



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 6H1V / pdb_00006h1v
Title : The crystal structure of Pol2CORE in complex with DNA and an incoming nucleotide, carrying an Fe-S cluster
Authors : Parkash, V.; Johansson, E.
Deposited on : 2018-07-12
Resolution : 2.70 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

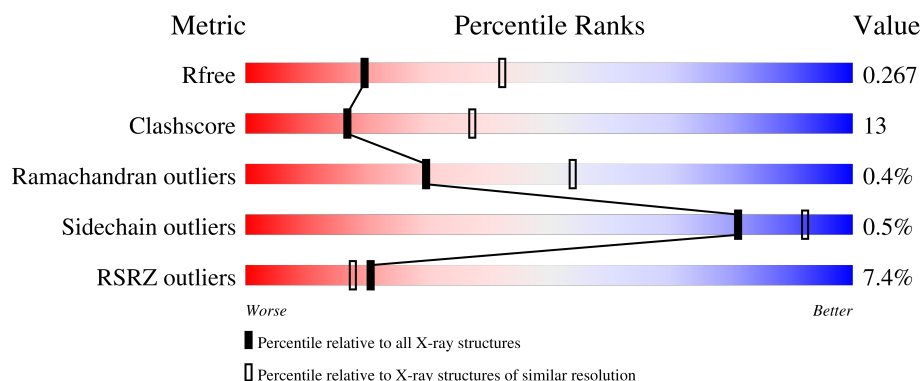
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1187	 7% 71% 23% 6%
2	P	11	 64% 27% 9%
3	T	16	 94% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9002 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1114	8428	5423	1414	1551	40	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	UNP P21951

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	11	221	106	38	66	11	4	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*AP*TP*TP*GP*AP*AP*CP*GP*CP*GP*GP*TP*TP*A)-3').

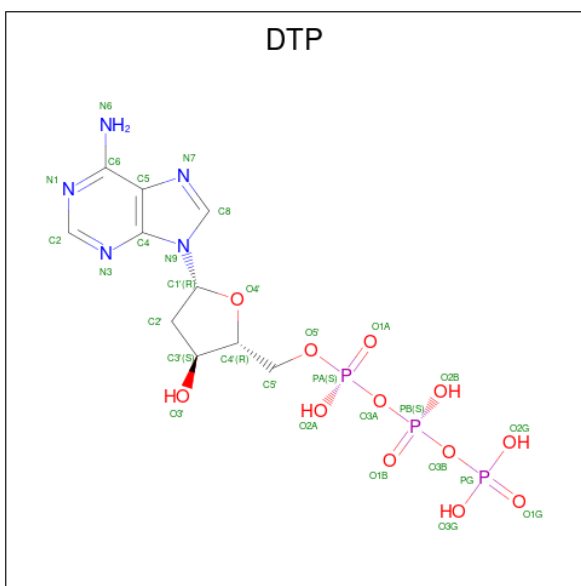
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	15	308	147	54	92	15	4	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	S		0	0
			8	4	4			

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



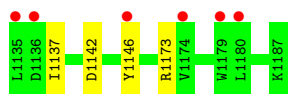
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	P	1	Total 1	O 1	0	0



- Molecule 2: DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP*(DOC))-3')

Chain P: 64% 27% 9%



- Molecule 3: DNA (5'-D(P*AP*AP*TP*TP*GP*AP*AP*CP*GP*CP*GP*GP*TP*TP*A)-3')

Chain T: 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.21Å 70.04Å 149.93Å 90.00° 109.43° 90.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.99-2.70) 97.9 (19.99-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.239 , 0.266 0.244 , 0.267	Depositor DCC
R_{free} test set	1968 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9002	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: MG, DOC, SF4, 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	0.31	1/8627 (0.0%)	0.49	4/11752 (0.0%)
2	P	0.22	0/226	0.42	0/346
3	T	0.23	0/344	0.45	0/529
All	All	0.30	1/9197 (0.0%)	0.49	4/12627 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	889	GLU	CA-C	7.24	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	LYS	N-CA-C	-6.65	103.51	111.69
1	A	33	SER	N-CA-C	-6.22	104.50	111.28
1	A	799	ASP	CA-C-N	6.05	127.40	119.84
1	A	799	ASP	C-N-CA	6.05	127.40	119.84

There are no chirality outliers.

There are no planarity outliers.

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	8428	0	7792	214	0
2	P	221	0	125	2	0
3	T	308	0	171	0	0
4	A	8	0	0	0	0
5	A	30	0	12	1	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
7	P	1	0	0	0	0
All	All	9002	0	8100	216	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 13.

