:MET:HE3	1:D:244:SER:HB2	1.21	1.14
1:A:565:ILE:O	1:A:566:LYS:HB2	1.45	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:257:LEU:HD22	1:D:262:GLY:HA3	1.41	1.02
1:D:601:MET:HE1	1:D:610:VAL:HG22	1.44	1.00
1:B:2:LYS:HE3	5:B:1182:HOH:O	1.67	0.94
1:D:601:MET:CE	1:D:610:VAL:HG22	1.98	0.94
1:B:601:MET:HE1	1:B:610:VAL:HG22	1.51	0.93
1:B:63:LYS:HB3	1:B:64:LYS:O	1.66	0.93
1:B:207:ARG:NH1	4:B:1009:CL:CL	2.41	0.90
1:B:601:MET:CE	1:B:610:VAL:HG22	2.02	0.88
1:A:65:ASN:H	1:A:65:ASN:HD22	1.21	0.88
1:C:512:TYR:O	1:C:527:LEU:O	1.93	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
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: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:A:601:MET:CE	1:A:627:VAL:HB	2.13	0.77
1:C:63:LYS:HB2	1:C:66:GLU:HG3	1.66	0.77
1:B:514:ARG:C	1:B:526:LEU:CB	2.53	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:A:65:ASN:H	1:A:65:ASN:ND2	1.84	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:B:514:ARG:C	1:B:526:LEU:HB2	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:601:MET:HE2	1:C:627:VAL:HB	1.72	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:601:MET:HE2	1:A:627:VAL:HB	1.71	0.70
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:D:257:LEU:HD22	1:D:262:GLY:CA	2.22	0.69
1:B:538:ASN:HD22	1:B:541:ILE:CD1	2.05	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
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: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:B:63:LYS:HB3	1:B:64:LYS:C	2.18	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:A:212:MET:HE3	1:A:213:GLY:N	2.14	0.63
1:B:514:ARG:C	1:B:526:LEU:HB3	2.18	0.62
1:A:284:ARG:NH2	1:A:608:ASP:OD1	2.32	0.62
1:A:122:TYR:O	1:A:125:ARG:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:601:MET:HE3	1:D:610:VAL:HG22	1.81	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: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:C:453:ASP:O	1:C:454:ASN:HB2	2.01	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
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: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:B:601:MET:HE3	1:B:610:VAL:HG22	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:212:MET:HE3	1:C:212:MET:HA	1.85	0.57
1:D:212:MET:HE1	1:D:244:SER:HB2	1.82	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: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: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:D:212:MET:CE	1:D:244:SER:CB	2.71	0.56
1:C:202:LYS:C	1:C:203:GLN:HE21	2.08	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
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:B:3:LEU:O	1:B:7:ILE:HG13	2.06	0.55
1:A:601:MET:HE3	1:A:627:VAL:HB	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:64:LYS:C	1:D:66:GLU:H	2.13	0.52
1:B:108:LYS:HE2	1:B:117:ASP:OD2	2.09	0.52
1:B:364:PHE:CD1	1:B:364:PHE:C	2.83	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:A:212:MET:HE3	1:A:213:GLY:H	1.74	0.52
1:B:551:GLU:HG3	1:B:552:LYS:H	1.75	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
1:C:212:MET:HE3	1:C:242:ASN:O	2.11	0.51
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: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:D:212:MET:HE2	1:D:214:ILE:CG1	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:72:LYS:O	1:B:110:ILE:HD11	2.13	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:B:601:MET:HE3	1:B:610:VAL:CG2	2.44	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: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
1:B:601:MET:CE	1:B:610:VAL:CG2	2.86	0.47
1:B:68:LEU:HD22	1:B:72:LYS:HD2	1.96	0.47
1:C:1:MET:HE2	1:C:9:ARG:HH21	1.79	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:237:VAL:HG13	1:C:237:VAL:O	2.15	0.46
1:A:52:VAL:HG21	1:A:364:PHE:CZ	2.51	0.46
1:B:67:LYS:O	1:B:71:ILE:HG13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:PRO:O	1:C:560:ASP:CG	2.54	0.46
1:D:450:ARG:NH1	1:D:478:GLU:HA	2.31	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:B:217:ILE:HA	1:B:222:ILE:HG12	1.98	0.45
1:D:126:ASN:OD1	1:D:126:ASN:C	2.53	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:D:476:THR:HA	1:D:479:PHE:O	2.17	0.45
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:C:218:ASN:HA	1:C:266:LEU:HD22	1.99	0.44
1:D:212:MET:HE1	1:D:244:SER:CB	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LYS:HE3	1:A:518:LYS:C	2.39	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:C:588:GLN:CD	1:C:623:ARG:HD3	2.39	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
1:A:562:PRO:O	1:A:565:ILE:O	2.38	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: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:59:ASN:HD22	1:A:59:ASN:C	2.24	0.41
1:A:65:ASN:O	1:A:66:GLU:HB3	2.20	0.41
1:A:128:LEU:HD13	1:B:179:GLY:HA3	2.02	0.41
1:A:538:ASN:HD22	1:A:538:ASN:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:O	1:A:550:ILE:HD12	2.21	0.41
1:D:212:MET:CE	1:D:214:ILE:HG12	2.50	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: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:C:460:MET:HE1	1:C:470:ARG:HD3	2.03	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
1:A:1:MET:HE3	5:A:1138:HOH:O	2.21	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: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%)	12 8
1	B	600/644 (93%)	572 (95%)	22 (4%)	6 (1%)	15 13
1	C	607/644 (94%)	576 (95%)	25 (4%)	6 (1%)	15 13
1	D	597/644 (93%)	555 (93%)	37 (6%)	5 (1%)	19 17
All	All	2410/2576 (94%)	2280 (95%)	105 (4%)	25 (1%)	15 13

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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	544/566 (96%)	514 (94%)	30 (6%)	21 21
1	B	537/566 (95%)	504 (94%)	33 (6%)	18 18
1	C	541/566 (96%)	496 (92%)	45 (8%)	11 9
1	D	535/566 (94%)	493 (92%)	42 (8%)	12 10
All	All	2157/2264 (95%)	2007 (93%)	150 (7%)	15 13

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	25	ASP
1	A	29	MET
1	A	42	GLU
1	A	46	ARG
1	A	54	THR
1	A	59	ASN
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	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	504	LEU
1	A	514	ARG
1	A	518	LYS
1	A	538	ASN
1	A	544	ARG
1	A	551	GLU
1	A	560	ASP
1	B	26	ARG
1	B	54	THR
1	B	68	LEU
1	B	90	ASN
1	B	189	SER
1	B	196	SER
1	B	198	ILE
1	B	207	ARG
1	B	215	LEU
1	B	230	LYS
1	B	243	LEU
1	B	257	LEU

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Mol	Chain	Res	Type
1	B	278	LYS
1	B	289	ASN
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	502	SER
1	B	504	LEU
1	B	512	TYR
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	596	SER
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	104	ASP
1	C	111	ASP
1	C	123	ARG
1	C	181	HIS
1	C	189	SER
1	C	192	HIS
1	C	196	SER
1	C	198	ILE
1	C	212	MET
1	C	215	LEU

