



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:03 AM UTC

PDB ID : 1UBG / pdb_00001ubg
Title : MsREcA-dATP complex
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Deposited on : 2003-04-04
Resolution : 3.50 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

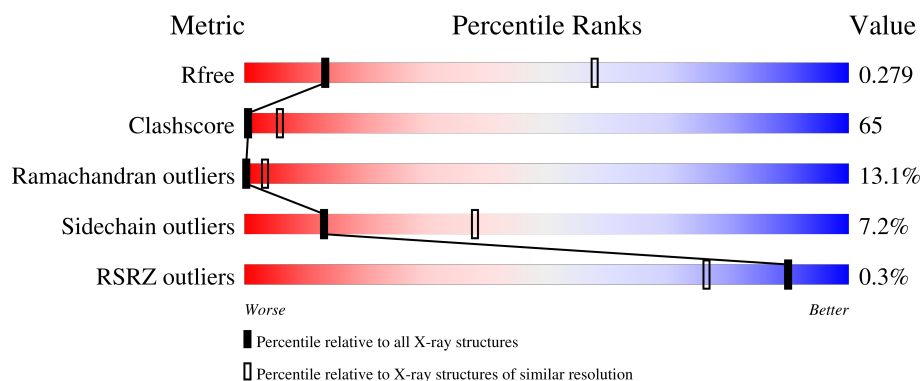
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	349	26% 47% 19% • 5%

2 Entry composition [i](#)

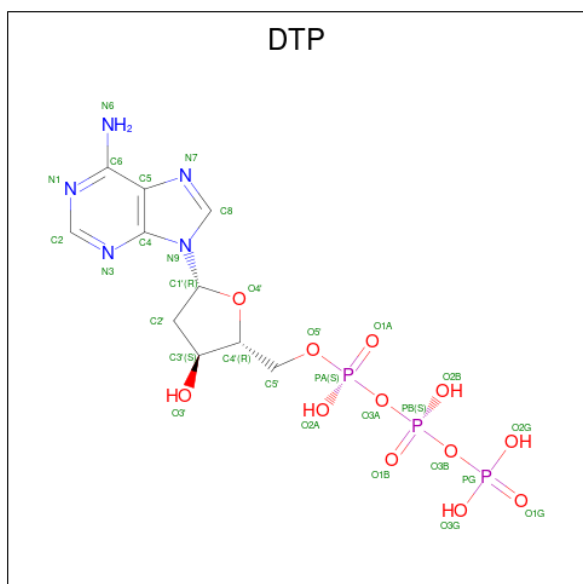
There are 3 unique types of molecules in this entry. The entry contains 2486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RecA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2389	1486	423	472	8			

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total 67 O 67	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	102.96Å 102.96Å 73.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.97 – 3.50 14.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.7 (14.97-3.50) 83.5 (14.97-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 3.46Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.286 0.218 , 0.279	Depositor DCC
R_{free} test set	518 reflections (10.40%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2486	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	0/2417	1.43	45/3269 (1.4%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASN	N-CA-C	-15.12	93.09	112.90
1	A	155	ALA	N-CA-C	-12.88	90.91	110.10
1	A	4	GLN	N-CA-C	-11.93	92.81	110.46
1	A	207	SER	CA-C-N	10.40	132.84	119.84
1	A	207	SER	C-N-CA	10.40	132.84	119.84
1	A	290	GLY	N-CA-C	-9.39	101.48	115.00
1	A	156	GLU	N-CA-C	9.05	123.83	110.17
1	A	5	ALA	N-CA-C	8.75	129.14	109.81
1	A	196	GLN	N-CA-C	8.69	129.31	110.80
1	A	47	ILE	N-CA-C	-8.36	102.09	110.62
1	A	51	VAL	N-CA-C	-8.07	102.01	113.07
1	A	141	ASP	N-CA-C	-7.98	101.43	112.12
1	A	68	GLY	CA-C-N	7.83	129.62	119.84
1	A	68	GLY	C-N-CA	7.83	129.62	119.84
1	A	34	GLU	N-CA-C	-7.66	104.07	113.41
1	A	77	VAL	N-CA-C	-7.63	103.25	110.42
1	A	105	TYR	N-CA-C	-6.97	102.25	111.24
1	A	7	ASP	N-CA-C	-6.66	100.18	110.10
1	A	2	ALA	N-CA-C	-6.13	97.75	110.80
1	A	172	LEU	N-CA-C	-6.11	103.94	111.33
1	A	58	LEU	CA-C-N	6.11	127.47	119.84
1	A	58	LEU	C-N-CA	6.11	127.47	119.84
1	A	29	MET	N-CA-C	6.00	118.41	108.99
1	A	197	LEU	N-CA-C	5.95	123.47	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASN	N-CA-C	5.92	119.72	111.56
1	A	328	LYS	N-CA-C	-5.88	105.95	113.01
1	A	195	ASN	N-CA-C	-5.74	100.69	109.41
1	A	210	THR	N-CA-C	-5.59	99.03	109.32
1	A	148	VAL	N-CA-C	-5.54	105.79	113.00
1	A	36	ARG	N-CA-C	5.50	122.51	110.80
1	A	307	ALA	N-CA-C	-5.47	106.11	112.89
1	A	171	ARG	N-CA-C	-5.39	99.32	110.80
1	A	166	VAL	N-CA-C	5.36	120.48	109.34
1	A	14	LEU	N-CA-C	-5.35	105.11	111.69
1	A	163	ASP	N-CA-C	5.33	122.14	110.80
1	A	124	GLY	N-CA-C	-5.27	108.87	114.67
1	A	322	GLU	N-CA-C	-5.19	105.06	111.33
1	A	92	ALA	N-CA-C	5.13	117.09	108.73
1	A	90	GLY	N-CA-C	5.12	117.96	112.33
1	A	249	VAL	N-CA-C	5.09	119.23	112.76
1	A	162	GLY	N-CA-C	5.05	125.14	113.18
1	A	25	LYS	N-CA-C	5.04	119.28	111.56
1	A	120	GLN	CA-C-N	5.02	126.12	119.84
1	A	120	GLN	C-N-CA	5.02	126.12	119.84
1	A	222	SER	N-CA-C	-5.02	107.21	113.38

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	2389	0	2345	309	0
2	A	30	0	12	4	0
3	A	67	0	0	6	0
All	All	2486	0	2357	309	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 65.