All (216) 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:294:THR:HG22	1:A:309:MET:CE	1.63	1.28
1:A:303:SER:HA	1:A:386:PHE:CE1	1.80	1.15
1:A:294:THR:HG22	1:A:309:MET:HE3	1.12	1.10
1:A:294:THR:CG2	1:A:309:MET:HE3	1.83	1.07
1:A:307:GLN:HA	1:A:390:ARG:HH12	1.36	0.87
1:A:303:SER:HA	1:A:386:PHE:HE1	1.36	0.85
1:A:303:SER:CA	1:A:386:PHE:CE1	2.60	0.84
1:A:291:ILE:HG12	1:A:383:ASP:OD1	1.79	0.83
1:A:1002:ILE:HD12	1:A:1003:PHE:H	1.43	0.83
1:A:294:THR:HG22	1:A:309:MET:HE2	1.60	0.82
1:A:294:THR:CG2	1:A:309:MET:HG3	2.10	0.81
1:A:303:SER:CA	1:A:386:PHE:HE1	1.93	0.81
1:A:835:MET:HE1	1:A:844:MET:HA	1.63	0.79
1:A:380:ASP:OD1	1:A:419:HIS:CE1	2.36	0.78
1:A:1002:ILE:HD12	1:A:1003:PHE:N	1.98	0.78
1:A:307:GLN:HA	1:A:390:ARG:NH1	2.00	0.77
1:A:169:ILE:C	1:A:170:ILE:HD12	2.09	0.77
1:A:653:ARG:NH1	1:A:766:GLU:O	2.20	0.75
1:A:460:THR:HG23	1:A:461:PRO:HD3	1.69	0.74
1:A:708:THR:HB	1:A:720:VAL:HG11	1.68	0.73
1:A:163:CYS:HA	1:A:198:GLN:OE1	1.88	0.73
1:A:380:ASP:OD1	1:A:419:HIS:HE1	1.72	0.71
1:A:1111:ILE:HD11	1:A:1119:LYS:HA	1.72	0.70
1:A:559:GLU:HA	1:A:966:LYS:HZ2	1.55	0.70
1:A:607:VAL:HG21	1:A:610:PHE:HB2	1.73	0.70
1:A:656:PRO:HG2	1:A:841:TRP:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ASP:HB3	1:A:933:ILE:HG12	1.74	0.70
1:A:310:MET:HE2	1:A:321:LEU:HD11	1.72	0.69
1:A:576:ILE:HD13	1:A:624:LEU:HD21	1.75	0.67
1:A:576:ILE:HG21	1:A:624:LEU:HD21	1.76	0.67
1:A:397:ASP:HB3	1:A:400:ASP:HB2	1.76	0.67
1:A:598:VAL:HG23	1:A:599:GLU:HG3	1.75	0.67
1:A:870:ARG:HB2	1:A:882:ILE:HD11	1.78	0.66
1:A:163:CYS:HB3	1:A:198:GLN:OE1	1.97	0.65
1:A:971:VAL:HG23	1:A:979:ALA:HB3	1.80	0.64
1:A:32:LEU:O	1:A:36:GLN:HB2	1.97	0.63
1:A:708:THR:HB	1:A:720:VAL:CG1	2.29	0.63
1:A:775:LYS:HG3	1:A:778:ARG:NH2	2.15	0.62
1:A:163:CYS:CB	1:A:198:GLN:OE1	2.48	0.62
1:A:986:LEU:HA	1:A:996:LYS:HD2	1.81	0.62
1:A:641:VAL:HG22	1:A:877:ASP:HB2	1.82	0.62
1:A:374:ILE:HG12	1:A:417:CYS:SG	2.40	0.61
1:A:559:GLU:HA	1:A:966:LYS:NZ	2.15	0.61
1:A:294:THR:HG23	1:A:309:MET:HG3	1.82	0.61
1:A:322:ILE:HG22	1:A:350:PHE:HB2	1.83	0.61
1:A:297:PRO:O	1:A:298:LEU:HB2	1.99	0.60
1:A:72:ILE:HD13	1:A:268:THR:HG21	1.83	0.60
1:A:978:LEU:HD21	1:A:981:LEU:HB2	1.83	0.60
1:A:159:TYR:CE2	1:A:209:ILE:HD11	2.36	0.60
1:A:384:TRP:HB2	1:A:385:PRO:HD3	1.83	0.60
1:A:1108:PRO:O	1:A:1111:ILE:HG22	2.02	0.59
1:A:303:SER:N	1:A:386:PHE:HE1	1.99	0.59
1:A:72:ILE:CD1	1:A:268:THR:HG21	2.32	0.59
1:A:609:ASN:O	1:A:613:ILE:HG22	2.02	0.58