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Mol	Chain	Res	Type
1	C	257	LEU
1	C	276	LYS
1	C	282	LEU
1	C	292	LYS
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	462	MET
1	C	464	ASN
1	C	480	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	573	LEU
1	C	627	VAL
1	D	14	GLU
1	D	24	ARG
1	D	31	ASP
1	D	32	LEU
1	D	33	ASP
1	D	54	THR
1	D	65	ASN
1	D	66	GLU
1	D	68	LEU
1	D	86	LEU
1	D	90	ASN
1	D	116	GLU
1	D	181	HIS
1	D	196	SER
1	D	199	SER
1	D	202	LYS
1	D	215	LEU
1	D	243	LEU

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Mol	Chain	Res	Type
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	458	PHE
1	D	474	LYS
1	D	478	GLU
1	D	504	LEU
1	D	514	ARG
1	D	526	LEU
1	D	535	GLU
1	D	536	LYS
1	D	540	GLU
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	627	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	59	ASN
1	A	65	ASN
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	35	ASN
1	B	112	GLN
1	B	454	ASN

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Mol	Chain	Res	Type
1	B	496	ASN
1	B	531	GLN
1	B	538	ASN
1	B	603	GLN
1	C	20	GLN
1	C	203	GLN
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	112	GLN
1	D	181	HIS
1	D	313	HIS
1	D	345	ASN
1	D	346	ASN
1	D	454	ASN
1	D	464	ASN
1	D	496	ASN
1	D	538	ASN
1	D	600	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 monosaccharides 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	$\#\|Z\| > 2$
3	DTP	C	1007	-	26,32,32	1.16	2 (7%)	30,50,50	1.51	6 (20%)
2	CDP	D	1003	-	24,26,26	1.68	6 (25%)	37,40,40	1.67	7 (18%)
3	DTP	B	1006	-	26,32,32	1.30	3 (11%)	30,50,50	1.69	4 (13%)
2	CDP	C	1004	-	24,26,26	1.65	3 (12%)	37,40,40	1.59	6 (16%)
3	DTP	C	1008	-	26,32,32	1.16	2 (7%)	30,50,50	1.38	2 (6%)
2	CDP	B	1001	-	24,26,26	1.16	2 (8%)	37,40,40	1.47	4 (10%)
3	DTP	A	1005	-	26,32,32	1.09	1 (3%)	30,50,50	1.53	4 (13%)
2	CDP	A	1002	-	24,26,26	1.54	3 (12%)	37,40,40	1.25	6 (16%)

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
3	DTP	C	1007	-	-	6/18/34/34	0/3/3/3
2	CDP	D	1003	-	-	1/16/32/32	0/2/2/2
3	DTP	B	1006	-	-	1/18/34/34	0/3/3/3
2	CDP	C	1004	-	-	3/16/32/32	0/2/2/2
3	DTP	C	1008	-	-	0/18/34/34	0/3/3/3
2	CDP	B	1001	-	-	1/16/32/32	0/2/2/2
3	DTP	A	1005	-	-	5/18/34/34	0/3/3/3
2	CDP	A	1002	-	-	8/16/32/32	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	CDP	O4'-C1'	5.37	1.54	1.42
2	C	1004	CDP	O4'-C1'	5.04	1.53	1.42
2	C	1004	CDP	C5'-C4'	-3.68	1.40	1.51
3	B	1006	DTP	C4-N3	-3.52	1.30	1.35
2	D	1003	CDP	PB-O3B	3.50	1.68	1.54
2	D	1003	CDP	O4'-C1'	3.24	1.49	1.42
3	C	1007	DTP	PG-O3G	3.20	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1003	CDP	C6-N1	2.96	1.45	1.38
2	D	1003	CDP	C6-C5	2.73	1.41	1.35
3	C	1008	DTP	PG-O3G	2.72	1.65	1.54
3	C	1008	DTP	O3'-C3'	2.62	1.48	1.43
3	A	1005	DTP	PG-O3G	2.59	1.64	1.54
2	C	1004	CDP	C6-C5	2.47	1.40	1.35
2	D	1003	CDP	C2-N1	2.37	1.45	1.40
3	B	1006	DTP	O3'-C3'	2.36	1.48	1.43
2	A	1002	CDP	C6-N1	2.34	1.43	1.38
3	C	1007	DTP	C4-N3	-2.32	1.32	1.35
3	B	1006	DTP	PA-O5'	2.30	1.68	1.59
2	B	1001	CDP	O4'-C1'	2.24	1.47	1.42
2	D	1003	CDP	C2'-C3'	2.18	1.59	1.53
2	B	1001	CDP	C6-C5	2.09	1.39	1.35
2	A	1002	CDP	PA-O2A	-2.08	1.45	1.55

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1008	DTP	N3-C2-N1	-5.45	120.16	128.68
3	B	1006	DTP	N3-C2-N1	-5.20	120.55	128.68
3	A	1005	DTP	N3-C2-N1	-4.99	120.88	128.68
2	B	1001	CDP	O4'-C4'-C5'	-4.99	92.96	109.37
2	D	1003	CDP	C5'-C4'-C3'	-4.87	96.92	115.18
2	C	1004	CDP	C4'-O4'-C1'	-4.71	99.07	109.47
3	C	1007	DTP	N3-C2-N1	-4.68	121.36	128.68
3	B	1006	DTP	O3G-PG-O3B	-4.63	89.09	104.64
2	C	1004	CDP	C2'-C1'-N1	3.95	124.39	113.22
2	C	1004	CDP	O4'-C4'-C3'	-3.29	98.61	105.11
2	D	1003	CDP	O3'-C3'-C2'	3.15	122.01	111.82
2	D	1003	CDP	O4'-C4'-C5'	3.11	119.61	109.37
2	A	1002	CDP	C4'-O4'-C1'	-2.91	103.06	109.47
2	D	1003	CDP	O2-C2-N3	-2.87	117.67	122.33
3	C	1007	DTP	PB-O3B-PG	-2.85	123.04	132.83
2	D	1003	CDP	O4'-C1'-N1	-2.74	102.09	108.36
2	A	1002	CDP	O4'-C1'-N1	2.65	114.43	108.36
2	C	1004	CDP	C5'-C4'-C3'	-2.62	105.38	115.18
3	A	1005	DTP	C2'-C1'-N9	-2.55	108.38	114.27
3	B	1006	DTP	PB-O3B-PG	-2.54	124.11	132.83
2	D	1003	CDP	C2'-C1'-N1	2.47	120.22	113.22
3	C	1008	DTP	O2G-PG-O1G	2.46	120.30	110.68
2	B	1001	CDP	C5'-C4'-C3'	2.41	124.22	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	CDP	O3A-PB-O1B	-2.40	97.85	111.19
2	A	1002	CDP	O4'-C4'-C3'	-2.38	100.40	105.11
3	A	1005	DTP	PA-O3A-PB	-2.38	124.65	132.83
3	B	1006	DTP	PA-O3A-PB	-2.35	124.78	132.83
3	C	1007	DTP	PA-O3A-PB	-2.33	124.84	132.83
2	C	1004	CDP	C5-C6-N1	-2.30	117.95	121.81
2	A	1002	CDP	O2B-PB-O1B	2.29	119.63	110.68
2	A	1002	CDP	O2B-PB-O3B	2.26	116.28	107.64
3	A	1005	DTP	O2G-PG-O3B	2.25	112.19	104.64
3	C	1007	DTP	C5-C6-N6	2.20	123.69	120.35
3	C	1007	DTP	C4-C5-N7	-2.18	107.12	109.40
3	C	1007	DTP	O2G-PG-O1G	2.15	119.09	110.68
2	C	1004	CDP	O2A-PA-O1A	2.09	122.56	112.24
2	A	1002	CDP	O2A-PA-O1A	2.07	122.47	112.24
2	B	1001	CDP	O2B-PB-O3A	2.03	111.45	104.64
2	D	1003	CDP	C1'-N1-C2	2.02	122.94	118.42

There are no chirality outliers.