All (309) 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:210:THR:O	1:A:211:THR:HG23	1.56	1.05
1:A:156:GLU:O	1:A:157:ILE:HG22	1.60	1.00
1:A:209:GLU:HG2	1:A:210:THR:H	1.28	0.96
1:A:60:ARG:HB3	1:A:60:ARG:NH1	1.81	0.95
1:A:171:ARG:O	1:A:175:GLN:HG2	1.67	0.94
1:A:60:ARG:HB3	1:A:60:ARG:HH11	1.33	0.93
1:A:58:LEU:HD22	1:A:64:ILE:HD13	1.47	0.92
1:A:181:THR:HA	1:A:184:LEU:HD12	1.53	0.87
1:A:157:ILE:CG2	1:A:160:GLU:HB3	2.05	0.87
1:A:50:ASP:HB2	1:A:56:GLY:C	1.99	0.86
1:A:157:ILE:HG21	1:A:160:GLU:HB3	1.57	0.86
1:A:254:SER:HB2	1:A:255:PRO:HD2	1.55	0.86
1:A:173:MET:O	1:A:177:LEU:HD23	1.75	0.86
1:A:63:VAL:HG13	1:A:221:ALA:HA	1.58	0.85
1:A:147:SER:O	1:A:151:LEU:HD13	1.77	0.84
1:A:218:LYS:O	1:A:218:LYS:HD3	1.78	0.83
1:A:13:GLU:HG2	1:A:16:MET:HE2	1.59	0.83
1:A:180:MET:HG2	1:A:184:LEU:HG	1.61	0.83
1:A:209:GLU:HG2	1:A:210:THR:N	1.95	0.82
1:A:51:VAL:HG21	1:A:279:MET:HE1	1.65	0.78
1:A:29:MET:HE1	1:A:254:SER:C	2.10	0.77
1:A:8:ARG:HG3	1:A:9:GLU:H	1.47	0.77
1:A:145:ILE:N	1:A:145:ILE:HD12	2.00	0.76
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.98	0.76
1:A:235:ASP:CB	1:A:240:VAL:HG13	2.15	0.76
1:A:267:GLY:O	1:A:268:GLN:HB2	1.86	0.75
1:A:41:VAL:HG21	1:A:55:ILE:O	1.85	0.74
1:A:74:LYS:HE3	2:A:350:DTP:O2B	1.88	0.73
1:A:13:GLU:HA	1:A:16:MET:HB3	1.71	0.72
1:A:47:ILE:O	1:A:51:VAL:HG13	1.90	0.71
1:A:192:ILE:HG21	3:A:417:HOH:O	1.89	0.71
1:A:141:ASP:O	1:A:189:THR:HG23	1.90	0.71
1:A:195:ASN:O	1:A:196:GLN:HB3	1.89	0.71
1:A:243:ARG:HD3	1:A:261:GLU:OE1	1.90	0.71
1:A:20:ASP:HA	1:A:24:GLY:O	1.91	0.70
1:A:18:GLN:NE2	1:A:22:ASN:HD21	1.89	0.70
1:A:280:GLY:HA3	1:A:286:ILE:HD12	1.73	0.70
1:A:265:LEU:HD21	1:A:271:SER:HB2	1.73	0.69
1:A:161:MET:HE3	1:A:161:MET:HA	1.75	0.68
1:A:253:VAL:HG22	1:A:253:VAL:O	1.93	0.68
1:A:6:PRO:CG	1:A:11:ALA:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HZ2	1:A:194:ILE:HG23	1.59	0.68
1:A:130:ILE:O	1:A:134:LEU:HB2	1.93	0.67
1:A:173:MET:C	1:A:177:LEU:HD23	2.18	0.67
1:A:128:LEU:HD13	1:A:176:ALA:CB	2.25	0.66
1:A:254:SER:HB2	1:A:255:PRO:CD	2.26	0.66
1:A:136:ARG:NH1	1:A:183:ALA:HB2	2.10	0.66
1:A:284:GLY:O	1:A:286:ILE:N	2.29	0.66
1:A:293:PHE:HE2	1:A:304:LYS:N	1.93	0.66
1:A:132:ASP:O	1:A:136:ARG:HG3	1.96	0.65
1:A:209:GLU:O	1:A:210:THR:HG22	1.97	0.65
