



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 1H7A / pdb_00001h7a
Title : Structural basis for allosteric substrate specificity regulation in class III ribonucleotide reductases: NRDD in complex with dATP
Authors : Larsson, K.-M.; Andersson, J.; Sjoeborg, B.-M.; Nordlund, P.; Logan, D.T.
Deposited on : 2001-07-04
Resolution : 2.75 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

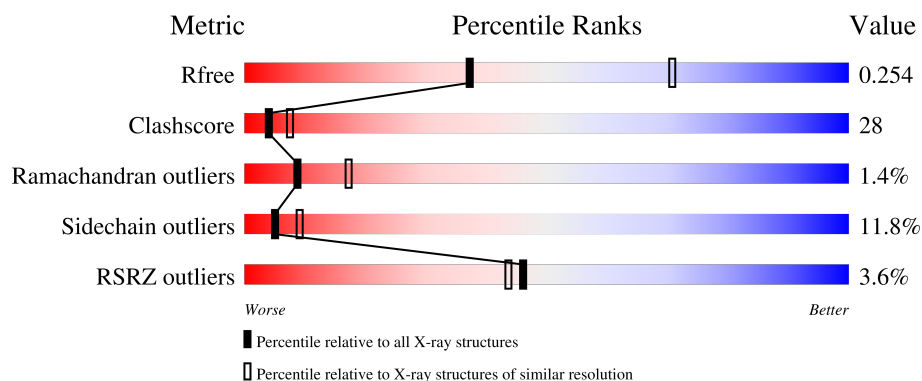
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	605	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FE2	A	1591	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4517 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.

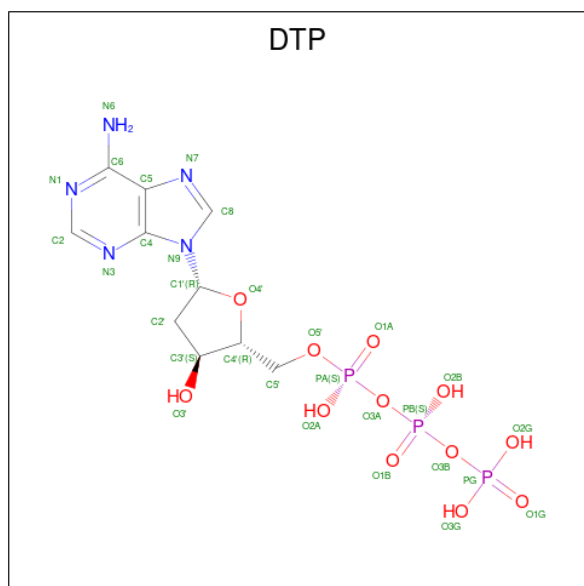
- Molecule 1 is a protein called ANAEROBIC RIBONUCLEOTIDE-TRIPHOSPHATE REDUCTASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	4427	2814	748	836	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	GLY	engineered mutation	UNP Q9T0V5

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



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

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.36Å 98.36Å 244.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.75 29.87 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.6 (29.87-2.75) 92.5 (29.87-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.258 0.212 , 0.254	Depositor DCC
R_{free} test set	2513 reflections (8.46%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4517	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, FE2, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	1/4525 (0.0%)	1.18	38/6125 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	MET	SD-CE	-5.28	1.66	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	GLY	N-CA-C	13.37	130.76	113.24
1	A	244	LEU	N-CA-C	9.78	126.41	113.30
1	A	398	SER	N-CA-C	9.11	123.58	108.73
1	A	140	VAL	N-CA-C	-8.45	102.63	111.58
1	A	328	ILE	N-CA-C	-8.13	95.87	107.75
1	A	62	ILE	N-CA-C	-7.67	103.32	110.53
1	A	110	ALA	N-CA-C	-7.17	101.85	111.96
1	A	162	TYR	N-CA-C	-7.07	103.27	110.97
1	A	446	GLU	N-CA-C	-7.04	103.69	111.36
1	A	28	ARG	N-CA-C	-7.00	104.89	113.50
1	A	268	ASP	N-CA-C	-6.93	100.26	110.52
1	A	556	GLU	N-CA-C	-6.90	104.98	113.19
1	A	415	ILE	N-CA-C	-6.78	106.20	112.43
1	A	90	ASN	CA-C-N	-6.60	116.55	122.43
1	A	90	ASN	C-N-CA	-6.60	116.55	122.43
1	A	187	SER	N-CA-C	-6.49	101.17	110.59
1	A	313	GLY	N-CA-C	6.37	119.22	110.56
1	A	176	GLN	N-CA-C	-6.16	104.83	112.90
1	A	381	LYS	N-CA-C	-6.15	101.10	110.07
1	A	371	TYR	N-CA-C	6.11	120.80	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ALA	N-CA-C	-6.01	104.84	111.82
1	A	420	LEU	N-CA-C	-5.98	104.76	111.28
1	A	520	LEU	N-CA-C	-5.94	104.72	111.07
1	A	530	HIS	N-CA-C	5.68	120.34	112.90
1	A	215	LEU	N-CA-C	5.61	117.39	111.28
1	A	80	CYS	N-CA-C	5.59	116.73	107.73
1	A	143	THR	N-CA-C	-5.57	105.36	111.82
1	A	77	THR	N-CA-C	-5.55	101.69	109.69
1	A	482	GLU	N-CA-C	-5.46	102.67	110.59
1	A	393	GLY	N-CA-C	5.45	122.84	115.32
1	A	494	ALA	CA-C-N	-5.42	113.31	119.28
1	A	494	ALA	C-N-CA	-5.42	113.31	119.28
1	A	177	ALA	N-CA-C	-5.35	105.09	111.03
1	A	418	GLU	N-CA-C	5.23	119.75	112.90
1	A	103	LYS	N-CA-C	-5.20	106.17	112.88
1	A	422	LYS	N-CA-C	-5.17	105.77	111.71
1	A	314	VAL	N-CA-C	5.09	115.07	108.35
1	A	243	ASN	N-CA-C	5.08	120.34	114.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4427	0	4375	242	1
2	A	30	0	12	1	0
3	A	1	0	0	2	0
4	A	1	0	0	0	0
5	A	58	0	0	1	1
All	All	4517	0	4387	242	2