All (25) 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	B	1006	DTP	C5'-O5'-PA-O3A
3	C	1007	DTP	PG-O3B-PB-O2B
3	C	1007	DTP	C5'-O5'-PA-O1A
2	A	1002	CDP	O4'-C1'-N1-C6
2	C	1004	CDP	O4'-C1'-N1-C6
2	A	1002	CDP	O4'-C1'-N1-C2
2	C	1004	CDP	O4'-C1'-N1-C2
2	A	1002	CDP	O4'-C4'-C5'-O5'
3	C	1007	DTP	PG-O3B-PB-O1B
2	A	1002	CDP	PA-O3A-PB-O1B
2	C	1004	CDP	C2'-C1'-N1-C6
2	B	1001	CDP	PA-O3A-PB-O1B
2	A	1002	CDP	PA-O3A-PB-O2B
3	C	1007	DTP	PB-O3B-PG-O3G
2	A	1002	CDP	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
3	A	1005	DTP	PG-O3B-PB-O1B
3	A	1005	DTP	PG-O3B-PB-O2B
3	C	1007	DTP	C5'-O5'-PA-O2A
3	A	1005	DTP	PB-O3B-PG-O1G

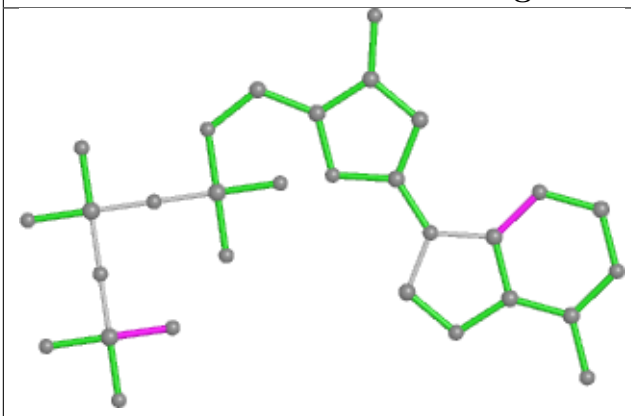
There are no ring outliers.

3 monomers are involved in 3 short contacts:

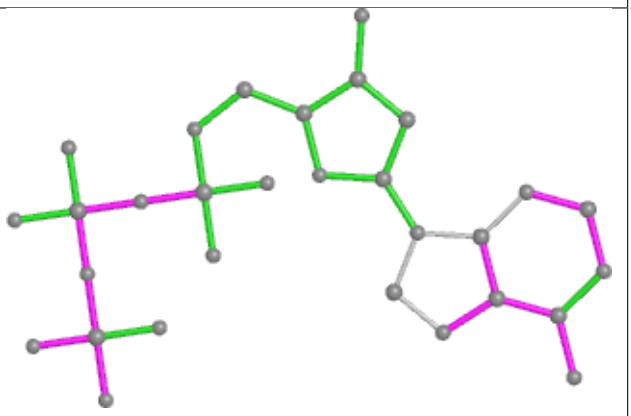
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1003	CDP	1	0
2	B	1001	CDP	1	0
2	A	1002	CDP	1	0

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 then 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.