1:A:7:ASP:O	1:A:8:ARG:C	2.40	0.65
1:A:58:LEU:HD13	1:A:192:ILE:HD11	1.78	0.65
1:A:199:GLU:O	1:A:200:LYS:HG3	1.97	0.64
1:A:210:THR:O	1:A:211:THR:CG2	2.40	0.64
1:A:14:LEU:HD13	1:A:14:LEU:O	1.98	0.64
1:A:183:ALA:O	1:A:185:ASN:N	2.31	0.64
1:A:321:ILE:H	1:A:321:ILE:HD12	1.62	0.64
1:A:177:LEU:HB3	1:A:220:TYR:CD2	2.33	0.64
1:A:180:MET:HG2	1:A:184:LEU:CG	2.28	0.64
1:A:62:ARG:HG2	1:A:62:ARG:HH21	1.63	0.64
1:A:161:MET:HG3	1:A:162:GLY:H	1.63	0.63
1:A:8:ARG:HG3	1:A:9:GLU:N	2.13	0.63
1:A:71:SER:O	1:A:229:ARG:HD3	1.99	0.63
1:A:134:LEU:O	1:A:140:LEU:HD23	1.98	0.63
1:A:194:ILE:HD12	1:A:194:ILE:N	2.14	0.63
1:A:247:LYS:O	1:A:249:VAL:HG13	1.98	0.63
1:A:237:THR:HG23	1:A:238:ASP:N	2.14	0.63
1:A:85:ALA:O	1:A:90:GLY:HA3	1.98	0.63
1:A:272:ARG:O	1:A:276:LEU:HD23	1.98	0.63
1:A:323:LYS:O	1:A:326:LYS:N	2.33	0.62
1:A:328:LYS:HD2	1:A:328:LYS:O	2.00	0.62
1:A:116:LEU:HD23	1:A:117:LEU:N	2.15	0.62
1:A:61:GLY:O	1:A:62:ARG:HD3	2.00	0.62
1:A:233:LEU:HD23	1:A:243:ARG:N	2.15	0.61
1:A:117:LEU:HD12	1:A:140:LEU:HD11	1.82	0.61
1:A:46:SER:OG	1:A:48:SER:HB3	2.00	0.61
1:A:233:LEU:HD23	1:A:242:ASN:C	2.25	0.61
1:A:293:PHE:HE2	1:A:304:LYS:H	1.47	0.60
1:A:240:VAL:HB	1:A:265:LEU:HD12	1.83	0.60
1:A:65:GLU:OE1	1:A:217:LEU:HG	2.01	0.60
1:A:163:ASP:C	1:A:165:HIS:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:CE1	1:A:109:LEU:HD22	2.37	0.59
1:A:109:LEU:CD2	1:A:269:GLY:HA3	2.32	0.59
1:A:230:ILE:CG2	1:A:243:ARG:HG2	2.32	0.59
1:A:66:ILE:HG22	1:A:74:LYS:HG3	1.85	0.59
1:A:13:GLU:HG2	1:A:16:MET:CE	2.32	0.59
1:A:78:ALA:O	1:A:81:ALA:HB3	2.03	0.58
1:A:75:THR:HA	1:A:78:ALA:HB3	1.84	0.58
1:A:136:ARG:HH12	1:A:183:ALA:HB2	1.67	0.58
1:A:305:GLU:O	1:A:308:ARG:HB3	2.03	0.58
1:A:30:ARG:HB2	1:A:33:GLU:HG2	1.85	0.58
1:A:74:LYS:O	1:A:77:VAL:HB	2.03	0.58
1:A:180:MET:O	1:A:184:LEU:HG	2.03	0.58
1:A:321:ILE:O	1:A:325:ILE:HG13	2.04	0.58
1:A:209:GLU:CG	1:A:210:THR:H	2.09	0.57
1:A:290:GLY:O	1:A:292:TRP:HD1	1.87	0.57
1:A:6:PRO:HG2	1:A:11:ALA:HB2	1.85	0.57
1:A:14:LEU:HD13	1:A:14:LEU:C	2.29	0.57
1:A:58:LEU:HB3	1:A:64:ILE:CD1	2.34	0.57
1:A:41:VAL:O	1:A:41:VAL:HG13	2.04	0.57
1:A:49:LEU:O	1:A:52:ALA:HB3	2.05	0.57
1:A:93:ALA:HB2	1:A:140:LEU:CD1	2.34	0.57
1:A:272:ARG:O	1:A:276:LEU:CD2	2.52	0.57