1:A:319:GLY:HA3	1:A:347:PHE:CE1	2.38	0.58
1:A:307:GLN:CA	1:A:390:ARG:HH12	2.15	0.58
1:A:694:MET:HA	1:A:697:TYR:HB3	1.85	0.58
1:A:1031:ASP:OD2	1:A:1173:ARG:NH2	2.37	0.58
1:A:426:VAL:HA	1:A:430:SER:HB3	1.87	0.57
1:A:379:GLY:HA2	1:A:383:ASP:HB2	1.86	0.57
1:A:163:CYS:CA	1:A:198:GLN:OE1	2.53	0.56
1:A:927:LYS:HD3	1:A:935:GLU:HB2	1.87	0.56
1:A:38:LEU:HD12	1:A:38:LEU:O	2.06	0.56
1:A:50:MET:HG2	1:A:416:TYR:CE2	2.41	0.56
1:A:956:PRO:HB2	1:A:965:ILE:HD11	1.87	0.55
1:A:791:TRP:C	1:A:813:ILE:HD11	2.31	0.55
1:A:559:GLU:HG2	1:A:874:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:PHE:HE2	1:A:1137:ILE:HA	1.70	0.55
1:A:310:MET:HE1	1:A:471:SER:HA	1.88	0.55
1:A:388:HIS:HB2	1:A:398:MET:HE1	1.89	0.55
1:A:606:LYS:HB3	1:A:895:LEU:HD22	1.88	0.55
1:A:160:LEU:HD11	1:A:206:LEU:HD21	1.88	0.55
1:A:553:TYR:HE1	1:A:835:MET:HE3	1.72	0.55
1:A:194:VAL:HG13	1:A:195:ASN:N	2.23	0.54
1:A:1111:ILE:HG23	1:A:1112:PHE:CD1	2.42	0.54
1:A:169:ILE:O	1:A:170:ILE:HD12	2.07	0.53
1:A:156:VAL:HG13	1:A:160:LEU:HD12	1.91	0.53
1:A:653:ARG:HG3	1:A:923:TYR:CE2	2.43	0.53
1:A:294:THR:HG22	1:A:309:MET:HG3	1.91	0.53
1:A:594:PHE:CE1	1:A:598:VAL:HG21	2.43	0.53
1:A:54:ARG:HE	1:A:132:THR:HG21	1.75	0.52
1:A:244:GLU:OE2	1:A:252:ARG:NH2	2.43	0.52
1:A:578:PRO:HA	1:A:581:ILE:HD12	1.91	0.52
1:A:402:ILE:HG22	1:A:404:PHE:HD1	1.75	0.52
1:A:1111:ILE:HG23	1:A:1112:PHE:HD1	1.75	0.52
1:A:112:GLN:NE2	1:A:194:VAL:HG11	2.24	0.52
1:A:992:LEU:CD2	1:A:994:LEU:HB3	2.40	0.52
1:A:294:THR:CA	1:A:309:MET:HE3	2.39	0.51
1:A:443:THR:HG23	1:A:447:LEU:HD12	1.92	0.51
1:A:69:ILE:O	1:A:72:ILE:HG13	2.09	0.51
1:A:875:ASP:O	1:A:877:ASP:N	2.44	0.51
1:A:1115:ASP:O	1:A:1119:LYS:HG3	2.10	0.51
1:A:775:LYS:HG3	1:A:778:ARG:HH21	1.74	0.51
1:A:35:GLN:O	1:A:35:GLN:HG3	2.11	0.51
1:A:798:ILE:HD11	1:A:805:ALA:HB1	1.93	0.51
1:A:241:ASP:OD1	1:A:242:ILE:N	2.44	0.50
1:A:159:TYR:HE2	1:A:209:ILE:HD11	1.76	0.50
1:A:384:TRP:N	1:A:385:PRO:CD	2.74	0.50
1:A:306:ASP:O	1:A:390:ARG:NH1	2.44	0.50
1:A:553:TYR:CE1	1:A:835:MET:HE3	2.47	0.50
1:A:596:VAL:HG11	1:A:604:VAL:HG12	1.92	0.50
1:A:322:ILE:HG13	1:A:358:LEU:HD12	1.93	0.49
1:A:337:TYR:HE2	1:A:452:ILE:HD11	1.77	0.49
1:A:604:VAL:O	1:A:607:VAL:HG22	2.12	0.49
1:A:921:HIS:HD1	1:A:938:SER:HG	1.61	0.49
1:A:500:ILE:HG22	1:A:502:LEU:HD12	1.94	0.49
1:A:244:GLU:HG2	1:A:531:LEU:HB2	1.95	0.49
1:A:287:MET:HE3	1:A:289:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:HE2	1:A:419:HIS:HB2	1.78	0.49