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 28.

All (242) 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:A:87:MET:HG2	1:A:374:GLY:HA3	1.39	1.01
1:A:559:PHE:HB2	1:A:572:MET:HE1	1.39	1.00
1:A:29:VAL:HG12	1:A:31:PRO:HD2	1.46	0.97
1:A:94:LEU:HD11	1:A:118:GLN:HG3	1.52	0.91
1:A:258:LEU:HD12	1:A:520:LEU:HD13	1.55	0.86
1:A:166:LYS:HA	1:A:166:LYS:HE2	1.55	0.86
1:A:546:CYS:HG	3:A:1591:FE2:FE	0.57	0.85
1:A:227:ILE:HB	1:A:573:ASN:OD1	1.78	0.84
1:A:582:LEU:N	1:A:582:LEU:HD12	1.92	0.83
1:A:151:ALA:HA	1:A:156:ILE:HD12	1.58	0.83
1:A:240:GLU:HA	1:A:244:LEU:HD21	1.59	0.82
1:A:218:ARG:NH2	1:A:232:PRO:O	2.12	0.82
1:A:417:ARG:HH11	1:A:417:ARG:HB2	1.44	0.82
1:A:420:LEU:HD12	1:A:423:MET:HE3	1.65	0.78
1:A:263:LYS:C	1:A:264:ARG:HG2	2.08	0.76
1:A:244:LEU:H	1:A:244:LEU:HD23	1.49	0.76
1:A:486:PRO:HB3	1:A:508:VAL:HG21	1.67	0.75
1:A:158:ASP:HB3	1:A:161:ASN:HB3	1.70	0.74
1:A:55:MET:O	1:A:59:GLU:HG2	1.86	0.74
1:A:417:ARG:HH11	1:A:417:ARG:CB	2.01	0.74
1:A:420:LEU:HD12	1:A:423:MET:CE	2.18	0.74
1:A:417:ARG:HH11	1:A:417:ARG:CG	2.02	0.73
1:A:258:LEU:HD12	1:A:520:LEU:CD1	2.19	0.73
1:A:87:MET:CG	1:A:374:GLY:HA3	2.17	0.73
1:A:507:TYR:HA	1:A:535:GLY:O	1.88	0.72
1:A:167:THR:HG22	1:A:209:MET:HE1	1.69	0.72
1:A:129:PHE:HB2	1:A:197:ILE:CD1	2.20	0.72
1:A:204:ASP:HB3	1:A:207:GLU:HG3	1.73	0.71
1:A:85:LYS:O	1:A:89:GLU:HB2	1.90	0.71
1:A:459:LYS:HD3	1:A:460:TYR:HE1	1.56	0.70
1:A:428:LYS:O	1:A:432:GLU:HG3	1.91	0.70
1:A:484:ILE:HD12	1:A:484:ILE:H	1.55	0.70
1:A:560:VAL:HG12	1:A:567:THR:HG22	1.73	0.69
1:A:509:GLU:C	1:A:510:LEU:HD12	2.17	0.69
1:A:480:VAL:HG23	1:A:481:GLU:N	2.09	0.68
1:A:553:THR:O	1:A:560:VAL:HG22	1.94	0.67
1:A:459:LYS:HD3	1:A:460:TYR:CE1	2.29	0.67
1:A:538:MET:HB2	1:A:539:PRO:HD2	1.77	0.67
1:A:94:LEU:CD1	1:A:118:GLN:HG3	2.24	0.67
1:A:536:VAL:HG22	1:A:538:MET:HE2	1.76	0.66
1:A:539:PRO:HA	1:A:576:ARG:HE	1.61	0.66
1:A:543:CYS:HB2	1:A:552:MET:HE1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:HB3	1:A:161:ASN:CB	2.27	0.65
1:A:555:THR:C	1:A:557:ASN:H	2.03	0.65
1:A:555:THR:HG22	1:A:557:ASN:H	1.60	0.64
1:A:422:LYS:HE2	5:A:2040:HOH:O	1.98	0.64
1:A:82:VAL:CG1	1:A:87:MET:HE1	2.27	0.64
1:A:141:LYS:HG3	1:A:206:THR:HG21	1.81	0.63
1:A:167:THR:HG22	1:A:209:MET:CE	2.30	0.62
1:A:244:LEU:H	1:A:244:LEU:CD2	2.12	0.62
1:A:540:VAL:HG22	1:A:540:VAL:O	1.99	0.62
1:A:314:VAL:HG22	1:A:398:SER:HB2	1.82	0.62
1:A:582:LEU:HD12	1:A:582:LEU:H	1.62	0.61
1:A:151:ALA:HA	1:A:156:ILE:CD1	2.29	0.61
1:A:236:MET:HE1	1:A:253:ILE:HG22	1.83	0.61
1:A:208:ARG:HD2	1:A:250:ASN:OD1	2.01	0.60
1:A:319:LEU:HB2	1:A:320:PRO:HD3	1.84	0.60
1:A:582:LEU:N	1:A:582:LEU:CD1	2.65	0.60
1:A:87:MET:HE2	1:A:375:ALA:HA	1.84	0.59