1:A:310:PHE:HE1	1:A:317:VAL:HG11	1.70	0.57
1:A:95:ILE:HG12	1:A:131:ALA:HB2	1.85	0.57
1:A:148:VAL:HG13	1:A:173:MET:HE2	1.86	0.57
1:A:92:ALA:CB	1:A:142:ILE:HG23	2.34	0.57
1:A:92:ALA:HB2	1:A:142:ILE:HG23	1.85	0.57
1:A:61:GLY:HA2	1:A:185:ASN:OD1	2.05	0.56
1:A:277:ILE:O	1:A:281:VAL:HG13	2.04	0.56
1:A:95:ILE:N	1:A:95:ILE:HD12	2.20	0.56
1:A:244:THR:O	1:A:261:GLU:HA	2.06	0.56
1:A:145:ILE:N	1:A:145:ILE:CD1	2.68	0.56
1:A:67:TYR:HB3	1:A:195:ASN:HB3	1.88	0.56
1:A:163:ASP:O	1:A:165:HIS:N	2.39	0.56
1:A:309:LYS:O	1:A:313:GLU:HG2	2.06	0.55
1:A:19:ILE:HG21	1:A:28:VAL:HG23	1.89	0.55
1:A:317:VAL:HG22	1:A:321:ILE:HD11	1.89	0.55
1:A:265:LEU:CD2	1:A:271:SER:HB2	2.37	0.55
1:A:148:VAL:HG12	1:A:148:VAL:O	2.06	0.55
1:A:141:ASP:O	1:A:189:THR:CG2	2.55	0.54
1:A:237:THR:HG23	1:A:238:ASP:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:HG23	1:A:211:THR:N	2.22	0.54
1:A:92:ALA:HB2	1:A:142:ILE:CG2	2.38	0.54
1:A:214:GLY:O	1:A:215:LYS:C	2.49	0.54
1:A:55:ILE:CD1	1:A:59:PRO:HB3	2.37	0.54
1:A:40:SER:O	1:A:41:VAL:HB	2.06	0.54
1:A:29:MET:SD	1:A:254:SER:O	2.66	0.53
1:A:74:LYS:HZ2	1:A:194:ILE:CG2	2.22	0.53
1:A:62:ARG:HD2	1:A:222:SER:OG	2.07	0.53
1:A:169:GLN:O	1:A:171:ARG:N	2.42	0.53
1:A:8:ARG:CG	1:A:9:GLU:H	2.19	0.53
1:A:47:ILE:HG23	1:A:279:MET:HG3	1.91	0.53
1:A:157:ILE:HG23	1:A:160:GLU:HB3	1.85	0.53
1:A:18:GLN:O	1:A:22:ASN:ND2	2.42	0.53
1:A:195:ASN:O	1:A:196:GLN:CB	2.54	0.53
1:A:265:LEU:N	1:A:265:LEU:HD22	2.23	0.53
1:A:59:PRO:HG2	1:A:59:PRO:O	2.07	0.53
1:A:146:ASP:O	1:A:147:SER:HB2	2.09	0.53
1:A:192:ILE:CD1	3:A:417:HOH:O	2.57	0.53
1:A:73:GLY:O	1:A:74:LYS:C	2.53	0.52
1:A:242:ASN:N	1:A:242:ASN:HD22	2.08	0.52
1:A:321:ILE:HD12	1:A:321:ILE:N	2.25	0.52
1:A:141:ASP:C	1:A:189:THR:HG23	2.34	0.52
1:A:276:LEU:O	1:A:280:GLY:N	2.40	0.52
1:A:1:MET:O	1:A:2:ALA:HB2	2.08	0.52
1:A:223:VAL:HA	1:A:250:LYS:O	2.09	0.52
1:A:208:PRO:O	1:A:209:GLU:O	2.27	0.52
1:A:280:GLY:HA3	1:A:286:ILE:CD1	2.39	0.52
1:A:282:GLU:O	1:A:282:GLU:HG2	2.09	0.52
1:A:317:VAL:HG22	1:A:321:ILE:CD1	2.40	0.52
1:A:154:ARG:O	1:A:155:ALA:C	2.50	0.52
1:A:120:GLN:O	1:A:121:PRO:O	2.27	0.51
1:A:168:LEU:O	1:A:169:GLN:C	2.53	0.51
1:A:5:ALA:HB3	1:A:6:PRO:CD	2.40	0.51
1:A:55:ILE:HD11	1:A:59:PRO:HB3	1.93	0.51