1:A:567:ARG:NH1	1:A:1015:CYS:SG	2.85	0.49
2:P:5:DC:H2'	2:P:6:DG:C8	2.48	0.48
1:A:581:ILE:HG23	1:A:621:LEU:HD22	1.95	0.48
1:A:294:THR:CG2	1:A:309:MET:CG	2.89	0.48
1:A:579:SER:O	1:A:583:GLU:HG3	2.13	0.48
1:A:294:THR:HG22	1:A:309:MET:CG	2.43	0.48
1:A:40:ALA:O	1:A:44:ASP:N	2.24	0.48
1:A:781:ARG:NH1	1:A:824:LYS:HB2	2.29	0.47
1:A:919:THR:HG22	1:A:940:ASN:CB	2.44	0.47
1:A:332:ILE:N	1:A:351:ASN:HD21	2.12	0.47
1:A:604:VAL:HA	1:A:607:VAL:HG13	1.96	0.47
1:A:1049:ASN:C	1:A:1050:ARG:HG2	2.39	0.47
1:A:416:TYR:CE2	1:A:417:CYS:HB2	2.50	0.47
1:A:994:LEU:HD12	1:A:1026:TRP:CZ3	2.50	0.47
1:A:406:PRO:HB3	1:A:412:TYR:CE1	2.50	0.47
1:A:686:ARG:HB2	1:A:755:ILE:HG22	1.96	0.47
1:A:1097:PRO:HD3	1:A:1126:TRP:O	2.15	0.47
1:A:347:PHE:CD2	1:A:475:VAL:HG22	2.50	0.46
1:A:458:LEU:C	1:A:461:PRO:HD2	2.39	0.46
1:A:338:THR:HG22	1:A:345:GLY:H	1.80	0.46
1:A:909:MET:O	1:A:913:ARG:HG3	2.16	0.46
1:A:628:ASN:HB2	1:A:629:ILE:HD12	1.97	0.46
1:A:677:CYS:O	1:A:764:GLN:HG2	2.16	0.46
1:A:561:LEU:HD13	1:A:871:PRO:HG2	1.97	0.46
1:A:1000:SER:O	1:A:1004:LYS:HE2	2.16	0.46
1:A:558:VAL:HG11	1:A:967:LYS:HE3	1.98	0.45
1:A:919:THR:HA	1:A:940:ASN:HB2	1.98	0.45
1:A:947:ASP:OD1	1:A:947:ASP:N	2.48	0.45
1:A:554:VAL:HG22	1:A:684:ALA:HB3	1.98	0.45
1:A:912:TYR:O	1:A:916:GLN:HG2	2.17	0.45
1:A:572:ASN:OD1	1:A:634:PRO:HG3	2.16	0.45
1:A:811:LYS:O	1:A:814:VAL:HG12	2.17	0.45
1:A:791:TRP:O	1:A:813:ILE:HD11	2.17	0.45
1:A:906:PRO:HA	1:A:909:MET:HG2	1.99	0.45
1:A:234:ASP:OD1	1:A:235:ALA:N	2.50	0.45
1:A:296:PRO:HG2	1:A:299:LYS:CB	2.47	0.45
1:A:373:VAL:HG23	1:A:420:MET:HG2	1.97	0.45
1:A:420:MET:HE1	1:A:493:ILE:HG21	1.99	0.45
1:A:338:THR:HG22	1:A:345:GLY:N	2.32	0.45
1:A:379:GLY:O	1:A:384:TRP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:C	1:A:170:ILE:CD1	2.86	0.44
1:A:379:GLY:O	1:A:385:PRO:HD3	2.17	0.44
1:A:577:ASP:OD1	1:A:579:SER:OG	2.35	0.44
1:A:595:SER:O	1:A:600:ASN:ND2	2.45	0.44
1:A:622:LEU:HD23	1:A:622:LEU:HA	1.82	0.44
1:A:502:LEU:HD11	1:A:518:MET:HG3	2.00	0.44
1:A:845:GLU:OE1	1:A:845:GLU:N	2.48	0.44
1:A:992:LEU:HD21	1:A:994:LEU:HB3	2.00	0.44
1:A:517:GLU:HB2	1:A:833:TYR:CE1	2.53	0.44
1:A:1004:LYS:HD3	1:A:1004:LYS:N	2.33	0.44
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.42	0.44
1:A:795:LEU:HD13	1:A:809:ALA:HB3	2.00	0.44
1:A:920:ASN:O	1:A:938:SER:HA	2.18	0.44
1:A:644:MET:SD	1:A:877:ASP:HB3	2.58	0.43
1:A:68:ASP:OD1	1:A:70:ASP:N	2.45	0.43