1:A:563:ILE:O	1:A:563:ILE:HG13	2.01	0.59
1:A:556:GLU:CD	1:A:556:GLU:N	2.61	0.58
1:A:370:LEU:HA	1:A:375:ALA:HB3	1.85	0.58
1:A:258:LEU:CD1	1:A:520:LEU:HD13	2.33	0.58
1:A:486:PRO:CB	1:A:508:VAL:HG21	2.32	0.58
1:A:575:ILE:HG23	1:A:582:LEU:HB3	1.85	0.58
1:A:555:THR:C	1:A:557:ASN:N	2.62	0.58
1:A:240:GLU:CA	1:A:244:LEU:HD21	2.33	0.58
1:A:420:LEU:HA	1:A:423:MET:HE3	1.85	0.57
1:A:563:ILE:O	1:A:564:CYS:HB3	2.04	0.57
1:A:137:SER:HB3	1:A:138:PRO:HD3	1.87	0.57
1:A:587:GLU:O	1:A:588:ARG:HB2	2.04	0.57
1:A:474:ASN:HD22	1:A:477:HIS:CE1	2.21	0.57
1:A:417:ARG:HH11	1:A:417:ARG:HG3	1.69	0.57
1:A:546:CYS:HG	1:A:564:CYS:HG	0.65	0.56
1:A:480:VAL:CG2	1:A:481:GLU:N	2.68	0.56
1:A:349:PHE:HB2	1:A:430:TRP:CZ2	2.40	0.56
1:A:486:PRO:HB3	1:A:508:VAL:CG2	2.35	0.56
1:A:555:THR:HG22	1:A:556:GLU:N	2.21	0.55
1:A:166:LYS:HE2	1:A:166:LYS:CA	2.33	0.55
1:A:417:ARG:HB2	1:A:417:ARG:NH1	2.19	0.55
1:A:559:PHE:HB2	1:A:572:MET:CE	2.25	0.55
1:A:240:GLU:HA	1:A:244:LEU:CD2	2.32	0.55
1:A:254:LYS:HE2	1:A:521:GLU:OE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:CYS:SG	1:A:564:CYS:SG	3.05	0.55
1:A:30:PHE:HB2	1:A:31:PRO:HD3	1.89	0.55
1:A:27:SER:HA	1:A:32:THR:HG21	1.89	0.54
1:A:490:ILE:CD1	1:A:527:ALA:HA	2.37	0.54
1:A:56:LYS:HE3	1:A:56:LYS:HA	1.87	0.54
1:A:195:VAL:HG13	1:A:232:PRO:HB3	1.90	0.54
1:A:401:TYR:OH	1:A:442:SER:HB3	2.07	0.54
1:A:486:PRO:O	1:A:490:ILE:HG23	2.07	0.53
1:A:189:ASN:HD22	1:A:189:ASN:N	2.05	0.53
1:A:485:THR:O	1:A:486:PRO:C	2.49	0.53
1:A:487:PHE:HD2	1:A:526:TYR:CD2	2.25	0.53
1:A:182:VAL:O	1:A:192:THR:HG23	2.08	0.53
1:A:54:ILE:HD13	1:A:351:ALA:HA	1.91	0.53
1:A:555:THR:HG22	1:A:557:ASN:N	2.24	0.53
1:A:417:ARG:HG3	1:A:417:ARG:NH1	2.23	0.53
1:A:129:PHE:HB2	1:A:197:ILE:HD13	1.89	0.53
1:A:409:ILE:HD13	1:A:465:ASP:HB3	1.92	0.53
1:A:489:LYS:O	1:A:493:GLU:HG3	2.09	0.53
1:A:509:GLU:O	1:A:510:LEU:HD12	2.09	0.53
1:A:537:ASN:HD22	1:A:577:ARG:HE	1.55	0.53
1:A:167:THR:CG2	1:A:209:MET:HE1	2.37	0.52
1:A:546:CYS:SG	1:A:564:CYS:HB3	2.49	0.52
1:A:574:THR:O	1:A:584:ASN:HA	2.10	0.52
1:A:83:ASP:HA	1:A:307:ASP:HB3	1.91	0.52
1:A:244:LEU:HD23	1:A:244:LEU:N	2.15	0.52
1:A:99:ILE:HG21	1:A:111:ILE:HD13	1.90	0.52
1:A:158:ASP:CB	1:A:161:ASN:HB3	2.39	0.52
1:A:241:GLY:HA2	1:A:248:ASP:OD1	2.09	0.52
1:A:402:ILE:HG12	1:A:403:GLY:N	2.25	0.52
1:A:31:PRO:HB2	1:A:190:GLY:HA3	1.91	0.52
1:A:244:LEU:CD2	1:A:244:LEU:N	2.73	0.51
1:A:105:ILE:HG13	1:A:140:VAL:HG22	1.92	0.51
1:A:160:LEU:HD12	1:A:160:LEU:N	2.25	0.51
1:A:221:GLY:CA	1:A:264:ARG:NH1	2.74	0.51
1:A:266:TYR:CZ	1:A:582:LEU:HD11	2.46	0.51
1:A:356:ILE:O	1:A:359:LEU:HB2	2.10	0.51
1:A:87:MET:HG2	1:A:374:GLY:CA	2.28	0.51
1:A:187:SER:HB3	1:A:189:ASN:ND2	2.25	0.51
1:A:512:ASP:OD2	1:A:514:LYS:HD2	2.10	0.51