1:A:209:GLU:O	1:A:210:THR:C	2.52	0.51
1:A:29:MET:HE1	1:A:254:SER:CA	2.41	0.51
1:A:119:SER:OG	1:A:130:ILE:CD1	2.58	0.50
1:A:233:LEU:HB2	1:A:241:GLY:C	2.37	0.50
1:A:50:ASP:HB2	1:A:57:GLY:N	2.26	0.50
1:A:152:VAL:HG23	1:A:152:VAL:O	2.11	0.50
1:A:325:ILE:HG22	1:A:329:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:HA	1:A:188:GLY:H	1.76	0.50
1:A:66:ILE:HG22	1:A:74:LYS:CG	2.41	0.50
1:A:207:SER:N	1:A:208:PRO:HD3	2.26	0.50
1:A:93:ALA:HB2	1:A:140:LEU:HD11	1.94	0.50
1:A:247:LYS:O	1:A:249:VAL:N	2.44	0.50
1:A:53:LEU:HD12	1:A:57:GLY:HA2	1.93	0.50
1:A:49:LEU:HA	1:A:260:ALA:CB	2.41	0.49
1:A:19:ILE:HG21	1:A:28:VAL:CG2	2.41	0.49
1:A:321:ILE:O	1:A:322:GLU:C	2.56	0.49
1:A:75:THR:O	1:A:79:LEU:N	2.43	0.49
1:A:98:GLU:CG	1:A:147:SER:OG	2.60	0.49
1:A:198:ARG:O	1:A:199:GLU:CB	2.60	0.49
1:A:323:LYS:O	1:A:324:LYS:C	2.56	0.49
1:A:148:VAL:HG21	1:A:217:LEU:CD2	2.42	0.49
1:A:29:MET:HE1	1:A:254:SER:HA	1.94	0.48
1:A:173:MET:O	1:A:174:SER:C	2.55	0.48
1:A:230:ILE:HG21	1:A:243:ARG:HG2	1.95	0.48
1:A:233:LEU:HD21	1:A:243:ARG:HB2	1.95	0.48
1:A:157:ILE:HD13	1:A:160:GLU:OE2	2.13	0.48
1:A:5:ALA:CB	1:A:6:PRO:CD	2.92	0.48
1:A:62:ARG:HG2	1:A:62:ARG:NH2	2.28	0.48
1:A:109:LEU:HD21	1:A:269:GLY:CA	2.43	0.48
1:A:119:SER:OG	1:A:130:ILE:HD12	2.14	0.48
1:A:235:ASP:O	1:A:237:THR:N	2.44	0.48
1:A:242:ASN:N	1:A:242:ASN:ND2	2.62	0.48
1:A:233:LEU:CD2	1:A:243:ARG:N	2.77	0.47
1:A:303:GLY:O	1:A:305:GLU:N	2.47	0.47
1:A:182:GLY:O	1:A:183:ALA:C	2.56	0.47
1:A:183:ALA:O	1:A:184:LEU:C	2.56	0.47
1:A:74:LYS:H	1:A:74:LYS:HD3	1.79	0.47
1:A:64:ILE:O	1:A:192:ILE:HA	2.14	0.47
1:A:223:VAL:HG12	1:A:225:LEU:CD1	2.45	0.47
1:A:163:ASP:C	1:A:165:HIS:N	2.73	0.47
1:A:95:ILE:HD11	1:A:143:ILE:HD11	1.96	0.47
1:A:200:LYS:HA	1:A:228:ARG:HH11	1.80	0.47
1:A:75:THR:O	1:A:76:THR:C	2.56	0.47
1:A:79:LEU:O	1:A:82:VAL:HB	2.14	0.47
1:A:94:PHE:CD1	1:A:94:PHE:C	2.92	0.47
1:A:192:ILE:HD12	3:A:417:HOH:O	2.15	0.47
1:A:209:GLU:C	1:A:210:THR:O	2.55	0.47
1:A:284:GLY:O	1:A:285:PHE:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:CA	1:A:24:GLY:O	2.62	0.47
1:A:98:GLU:CD	1:A:147:SER:HG	2.23	0.47
1:A:135:VAL:HG23	1:A:189:THR:HG21	1.95	0.47
1:A:49:LEU:HA	1:A:260:ALA:HB3	1.97	0.47
1:A:82:VAL:O	1:A:83:ALA:C	2.58	0.47