1:A:594:PHE:CZ	1:A:598:VAL:HG21	2.53	0.43
1:A:915:HIS:CD2	1:A:940:ASN:HD22	2.35	0.43
1:A:293:THR:O	1:A:309:MET:CE	2.67	0.43
1:A:1069:THR:HG21	1:A:1091:TYR:HB3	2.00	0.43
1:A:264:TRP:CZ2	1:A:282:ALA:HB2	2.54	0.43
1:A:294:THR:HA	1:A:309:MET:HE3	2.01	0.43
1:A:294:THR:CB	1:A:309:MET:HE3	2.46	0.43
1:A:337:TYR:CE1	1:A:339:PRO:HG3	2.53	0.43
1:A:858:ILE:HD12	1:A:858:ILE:HA	1.89	0.43
1:A:799:ASP:HA	1:A:800:PRO:HD3	1.75	0.43
1:A:798:ILE:CD1	1:A:805:ALA:HB1	2.49	0.42
1:A:880:TRP:CG	1:A:953:MET:HE1	2.54	0.42
1:A:1142:ASP:O	1:A:1146:TYR:HD1	2.01	0.42
1:A:496:LEU:HB3	1:A:507:THR:HG21	2.02	0.42
1:A:865:VAL:HA	1:A:868:VAL:HG12	2.01	0.42
1:A:919:THR:HG22	1:A:940:ASN:HB3	2.02	0.42
1:A:81:ASN:OD1	1:A:82:MET:N	2.52	0.42
1:A:591:ALA:O	1:A:594:PHE:HB3	2.20	0.42
1:A:645:TYR:CD2	5:A:1202:DTP:H2'1	2.54	0.42
1:A:338:THR:O	1:A:338:THR:OG1	2.37	0.42
1:A:652:ASN:HB2	1:A:654:LEU:HG	2.02	0.42
1:A:580:ALA:HB2	1:A:867:ARG:HB3	2.02	0.42
1:A:1087:LEU:HD11	1:A:1089:CYS:SG	2.60	0.42
1:A:65:ASP:OD1	1:A:67:LYS:N	2.53	0.42
1:A:314:MET:HE2	1:A:314:MET:HB3	1.96	0.42
1:A:365:HIS:O	1:A:369:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:10:DT:H2''	2:P:11:DOC:H6	2.01	0.42
1:A:460:THR:CG2	1:A:461:PRO:HD3	2.43	0.41
1:A:384:TRP:CB	1:A:385:PRO:HD3	2.47	0.41
1:A:595:SER:HA	1:A:599:GLU:OE1	2.20	0.41
1:A:124:GLU:H	1:A:124:GLU:HG2	1.63	0.41
1:A:194:VAL:CG1	1:A:195:ASN:N	2.84	0.41
1:A:369:VAL:HG23	1:A:371:PRO:HD3	2.03	0.41
1:A:543:TYR:OH	1:A:754:GLU:OE2	2.33	0.41
1:A:635:LEU:HD11	1:A:885:LYS:HA	2.03	0.41
1:A:287:MET:HG3	1:A:315:ILE:CG1	2.51	0.41
1:A:302:ASP:C	1:A:386:PHE:HE1	2.28	0.41
1:A:122:LEU:HD21	1:A:372:THR:HG21	2.03	0.41
1:A:319:GLY:HA3	1:A:347:PHE:CD1	2.55	0.41
1:A:426:VAL:O	1:A:430:SER:OG	2.32	0.41
1:A:588:LEU:O	1:A:592:LEU:HD12	2.21	0.41
1:A:958:SER:HB2	1:A:964:GLY:O	2.21	0.41
1:A:1087:LEU:HD12	1:A:1087:LEU:C	2.45	0.41
1:A:308:ILE:HD11	1:A:311:ILE:HD11	2.03	0.41
1:A:474:SER:OG	1:A:475:VAL:N	2.53	0.40
1:A:581:ILE:HG22	1:A:585:LEU:HD23	2.02	0.40
1:A:438:GLY:O	1:A:442:VAL:HG23	2.21	0.40
1:A:581:ILE:O	1:A:585:LEU:HD23	2.20	0.40
1:A:87:VAL:HG22	1:A:88:SER:H	1.85	0.40
1:A:607:VAL:HA	1:A:895:LEU:HD23	2.02	0.40
1:A:496:LEU:HD12	1:A:496:LEU:HA	1.87	0.40
1:A:580:ALA:HA	1:A:867:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1104/1187 (93%)	1035 (94%)	65 (6%)	4 (0%)	30 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	THR
1	A	802	ASP
1	A	328	ILE
1	A	800	PRO