1:A:526:TYR:CE1	1:A:530:HIS:CE1	2.99	0.51
1:A:321:ARG:HD3	1:A:456:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:THR:HG21	1:A:566:GLU:OE1	2.11	0.51
1:A:363:LYS:NZ	1:A:385:ASP:OD1	2.30	0.50
1:A:62:ILE:HG23	1:A:344:ARG:HD3	1.92	0.50
1:A:408:ASN:CG	1:A:414:ASP:HA	2.36	0.50
1:A:555:THR:N	1:A:558:GLY:O	2.37	0.49
1:A:225:ASP:OD1	1:A:225:ASP:N	2.46	0.49
1:A:480:VAL:HG23	1:A:481:GLU:HG3	1.94	0.49
1:A:487:PHE:HB3	1:A:526:TYR:CE2	2.48	0.49
1:A:266:TYR:CE2	1:A:582:LEU:HD11	2.48	0.49
1:A:56:LYS:HE3	1:A:56:LYS:CA	2.43	0.48
1:A:582:LEU:H	1:A:582:LEU:CD1	2.26	0.48
1:A:82:VAL:HG13	1:A:87:MET:HE1	1.94	0.48
1:A:160:LEU:H	1:A:160:LEU:CD1	2.26	0.48
1:A:469:LYS:HG3	1:A:471:TRP:CE3	2.49	0.48
1:A:513:MET:O	1:A:514:LYS:C	2.54	0.48
1:A:236:MET:CE	1:A:253:ILE:HG22	2.44	0.48
1:A:82:VAL:CG1	1:A:87:MET:CE	2.92	0.48
1:A:404:ILE:HD11	1:A:420:LEU:CD1	2.43	0.48
1:A:179:GLU:OE1	1:A:218:ARG:NH1	2.47	0.47
1:A:359:LEU:HB2	1:A:387:ILE:HD13	1.97	0.47
1:A:480:VAL:CG2	1:A:481:GLU:H	2.27	0.47
1:A:239:GLU:C	1:A:244:LEU:HD22	2.39	0.47
1:A:285:VAL:HG22	1:A:306:LEU:HD21	1.97	0.47
1:A:393:GLY:HA2	1:A:437:ALA:HB2	1.95	0.47
1:A:400:GLY:HA2	1:A:441:TYR:O	2.13	0.47
1:A:546:CYS:SG	1:A:564:CYS:CB	3.03	0.47
1:A:176:GLN:O	1:A:180:TYR:HD1	1.98	0.46
1:A:254:LYS:O	1:A:258:LEU:CD2	2.63	0.46
1:A:315:VAL:HG23	1:A:352:LEU:HD23	1.97	0.46
1:A:541:ASP:OD2	1:A:576:ARG:NH2	2.47	0.46
1:A:584:ASN:OD1	1:A:586:ASN:HB2	2.15	0.46
1:A:169:LYS:O	1:A:170:ASP:C	2.59	0.46
1:A:349:PHE:O	1:A:353:MET:HB2	2.16	0.46
1:A:261:ALA:HA	1:A:266:TYR:O	2.15	0.46
1:A:160:LEU:HD12	1:A:160:LEU:H	1.81	0.46
1:A:369:ILE:HD12	1:A:370:LEU:N	2.31	0.46
1:A:148:ILE:HD13	1:A:163:ALA:HB2	1.98	0.46
1:A:527:ALA:HB1	1:A:531:LEU:HD11	1.98	0.46
1:A:564:CYS:HG	3:A:1591:FE2:FE	0.27	0.46
1:A:575:ILE:CG2	1:A:582:LEU:HB3	2.45	0.46
1:A:163:ALA:O	1:A:164:GLN:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:O	1:A:475:SER:C	2.59	0.45
1:A:505:ILE:HG12	1:A:506:SER:N	2.31	0.45
1:A:189:ASN:HD22	1:A:189:ASN:H	1.64	0.45
1:A:440:LEU:HB3	1:A:500:ALA:HA	1.99	0.45
1:A:446:GLU:OE2	1:A:579:CYS:HB2	2.17	0.45
1:A:144:TYR:CE1	1:A:163:ALA:HB1	2.52	0.45
1:A:484:ILE:HD12	1:A:484:ILE:N	2.25	0.45
1:A:203:THR:O	1:A:204:ASP:C	2.59	0.45
1:A:114:GLN:OE1	2:A:1590:DTP:H2	2.17	0.45
1:A:415:ILE:O	1:A:418:GLU:HG2	2.16	0.45
1:A:111:ILE:O	1:A:115:ILE:HG13	2.16	0.45
1:A:278:ILE:HD13	1:A:497:HIS:O	2.18	0.45
1:A:369:ILE:HD12	1:A:370:LEU:H	1.82	0.44
1:A:505:ILE:HG12	1:A:506:SER:H	1.82	0.44
1:A:511:PRO:O	1:A:512:ASP:C	2.60	0.44
1:A:33:GLN:OE1	1:A:33:GLN:HA	2.16	0.44
1:A:159:ALA:O	1:A:161:ASN:N	2.51	0.44
1:A:233:LYS:O	1:A:234:LEU:HD23	2.17	0.44
1:A:132:VAL:HG11	1:A:197:ILE:HD12	1.99	0.44
1:A:464:LYS:O	1:A:465:ASP:HB2	2.17	0.44