1:A:241:GLY:C	1:A:242:ASN:ND2	2.73	0.47
1:A:74:LYS:HE3	2:A:350:DTP:PB	2.54	0.46
1:A:147:SER:HB3	1:A:150:ALA:H	1.80	0.46
1:A:273:GLU:O	1:A:274:GLY:C	2.58	0.46
1:A:48:SER:O	1:A:51:VAL:HG22	2.16	0.46
1:A:63:VAL:HG13	1:A:63:VAL:O	2.15	0.46
1:A:109:LEU:HD21	1:A:269:GLY:HA3	1.98	0.46
1:A:128:LEU:HD12	1:A:172:LEU:HG	1.97	0.46
1:A:204:MET:O	1:A:205:PHE:CB	2.63	0.46
1:A:253:VAL:O	1:A:254:SER:HB3	2.16	0.46
1:A:283:HIS:CD2	1:A:329:LEU:HD21	2.50	0.46
1:A:4:GLN:HA	1:A:4:GLN:NE2	2.30	0.46
1:A:78:ALA:HA	3:A:417:HOH:O	2.16	0.46
1:A:157:ILE:HG21	1:A:160:GLU:CB	2.39	0.46
1:A:209:GLU:O	1:A:210:THR:CG2	2.63	0.46
1:A:253:VAL:O	1:A:253:VAL:CG2	2.62	0.46
1:A:317:VAL:HG13	1:A:318:ALA:N	2.30	0.46
1:A:156:GLU:O	1:A:157:ILE:CG2	2.49	0.45
1:A:173:MET:CA	1:A:177:LEU:HD23	2.45	0.45
1:A:294:THR:HA	1:A:299:GLN:HA	1.97	0.45
1:A:98:GLU:HG3	1:A:146:ASP:OD1	2.16	0.45
1:A:194:ILE:N	1:A:194:ILE:CD1	2.78	0.45
1:A:71:SER:N	2:A:350:DTP:O3G	2.48	0.45
1:A:84:ASN:C	1:A:86:GLN:N	2.73	0.45
1:A:303:GLY:O	1:A:304:LYS:C	2.59	0.45
1:A:310:PHE:CD1	1:A:310:PHE:C	2.94	0.45
1:A:171:ARG:C	1:A:175:GLN:HG2	2.39	0.45
1:A:55:ILE:HD13	1:A:253:VAL:HG21	1.97	0.45
1:A:147:SER:O	1:A:151:LEU:CD1	2.56	0.45
1:A:328:LYS:O	1:A:329:LEU:HD23	2.17	0.45
1:A:30:ARG:O	1:A:32:GLY:N	2.50	0.44
1:A:143:ILE:O	1:A:143:ILE:HG23	2.17	0.44
1:A:68:GLY:O	1:A:69:PRO:O	2.35	0.44
1:A:82:VAL:HG13	1:A:92:ALA:CB	2.48	0.44
1:A:180:MET:O	1:A:184:LEU:CG	2.65	0.44
1:A:284:GLY:C	1:A:286:ILE:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HG12	1:A:158:GLU:N	2.33	0.44
1:A:294:THR:HG23	1:A:294:THR:O	2.18	0.44
1:A:74:LYS:N	2:A:350:DTP:O2B	2.50	0.44
1:A:93:ALA:O	1:A:143:ILE:HA	2.18	0.44
1:A:123:THR:HG21	1:A:154:ARG:HG2	1.99	0.44
1:A:200:LYS:HA	1:A:228:ARG:HD2	1.99	0.44
1:A:218:LYS:HD3	1:A:218:LYS:C	2.42	0.44
1:A:4:GLN:HE21	1:A:4:GLN:CA	2.29	0.44
1:A:248:VAL:O	1:A:248:VAL:HG13	2.18	0.44
1:A:321:ILE:H	1:A:321:ILE:CD1	2.28	0.44
1:A:213:GLY:O	1:A:214:GLY:O	2.37	0.43
1:A:36:ARG:HB3	3:A:359:HOH:O	2.17	0.43
1:A:175:GLN:O	1:A:176:ALA:C	2.61	0.43
1:A:118:VAL:HG12	1:A:119:SER:N	2.33	0.43
1:A:254:SER:CB	1:A:255:PRO:CD	2.95	0.43
1:A:78:ALA:CB	3:A:417:HOH:O	2.67	0.43
1:A:180:MET:HG2	1:A:184:LEU:CD1	2.49	0.43
1:A:238:ASP:O	1:A:239:ALA:HB2	2.19	0.43