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	821/1063 (77%)	817 (100%)	4 (0%)	81 92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	38	LEU
1	A	187	THR
1	A	798	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	419	HIS
1	A	528	ASN
1	A	535	HIS
1	A	859	GLN
1	A	940	ASN
1	A	1088	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	DOC	P	11	3,2	16,19,20	4.35	12 (75%)	20,26,29	0.89	1 (5%)

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	DOC	P	11	3,2	-	2/7/18/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	11	DOC	O4'-C4'	8.50	1.61	1.44
2	P	11	DOC	C2-N3	6.73	1.49	1.36
2	P	11	DOC	O4'-C1'	-6.55	1.27	1.42
2	P	11	DOC	C6-C5	5.96	1.48	1.35
2	P	11	DOC	C4-N3	4.62	1.43	1.34
2	P	11	DOC	C2-N1	4.12	1.48	1.40
2	P	11	DOC	C3'-C4'	-3.73	1.33	1.52
2	P	11	DOC	C4-N4	3.73	1.42	1.33
2	P	11	DOC	O2-C2	-3.22	1.17	1.23
2	P	11	DOC	C6-N1	3.08	1.45	1.38
2	P	11	DOC	C5-C4	2.77	1.49	1.42
2	P	11	DOC	C2'-C1'	2.73	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	11	DOC	C4'-O4'-C1'	-2.17	107.76	109.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	11	DOC	C3'-C4'-C5'-O5'
2	P	11	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	11	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	A	1201	1	0,12,12	-	-	-		
5	DTP	A	1202	6	31,32,32	3.07	11 (35%)	46,50,50	2.39	12 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	1201	1	-	-	0/6/5/5
5	DTP	A	1202	6	-	1/22/34/34	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1202	DTP	C3'-C4'	-8.45	1.30	1.53
5	A	1202	DTP	O4'-C4'	8.25	1.63	1.45
5	A	1202	DTP	PB-O3A	4.78	1.64	1.59
5	A	1202	DTP	O4'-C1'	-4.71	1.31	1.42
5	A	1202	DTP	PB-O3B	4.69	1.64	1.59
5	A	1202	DTP	PA-O3A	4.66	1.64	1.59
5	A	1202	DTP	C6-N6	4.43	1.45	1.34
5	A	1202	DTP	O3'-C3'	2.96	1.49	1.43
5	A	1202	DTP	C5-C4	-2.79	1.34	1.39
5	A	1202	DTP	C5-N7	-2.65	1.34	1.39
5	A	1202	DTP	C8-N9	-2.19	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1202	DTP	N6-C6-N1	-6.68	103.50	118.38
5	A	1202	DTP	N3-C2-N1	-5.91	119.63	128.58
5	A	1202	DTP	C5-C6-N6	5.11	135.94	123.29
5	A	1202	DTP	C5-C4-N3	-5.04	119.78	126.72
5	A	1202	DTP	C1'-N9-C8	4.89	144.05	126.95
5	A	1202	DTP	C4-N9-C1'	-4.71	107.63	126.50
5	A	1202	DTP	N9-C8-N7	-4.12	108.09	113.94
5	A	1202	DTP	C2-N3-C4	3.54	120.48	111.83
5	A	1202	DTP	N3-C4-N9	3.37	132.90	127.17
5	A	1202	DTP	C5-N7-C8	2.75	107.78	103.45
5	A	1202	DTP	C2'-C1'-N9	-2.63	108.44	114.63
5	A	1202	DTP	C4-N9-C8	2.45	108.31	105.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