1:A:468:ASP:OD1	1:A:469:LYS:N	2.50	0.44
1:A:492:ARG:HH11	1:A:492:ARG:HB3	1.82	0.44
1:A:511:PRO:O	1:A:513:MET:HG2	2.17	0.44
1:A:545:THR:HG23	1:A:571:LYS:HD2	2.00	0.44
1:A:263:LYS:O	1:A:264:ARG:HG2	2.18	0.44
1:A:312:LEU:HD13	1:A:395:SER:HB3	2.00	0.43
1:A:349:PHE:HB2	1:A:430:TRP:CE2	2.53	0.43
1:A:390:PHE:HB3	1:A:395:SER:HB2	2.01	0.43
1:A:555:THR:CG2	1:A:556:GLU:N	2.80	0.43
1:A:197:ILE:HD13	1:A:197:ILE:HA	1.68	0.43
1:A:291:ARG:O	1:A:503:GLY:HA2	2.18	0.43
1:A:555:THR:OG1	1:A:560:VAL:HG13	2.19	0.43
1:A:218:ARG:O	1:A:264:ARG:CD	2.67	0.43
1:A:239:GLU:HB2	1:A:272:ALA:HB3	2.01	0.43
1:A:480:VAL:CG2	1:A:481:GLU:HG3	2.49	0.43
1:A:480:VAL:C	1:A:482:GLU:H	2.26	0.43
1:A:485:THR:HG22	1:A:487:PHE:H	1.84	0.43
1:A:91:GLY:O	1:A:92:PHE:HB3	2.19	0.43
1:A:87:MET:CE	1:A:375:ALA:HA	2.47	0.43
1:A:250:ASN:HB3	1:A:253:ILE:HD12	2.01	0.43
1:A:417:ARG:CG	1:A:417:ARG:NH1	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:VAL:CG2	1:A:524:TRP:N	2.80	0.43
1:A:133:ASP:OD1	1:A:134:LYS:N	2.52	0.42
1:A:459:LYS:CD	1:A:460:TYR:CE1	3.01	0.42
1:A:198:THR:HG22	1:A:235:VAL:HB	2.01	0.42
1:A:246:LYS:H	1:A:246:LYS:HD2	1.83	0.42
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.84	0.42
1:A:564:CYS:SG	1:A:566:GLU:HB2	2.59	0.42
1:A:79:CYS:O	1:A:80:CYS:HB3	2.19	0.42
1:A:131:ASN:O	1:A:135:VAL:HG23	2.20	0.42
1:A:537:ASN:HD22	1:A:577:ARG:NE	2.18	0.41
1:A:584:ASN:HB3	1:A:587:GLU:OE1	2.20	0.41
1:A:290:CYS:HB3	1:A:291:ARG:HD3	2.03	0.41
1:A:332:PHE:CZ	1:A:411:VAL:HG12	2.55	0.41
1:A:165:SER:O	1:A:166:LYS:C	2.64	0.41
1:A:254:LYS:O	1:A:258:LEU:HD22	2.20	0.41
1:A:102:PRO:HG3	1:A:111:ILE:HD12	2.01	0.41
1:A:318:ASN:ND2	1:A:321:ARG:HB2	2.35	0.41
1:A:518:LYS:HD2	1:A:518:LYS:HA	1.87	0.41
1:A:99:ILE:HG22	1:A:100:GLU:N	2.36	0.41
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.82	0.41
1:A:204:ASP:OD1	1:A:205:TRP:N	2.53	0.41
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.75	0.41
1:A:62:ILE:HG22	1:A:63:ILE:HG23	2.01	0.41
1:A:252:ASP:OD1	1:A:252:ASP:N	2.54	0.41
1:A:490:ILE:HD13	1:A:527:ALA:HA	2.02	0.41
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.81	0.41
1:A:540:VAL:O	1:A:540:VAL:CG2	2.66	0.40
1:A:160:LEU:N	1:A:160:LEU:CD1	2.84	0.40
1:A:225:ASP:O	1:A:226:GLY:C	2.65	0.40
1:A:405:HIS:CE1	1:A:479:SER:HB2	2.55	0.40
1:A:469:LYS:HG3	1:A:471:TRP:CD2	2.56	0.40
1:A:36:LEU:O	1:A:40:ILE:HG12	2.22	0.40
1:A:378:VAL:HG21	1:A:389:LEU:HD13	2.03	0.40
1:A:487:PHE:CD2	1:A:526:TYR:CD2	3.08	0.40
1:A:466:VAL:HG12	1:A:467:THR:N	2.36	0.40
1:A:537:ASN:HB3	1:A:577:ARG:HE	1.87	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2002:HOH:O	5:A:2002:HOH:O[8_665]	1.33	0.87
1:A:162:TYR:OH	1:A:162:TYR:OH[8_665]	2.18	0.02