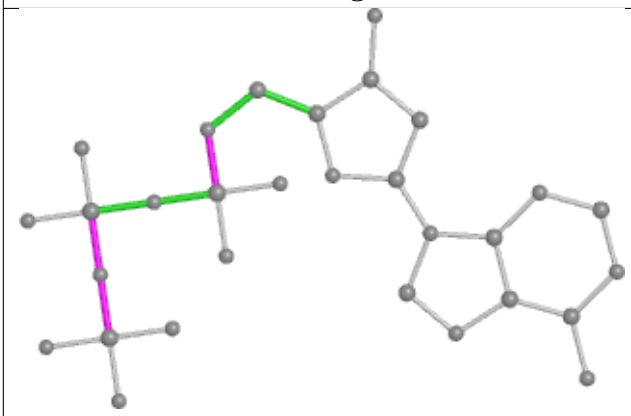
Ligand DTP C 1007



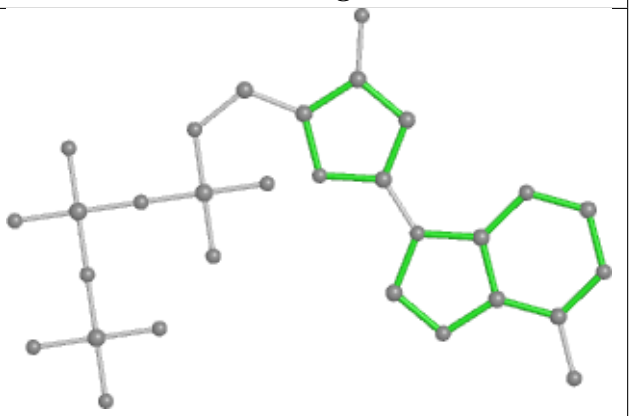
Bond lengths



Bond angles

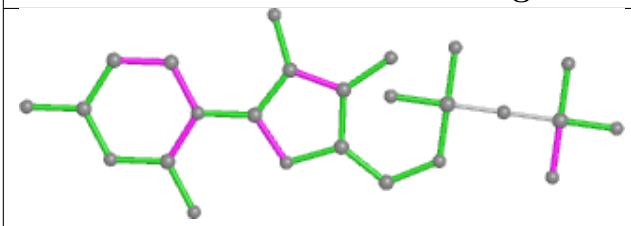


Torsions

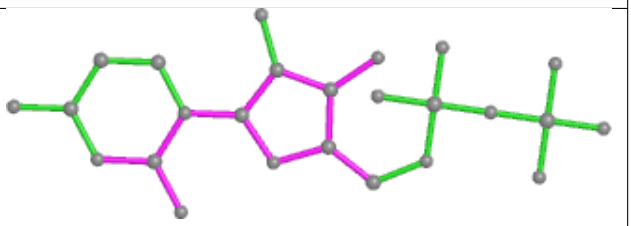


Rings

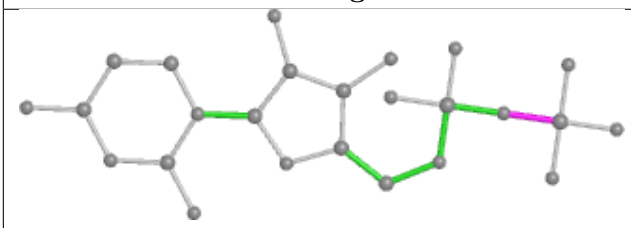
Ligand CDP D 1003



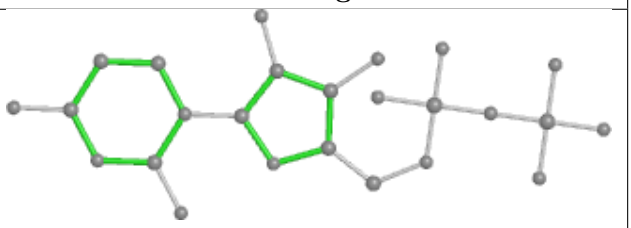
Bond lengths



Bond angles

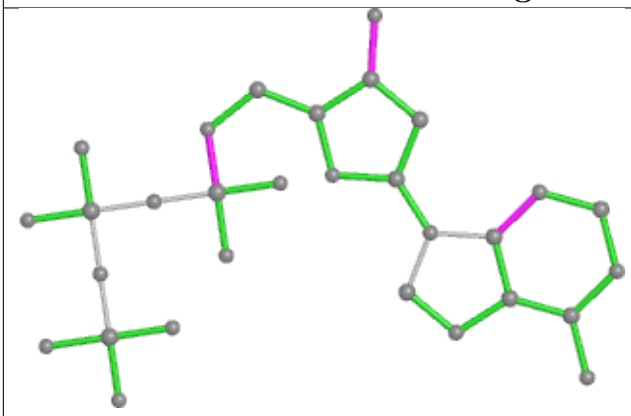


Torsions

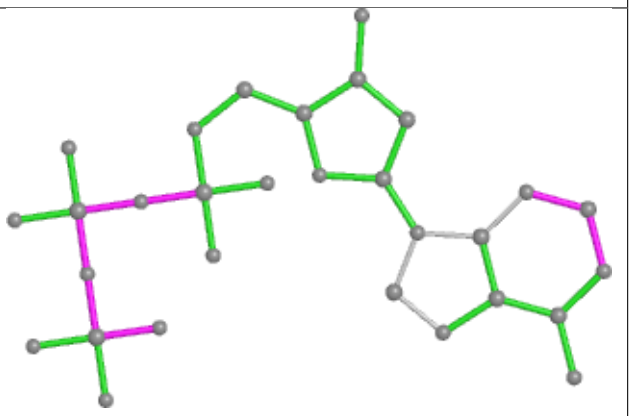


Rings

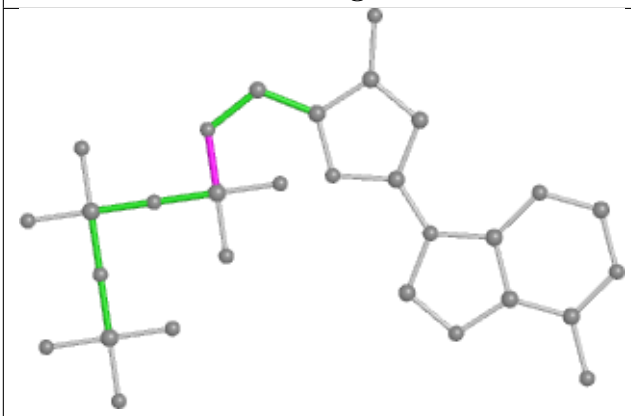
Ligand DTP B 1006



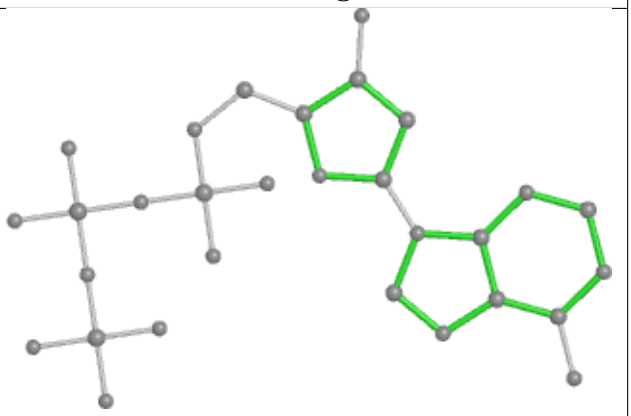
Bond lengths



Bond angles

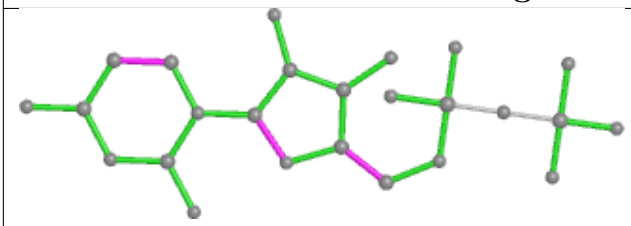


Torsions

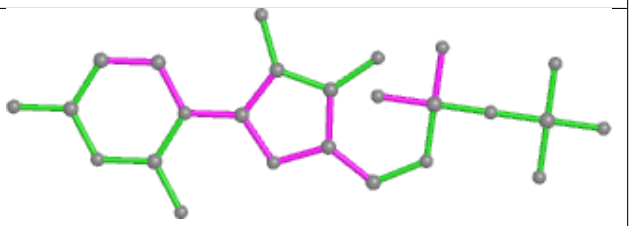


Rings

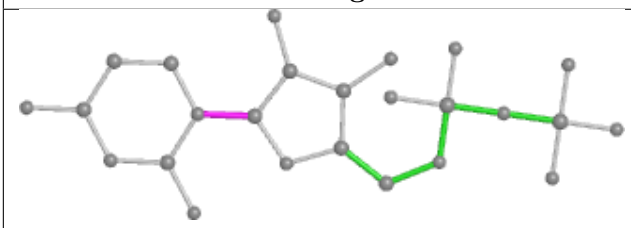
Ligand CDP C 1004



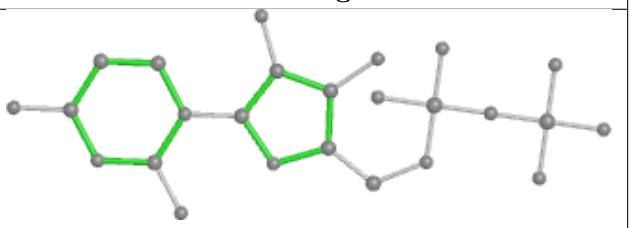
Bond lengths



Bond angles

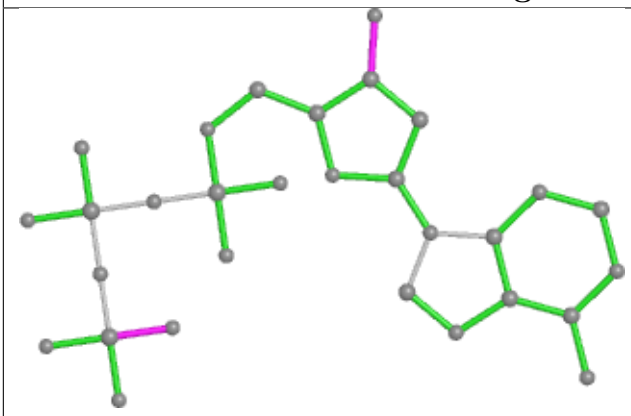


Torsions

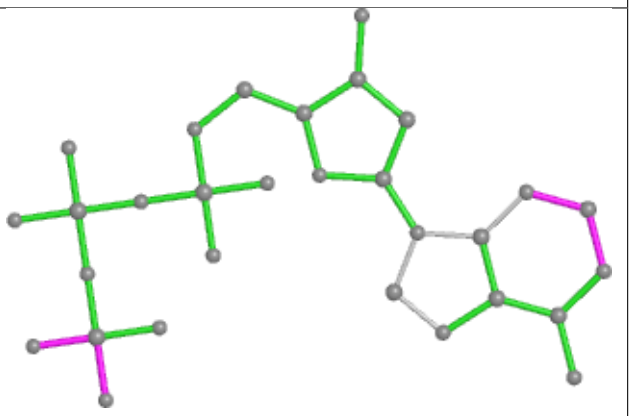


Rings

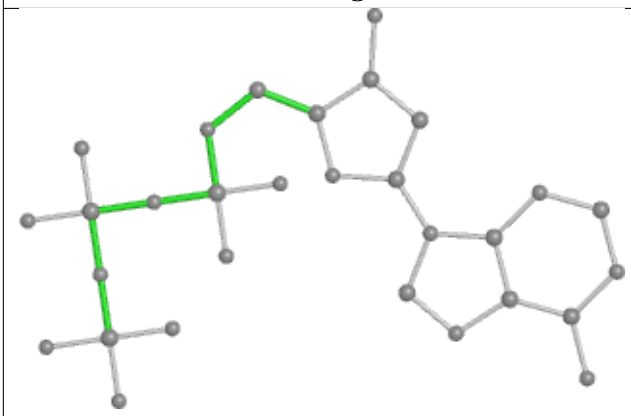
Ligand DTP C 1008



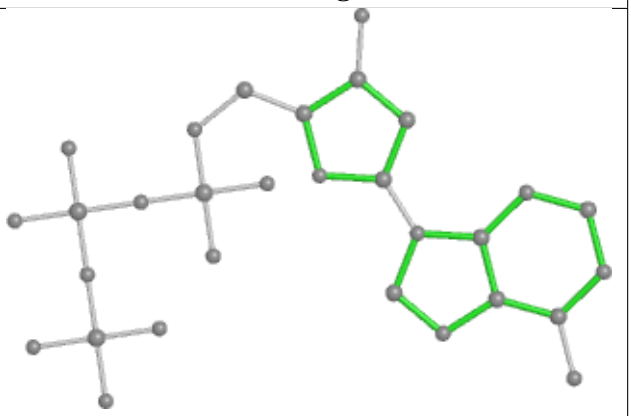
Bond lengths



Bond angles

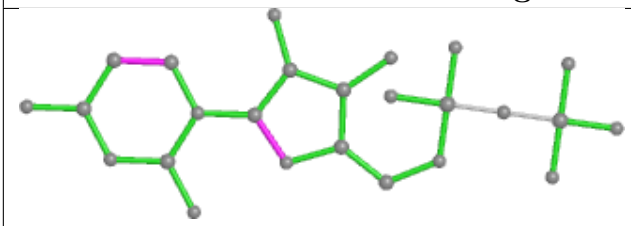


Torsions

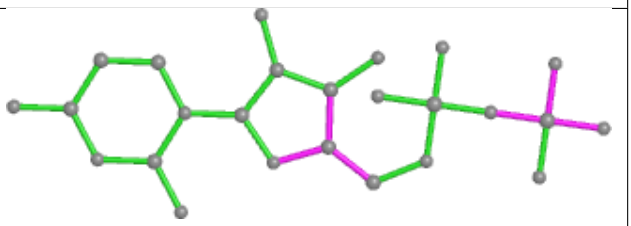


Rings

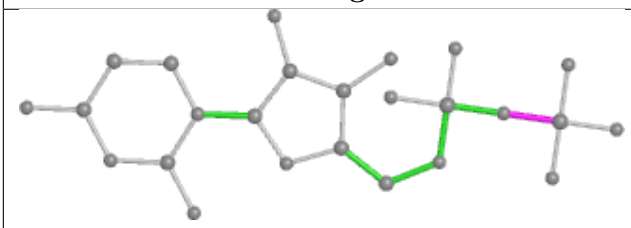