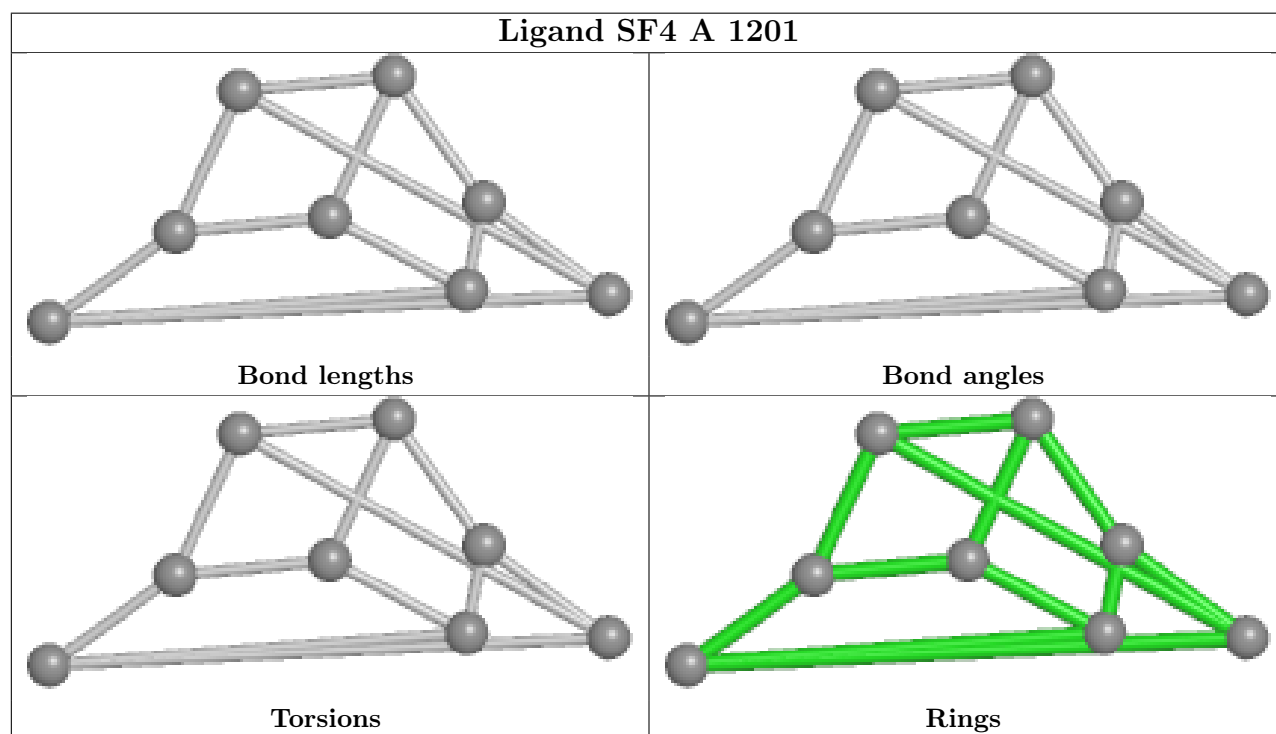
Mol	Chain	Res	Type	Atoms
5	A	1202	DTP	PB-O3B-PG-O1G