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	561/605 (93%)	498 (89%)	55 (10%)	8 (1%)	9	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	CYS
1	A	157	ALA
1	A	246	LYS
1	A	516	ASN
1	A	159	ALA
1	A	160	LEU
1	A	475	SER
1	A	588	ARG

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	485/524 (93%)	428 (88%)	57 (12%)	5	9

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	32	THR
1	A	36	LEU
1	A	56	LYS
1	A	62	ILE
1	A	104	SER
1	A	105	ILE
1	A	127	THR
1	A	134	LYS
1	A	142	ARG
1	A	148	ILE
1	A	149	GLU
1	A	187	SER
1	A	189	ASN
1	A	197	ILE
1	A	203	THR
1	A	216	LYS
1	A	217	ASN
1	A	218	ARG
1	A	238	VAL
1	A	258	LEU
1	A	264	ARG
1	A	283	VAL
1	A	290	CYS
1	A	291	ARG
1	A	301	THR
1	A	306	LEU
1	A	312	LEU
1	A	317	LEU
1	A	353	MET
1	A	355	ARG
1	A	366	VAL
1	A	369	ILE
1	A	399	LEU
1	A	409	ILE
1	A	417	ARG
1	A	418	GLU
1	A	420	LEU
1	A	427	LEU
1	A	433	ARG
1	A	440	LEU
1	A	442	SER
1	A	484	ILE