1:A:173:MET:HE3	1:A:177:LEU:HD21	2.01	0.43
1:A:1:MET:O	1:A:2:ALA:CB	2.66	0.43
1:A:295:TYR:CZ	1:A:296:GLU:OE2	2.72	0.42
1:A:181:THR:CA	1:A:184:LEU:HD12	2.37	0.42
1:A:200:LYS:HA	1:A:228:ARG:NH1	2.35	0.42
1:A:144:VAL:HG13	1:A:144:VAL:O	2.19	0.42
1:A:95:ILE:CD1	1:A:143:ILE:HD11	2.49	0.42
1:A:240:VAL:HG23	1:A:241:GLY:N	2.34	0.42
1:A:84:ASN:C	1:A:86:GLN:H	2.26	0.42
1:A:147:SER:C	1:A:149:ALA:H	2.27	0.42
1:A:82:VAL:HG13	1:A:92:ALA:HB3	2.02	0.42
1:A:263:ASP:O	1:A:270:ILE:HA	2.19	0.42
1:A:96:ASP:OD2	1:A:99:HIS:HA	2.19	0.42
1:A:327:GLU:C	1:A:329:LEU:H	2.26	0.42
1:A:156:GLU:H	1:A:156:GLU:HG2	1.60	0.41
1:A:62:ARG:HB3	1:A:222:SER:HB2	2.01	0.41
1:A:4:GLN:NE2	1:A:4:GLN:CA	2.83	0.41
1:A:317:VAL:O	1:A:318:ALA:C	2.63	0.41
1:A:124:GLY:C	1:A:172:LEU:HD21	2.45	0.41
1:A:128:LEU:HD13	1:A:176:ALA:HB2	1.99	0.41
1:A:147:SER:C	1:A:149:ALA:N	2.75	0.41
1:A:171:ARG:O	1:A:175:GLN:N	2.33	0.41
1:A:215:LYS:O	1:A:218:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:O	1:A:78:ALA:N	2.54	0.41
1:A:128:LEU:HD13	1:A:176:ALA:HB3	2.01	0.41
1:A:39:ILE:C	1:A:39:ILE:HD12	2.46	0.41
1:A:176:ALA:O	1:A:180:MET:N	2.53	0.41
1:A:251:ASN:OD1	1:A:253:VAL:HG12	2.20	0.41
1:A:61:GLY:C	1:A:185:ASN:CG	2.89	0.41
1:A:14:LEU:C	1:A:14:LEU:CD1	2.93	0.41
1:A:224:ARG:C	1:A:225:LEU:HD12	2.45	0.41
1:A:59:PRO:O	1:A:60:ARG:C	2.61	0.41
1:A:235:ASP:C	1:A:237:THR:N	2.79	0.40
1:A:254:SER:CB	1:A:255:PRO:HD2	2.38	0.40
1:A:80:HIS:O	1:A:81:ALA:C	2.62	0.40
1:A:177:LEU:O	1:A:178:ARG:C	2.63	0.40
1:A:304:LYS:O	1:A:308:ARG:HB2	2.21	0.40
1:A:94:PHE:C	1:A:94:PHE:HD1	2.30	0.40
1:A:18:GLN:HE21	1:A:22:ASN:HD21	1.64	0.40
1:A:98:GLU:HG2	1:A:147:SER:OG	2.21	0.40
1:A:186:ASN:N	1:A:186:ASN:HD22	2.18	0.40
1:A:237:THR:CG2	1:A:238:ASP:H	2.33	0.40
1:A:262:PHE:CD1	1:A:262:PHE:C	2.99	0.40
1:A:77:VAL:O	1:A:78:ALA:C	2.63	0.40
1:A:265:LEU:O	1:A:266:TYR:C	2.64	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	328/349 (94%)	226 (69%)	59 (18%)	43 (13%)	0 3

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	5	ALA
1	A	35	VAL
1	A	36	ARG
1	A	39	ILE
1	A	41	VAL
1	A	69	PRO
1	A	121	PRO
1	A	157	ILE
1	A	164	SER
1	A	166	VAL
1	A	169	GLN
1	A	184	LEU
1	A	200	LYS
1	A	201	ILE
1	A	205	PHE
1	A	208	PRO
1	A	209	GLU
1	A	214	GLY
1	A	215	LYS