Ligand CDP B 1001



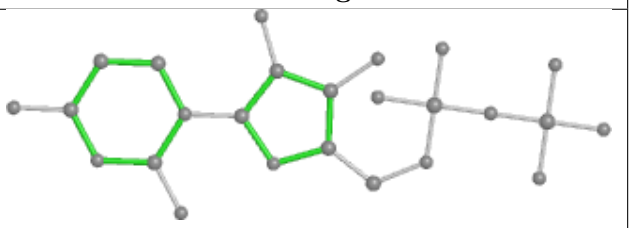
Bond lengths



Bond angles

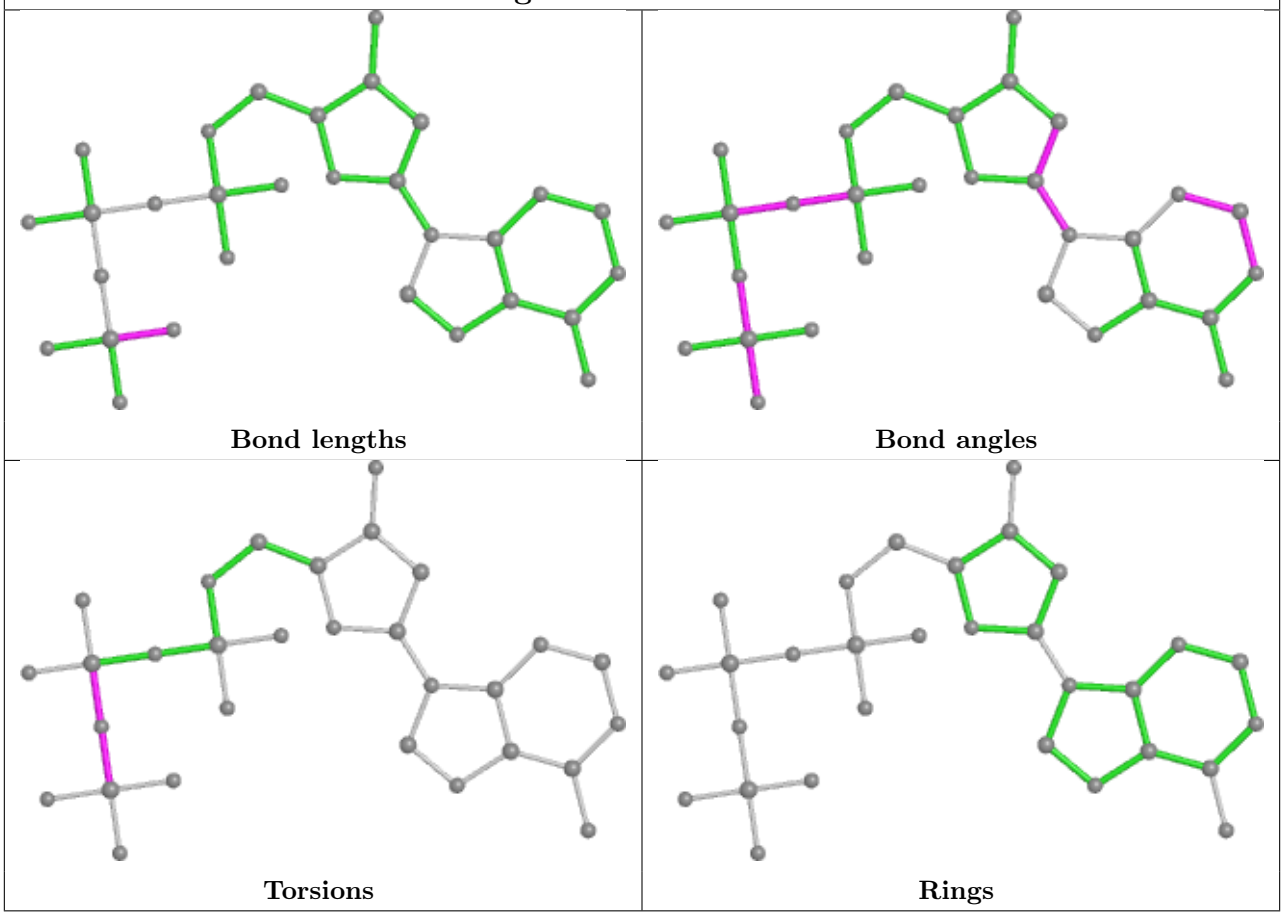


Torsions

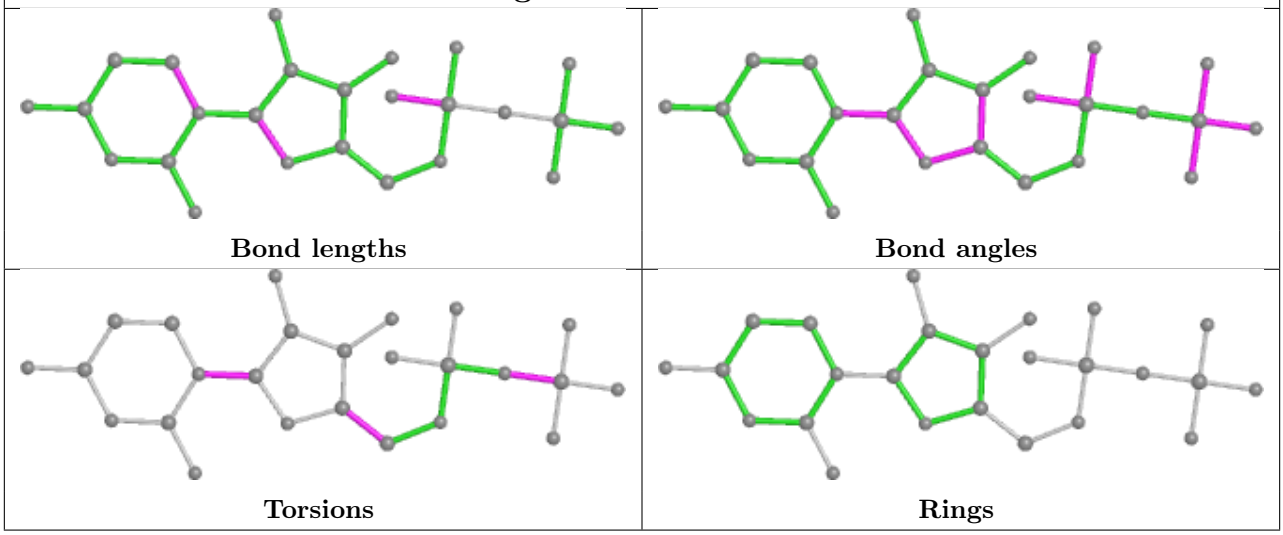


Rings

Ligand DTP A 1005



Ligand CDP A 1002



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	618/644 (95%)	-0.30	17 (2%)	53	55	13, 23, 49, 79	0
1	B	610/644 (94%)	-0.30	19 (3%)	49	52	12, 23, 54, 70	0
1	C	615/644 (95%)	-0.25	18 (2%)	51	55	16, 26, 52, 68	0
1	D	607/644 (94%)	-0.16	22 (3%)	42	44	19, 29, 56, 69	0
All	All	2450/2576 (95%)	-0.25	76 (3%)	49	52	12, 26, 53, 79	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	HIS	7.8
1	B	526	LEU	6.1
1	A	515	PHE	5.1
1	D	34	GLY	4.9
1	B	527	LEU	4.7
1	D	237	VAL	4.6
1	C	231	GLU	4.6
1	D	33	ASP	4.6
1	C	232	ASN	4.5
1	A	33	ASP	4.5
1	A	516	VAL	4.4
1	B	209	GLY	4.4
1	B	559	PRO	4.3
1	B	65	ASN	4.2
1	A	517	THR	4.2
1	A	519	GLU	4.2
1	B	560	ASP	4.1
1	A	182	GLY	4.1
1	A	34	GLY	4.0
1	A	518	LYS	4.0
1	A	525	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	32	LEU	3.9
1	C	524	GLU	3.7
1	C	34	GLY	3.7
1	A	209	GLY	3.5
1	A	237	VAL	3.4
1	D	560	ASP	3.4
1	C	180	THR	3.4
1	C	526	LEU	3.4
1	B	208	ARG	3.2
1	C	237	VAL	3.2
1	C	33	ASP	3.1
1	C	182	GLY	3.0
1	B	64	LYS	3.0
1	B	547	LYS	3.0
1	C	525	PRO	3.0
1	C	65	ASN	2.8