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Mol	Chain	Res	Type
1	A	488	GLU
1	A	490	ILE
1	A	492	ARG
1	A	505	ILE
1	A	515	ASN
1	A	520	LEU
1	A	523	VAL
1	A	531	LEU
1	A	536	VAL
1	A	540	VAL
1	A	556	GLU
1	A	564	CYS
1	A	582	LEU
1	A	588	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	147	HIS
1	A	189	ASN
1	A	255	GLN
1	A	274	ASN
1	A	335	GLN
1	A	372	GLN
1	A	426	HIS
1	A	474	ASN
1	A	529	GLN
1	A	537	ASN
1	A	586	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	DTP	A	1590	4	31,32,32	1.48	4 (12%)	46,50,50	1.08	2 (4%)

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	DTP	A	1590	4	-	5/22/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1590	DTP	PB-O3B	5.03	1.64	1.59
2	A	1590	DTP	C4-N3	2.54	1.39	1.34
2	A	1590	DTP	C1'-N9	2.33	1.51	1.46
2	A	1590	DTP	PG-O2G	-2.01	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1590	DTP	O3G-PG-O2G	2.27	116.33	107.80
2	A	1590	DTP	O2B-PB-O3A	2.01	112.70	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

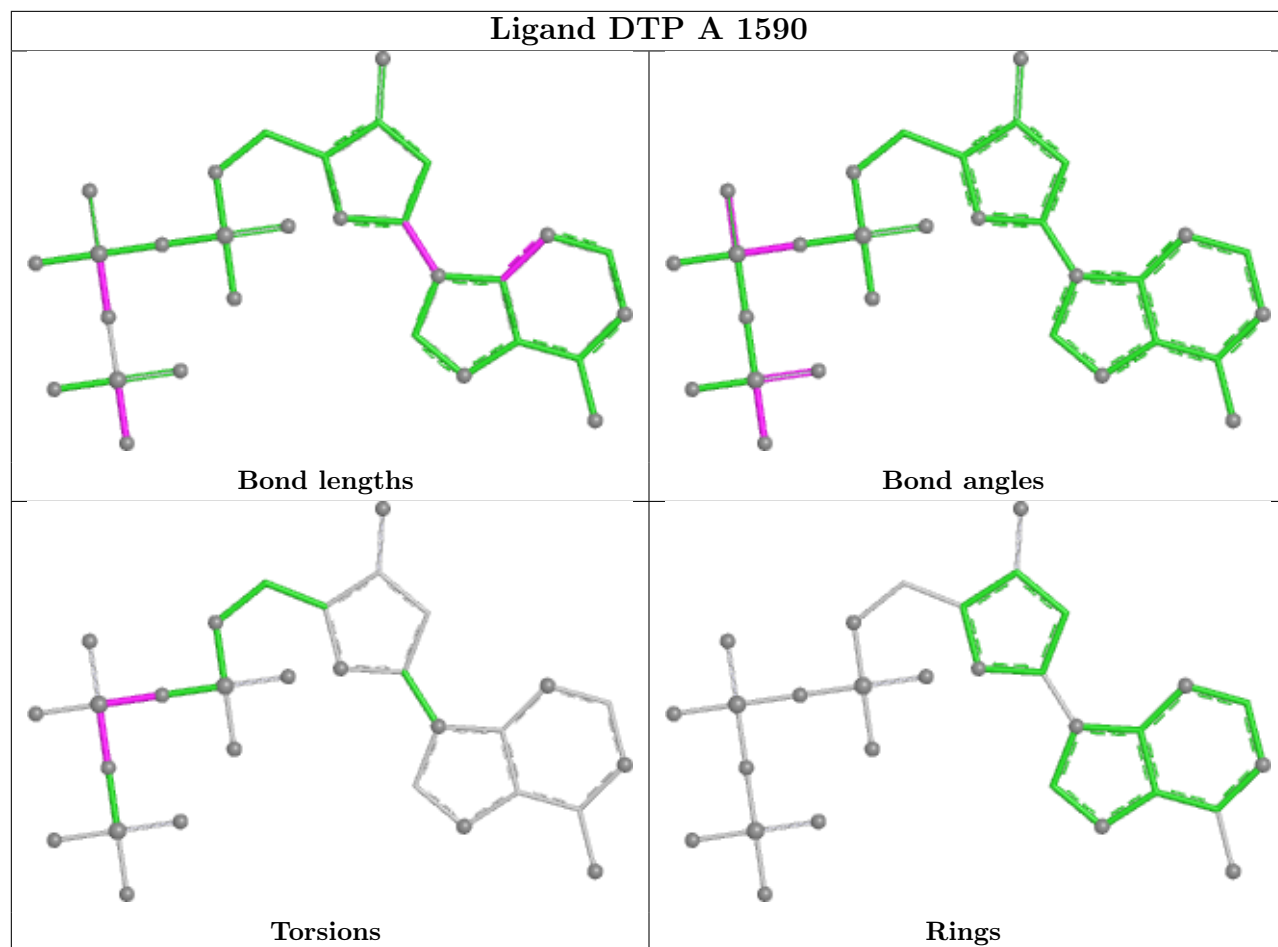
Mol	Chain	Res	Type	Atoms
2	A	1590	DTP	PA-O3A-PB-O3B
2	A	1590	DTP	PG-O3B-PB-O2B
2	A	1590	DTP	PG-O3B-PB-O1B
2	A	1590	DTP	PA-O3A-PB-O1B
2	A	1590	DTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1590	DTP	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.