1	A	237	THR
1	A	254	SER
1	A	268	GLN
1	A	285	PHE
1	A	304	LYS
1	A	31	LEU
1	A	147	SER
1	A	170	ALA
1	A	171	ARG
1	A	182	GLY
1	A	198	ARG
1	A	199	GLU
1	A	248	VAL
1	A	289	SER
1	A	74	LYS
1	A	267	GLY
1	A	296	GLU
1	A	168	LEU
1	A	175	GLN
1	A	233	LEU
1	A	323	LYS
1	A	273	GLU
1	A	167	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	237/275 (86%)	220 (93%)	17 (7%)	13	38

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	38	PRO
1	A	43	PRO
1	A	59	PRO
1	A	60	ARG
1	A	69	PRO
1	A	74	LYS
1	A	103	PRO
1	A	116	LEU
1	A	121	PRO
1	A	145	ILE
1	A	194	ILE
1	A	208	PRO
1	A	242	ASN
1	A	265	LEU
1	A	321	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	GLN
1	A	18	GLN
1	A	120	GLN
1	A	186	ASN
1	A	242	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	350	-	31,32,32	1.46	4 (12%)	46,50,50	1.22	5 (10%)

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	350	-	-	10/22/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	DTP	PG-O2G	-4.02	1.39	1.54
2	A	350	DTP	PB-O2B	-3.65	1.38	1.55
2	A	350	DTP	PA-O5'	-2.92	1.48	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	DTP	PA-O2A	-2.40	1.44	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	DTP	O2A-PA-O3A	4.01	118.12	107.27
2	A	350	DTP	O3A-PA-O1A	-3.55	100.04	110.70
2	A	350	DTP	C1'-N9-C8	3.01	137.48	126.95
2	A	350	DTP	C4-N9-C1'	-2.34	117.12	126.50
2	A	350	DTP	C2'-C3'-C4'	2.11	107.09	102.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	350	DTP	O4'-C4'-C5'-O5'
2	A	350	DTP	C3'-C4'-C5'-O5'
2	A	350	DTP	C2'-C1'-N9-C4
2	A	350	DTP	O4'-C1'-N9-C4
2	A	350	DTP	PB-O3B-PG-O1G
2	A	350	DTP	PG-O3B-PB-O1B
2	A	350	DTP	PA-O3A-PB-O1B
2	A	350	DTP	PB-O3B-PG-O2G
2	A	350	DTP	PB-O3B-PG-O3G
2	A	350	DTP	O4'-C1'-N9-C8

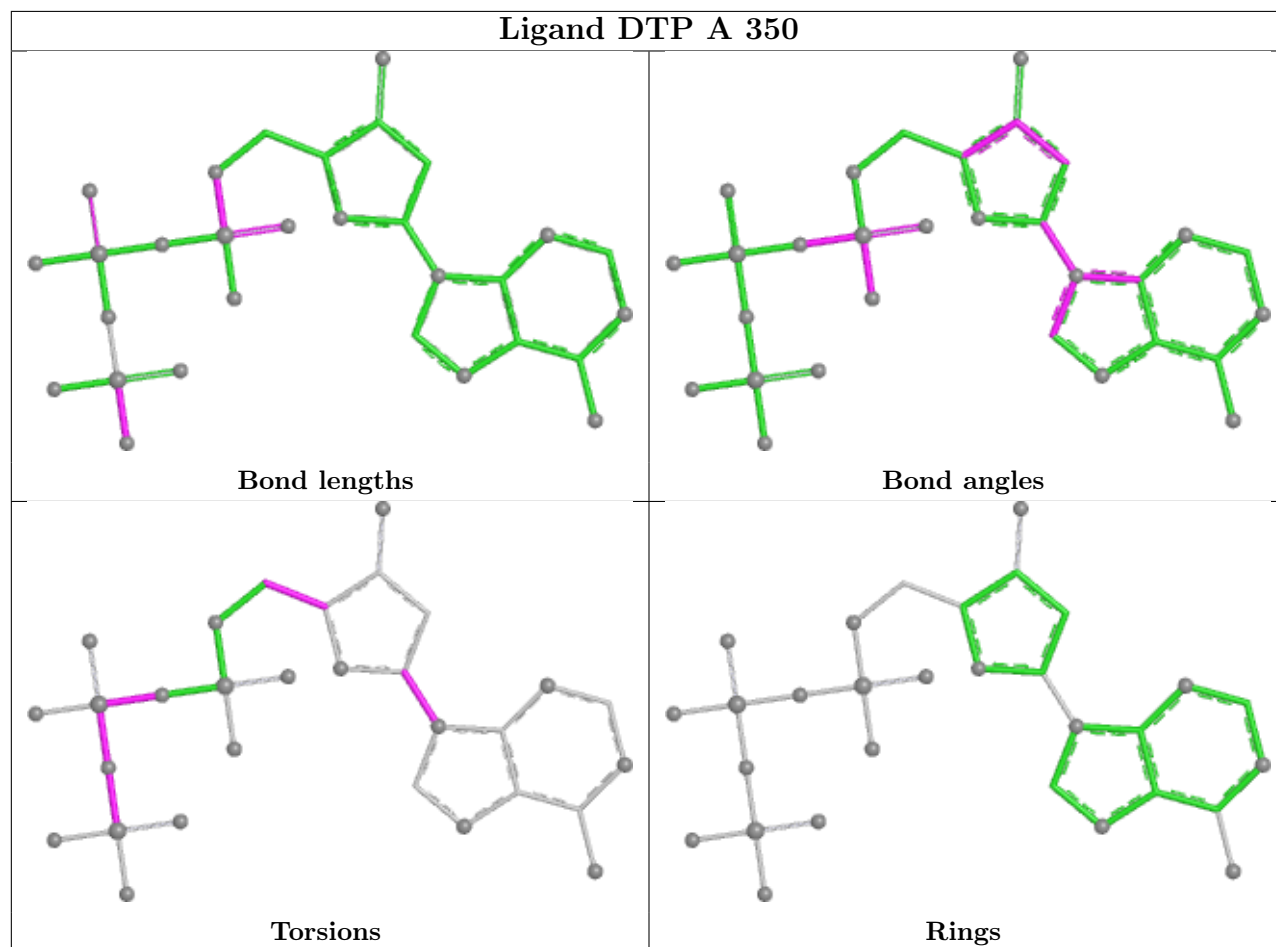
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	DTP	4	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	330/349 (94%)	-0.15	1 (0%)	90 76	13, 34, 108, 108	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	VAL	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](#)

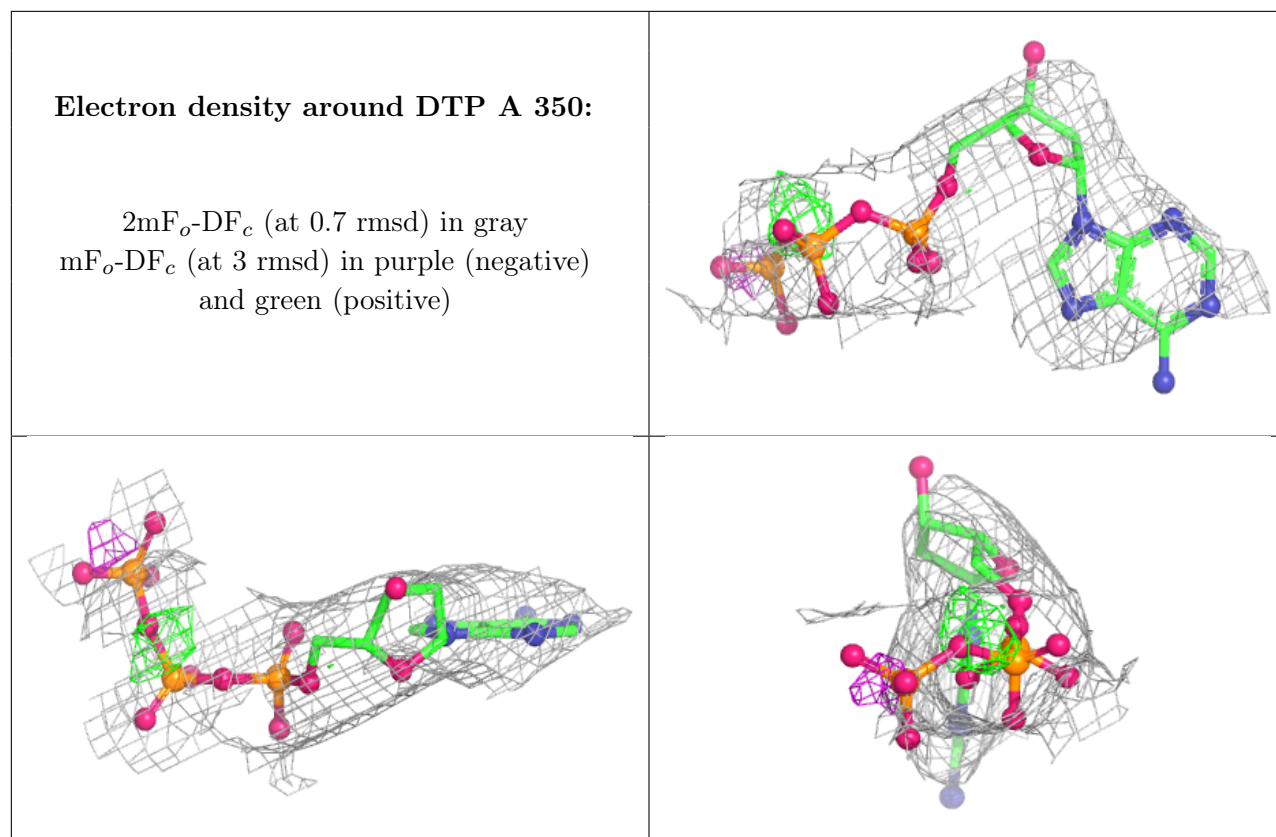
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	DTP	A	350	30/30	0.88	0.14	75,75,75,75	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.