1	D	514	ARG	2.8
1	D	32	LEU	2.8
1	D	515	PHE	2.8
1	D	63	LYS	2.7
1	B	551	GLU	2.7
1	D	60	PRO	2.7
1	C	35	ASN	2.7
1	C	209	GLY	2.6
1	D	559	PRO	2.6
1	C	63	LYS	2.6
1	D	555	LEU	2.5
1	A	176	PHE	2.5
1	A	524	GLU	2.5
1	B	237	VAL	2.5
1	D	631	GLY	2.5
1	A	63	LYS	2.4
1	D	526	LEU	2.4
1	D	35	ASN	2.4
1	D	64	LYS	2.4
1	A	346	ASN	2.4
1	B	514	ARG	2.3
1	B	633	LEU	2.3
1	B	33	ASP	2.3
1	D	202	LYS	2.3
1	A	178	ALA	2.3
1	B	540	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	547	LYS	2.2
1	D	551	GLU	2.2
1	C	64	LYS	2.2
1	D	65	ASN	2.2
1	B	538	ASN	2.1
1	B	453	ASP	2.1
1	D	230	LYS	2.1
1	D	453	ASP	2.1
1	A	64	LYS	2.1
1	B	346	ASN	2.1
1	D	13	VAL	2.0
1	C	24	ARG	2.0
1	B	528	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

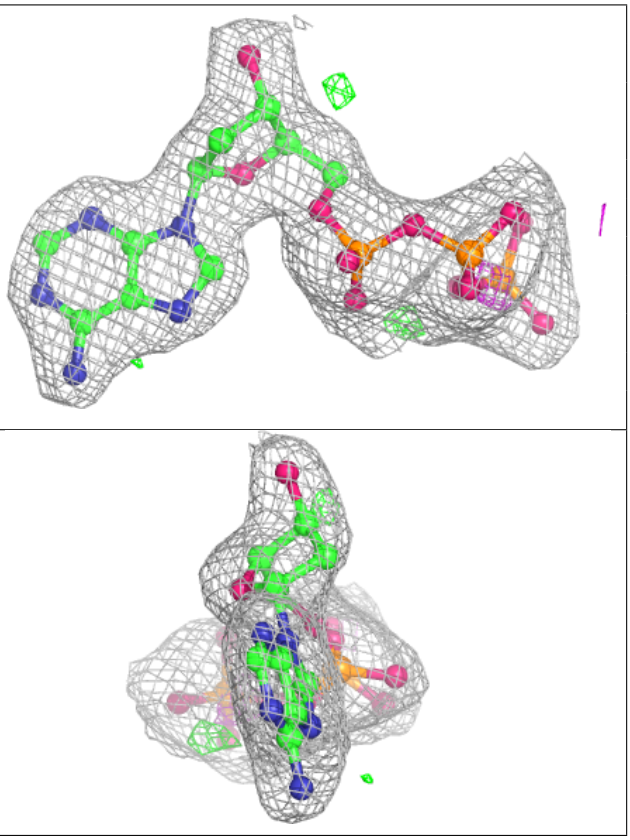
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	B	1009	1/1	0.89	0.22	58,58,58,58	0
3	DTP	C	1007	30/30	0.93	0.11	25,30,56,59	0
2	CDP	C	1004	25/25	0.93	0.22	23,50,64,64	0
2	CDP	A	1002	25/25	0.94	0.20	22,52,66,67	0
2	CDP	D	1003	25/25	0.94	0.19	26,43,58,59	0
3	DTP	A	1005	30/30	0.95	0.11	15,24,57,59	0
2	CDP	B	1001	25/25	0.96	0.15	22,32,41,41	0
3	DTP	C	1008	30/30	0.96	0.09	14,21,40,41	0
3	DTP	B	1006	30/30	0.96	0.10	13,21,40,42	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.