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	563/605 (93%)	-0.09	20 (3%) 46 44	25, 46, 89, 101	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ASN	3.6
1	A	557	ASN	3.5
1	A	589	GLY	3.5
1	A	586	ASN	3.4
1	A	27	SER	3.0
1	A	159	ALA	3.0
1	A	555	THR	2.7
1	A	588	ARG	2.7
1	A	447	ASN	2.6
1	A	548	SER	2.6
1	A	563	ILE	2.5
1	A	550	HIS	2.3
1	A	587	GLU	2.2
1	A	160	LEU	2.2
1	A	484	ILE	2.2
1	A	554	PRO	2.1
1	A	481	GLU	2.1
1	A	578	THR	2.0
1	A	154	TRP	2.0
1	A	244	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](#)

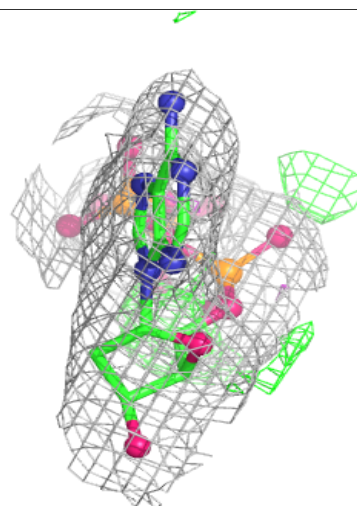
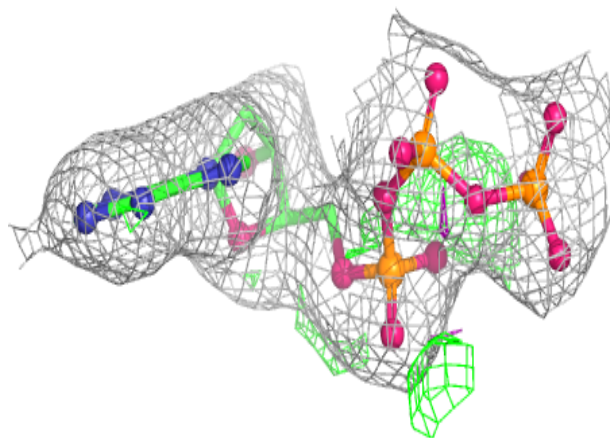
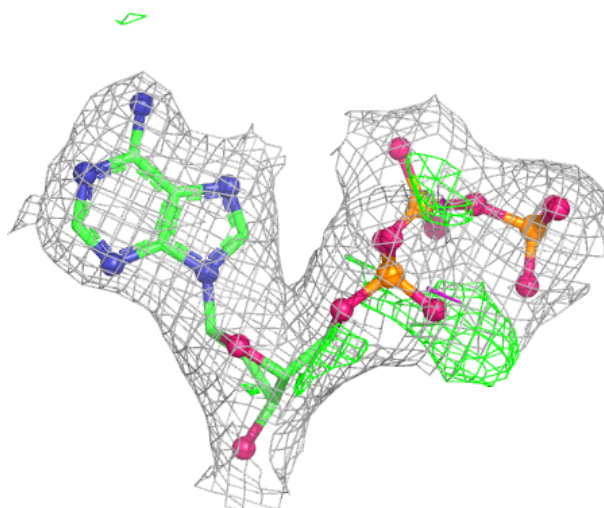
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	DTP	A	1590	30/30	0.95	0.08	38,44,66,67	0
3	FE2	A	1591	1/1	0.99	0.16	60,60,60,60	1
4	MG	A	1592	1/1	0.99	0.10	15,15,15,15	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 A 1590:

$2mF_o-DF_c$ (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.