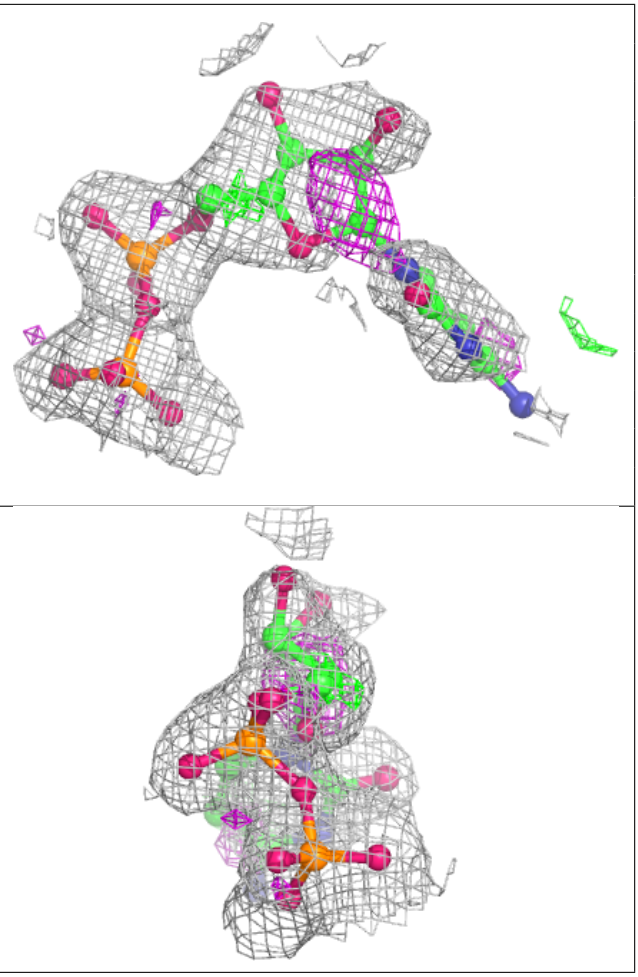
Electron density around DTP C 1007:

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



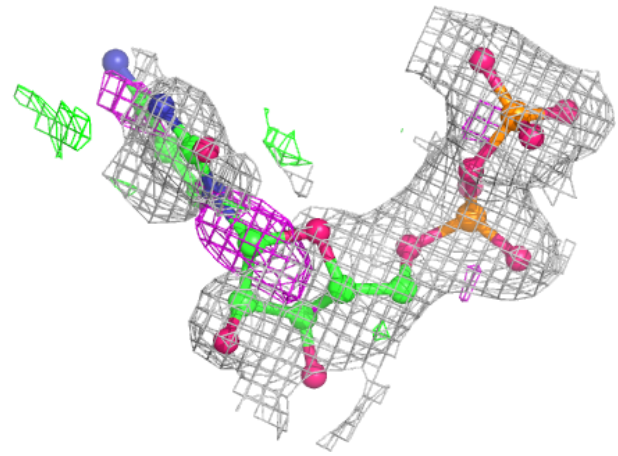
Electron density around CDP C 1004:

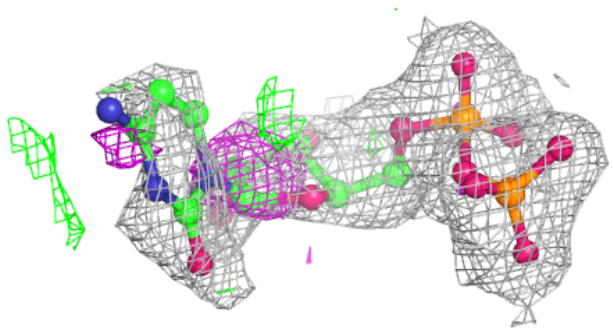
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

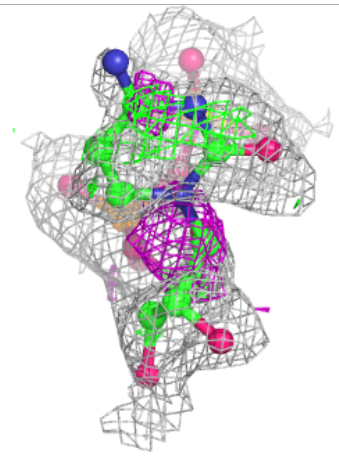


Electron density around CDP A 1002:

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

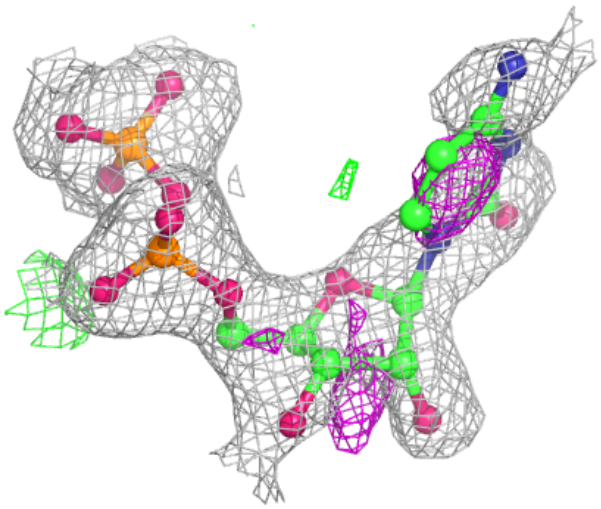


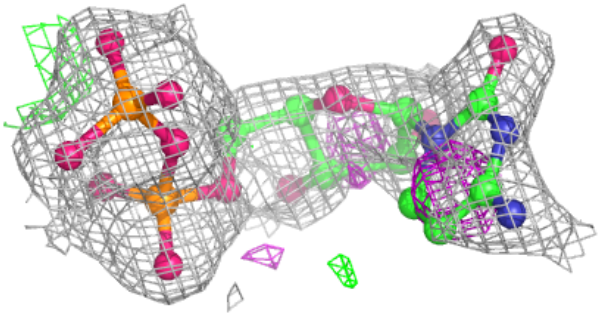




Electron density around CDP D 1003:

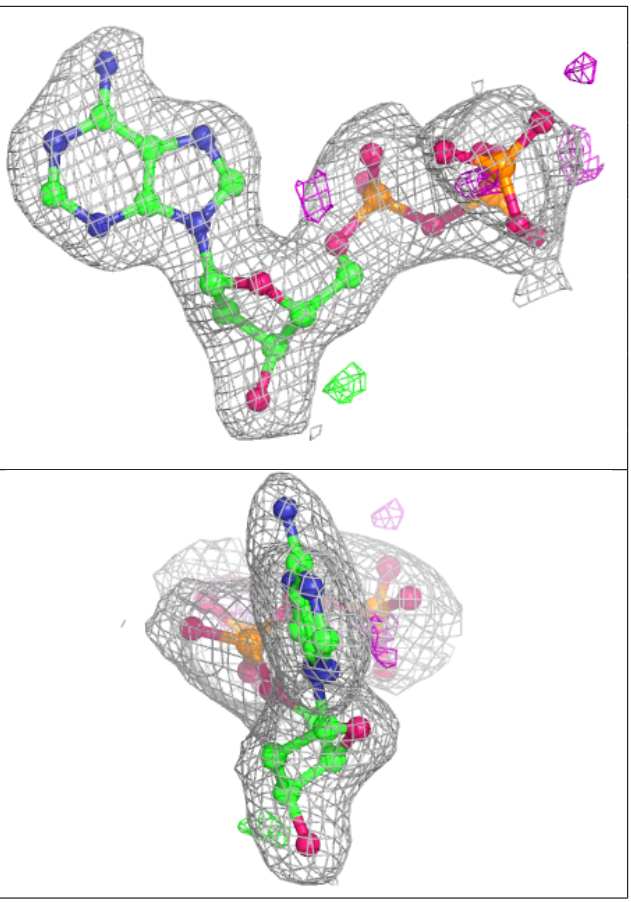
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around DTP 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)



Electron density around CDP B 1001:

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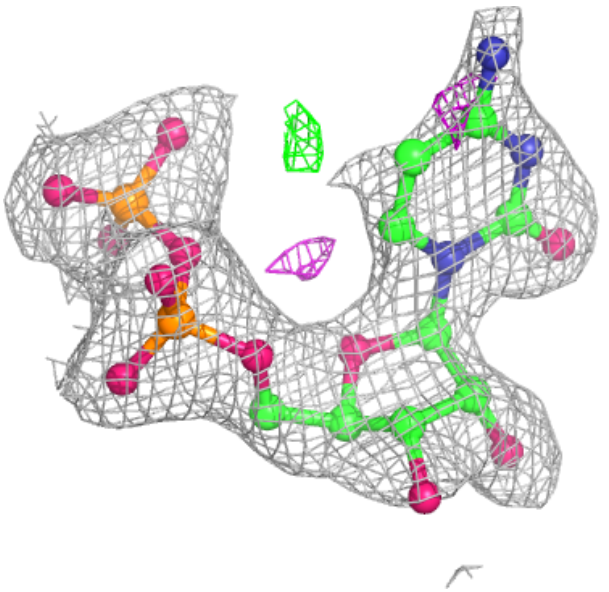
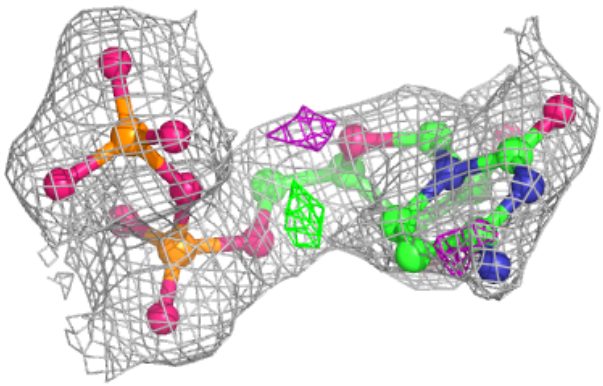
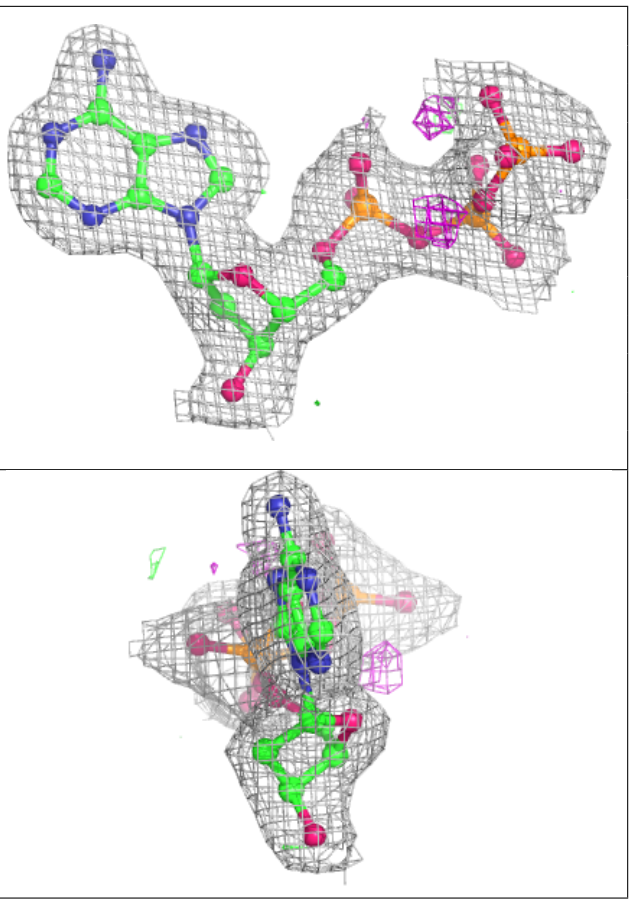
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





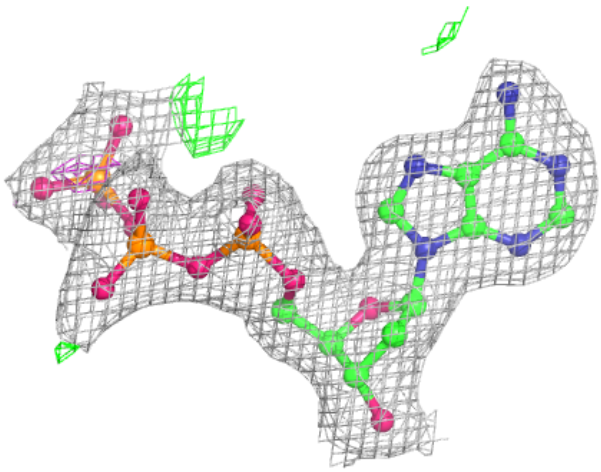
Electron density around DTP C 1008:

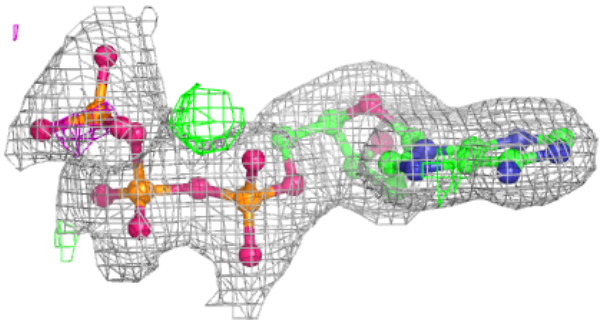
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

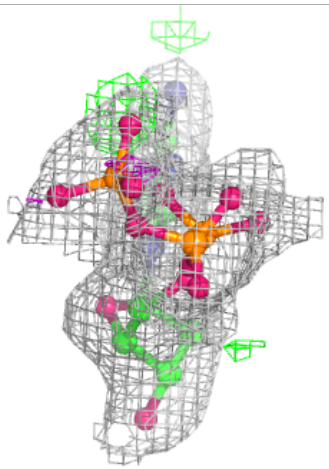


Electron density around DTP B 1006:

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







6.5 Other polymers (i)

There are no such residues in this entry.