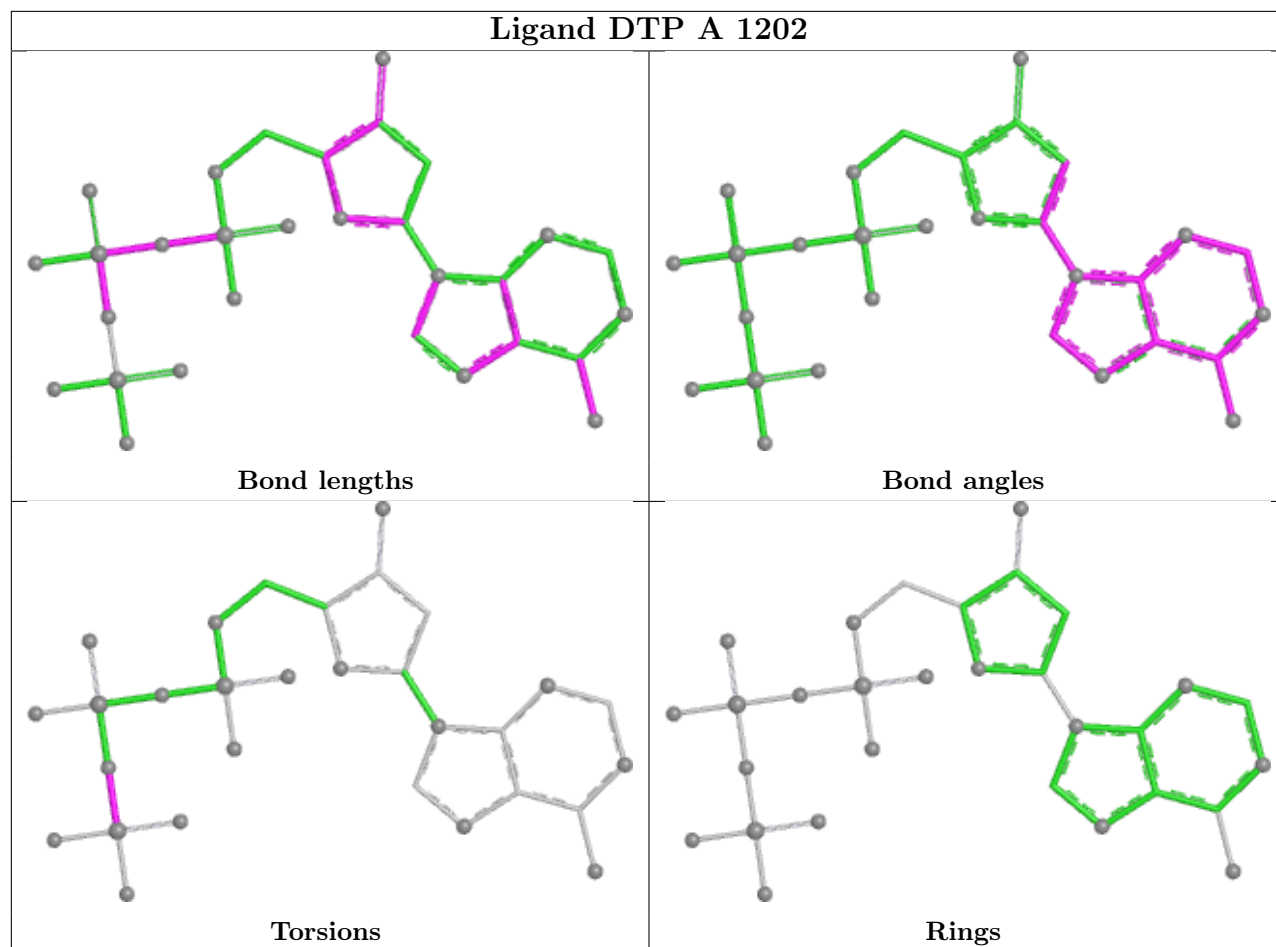
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1202	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1114/1187 (93%)	0.72	84 (7%) 20 17	28, 67, 101, 123	0
2	P	10/11 (90%)	0.20	0 100 100	31, 49, 71, 72	1 (10%)
3	T	15/16 (93%)	0.08	0 100 100	27, 50, 86, 91	1 (6%)
All	All	1139/1214 (93%)	0.71	84 (7%) 20 18	27, 66, 101, 123	2 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1100	ALA	5.3
1	A	1074	GLY	4.9
1	A	691	PRO	3.6
1	A	1030	LEU	3.5
1	A	1132	LEU	3.5
1	A	799	ASP	3.4
1	A	474	SER	3.4
1	A	747	TYR	3.3
1	A	1174	VAL	3.3
1	A	582	ASP	3.2
1	A	750	VAL	3.2
1	A	749	ARG	3.1
1	A	399	PHE	3.1
1	A	1078	GLY	3.0
1	A	1062	GLN	3.0
1	A	678	ALA	2.9
1	A	1179	TRP	2.9
1	A	709	PHE	2.8
1	A	1047	CYS	2.8
1	A	337	TYR	2.8
1	A	580	ALA	2.7
1	A	697	TYR	2.7
1	A	72	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	53	GLU	2.7
1	A	1120	ARG	2.7
1	A	1133	GLU	2.7
1	A	617	ILE	2.7
1	A	1128	LEU	2.7
1	A	1066	SER	2.7
1	A	64	PHE	2.6
1	A	303	SER	2.6
1	A	309	MET	2.6
1	A	1101	PRO	2.6
1	A	791	TRP	2.6
1	A	964	GLY	2.6
1	A	66	ALA	2.5
1	A	320	PHE	2.4
1	A	1007	LEU	2.4
1	A	1129	ASP	2.4
1	A	1052	MET	2.4
1	A	160	LEU	2.4
1	A	804	HIS	2.4
1	A	607	VAL	2.4
1	A	347	PHE	2.4
1	A	1015	CYS	2.4
1	A	1136	ASP	2.3
1	A	1126	TRP	2.3
1	A	335	PHE	2.3
1	A	1080	ASP	2.3
1	A	610	PHE	2.3
1	A	1180	LEU	2.3
1	A	327	ILE	2.3
1	A	1043	VAL	2.3
1	A	235	ALA	2.3
1	A	1070	ALA	2.3
1	A	1099	ASN	2.3
1	A	613	ILE	2.2
1	A	1040	GLU	2.2
1	A	354	ASP	2.2
1	A	475	VAL	2.2
1	A	339	PRO	2.2
1	A	321	LEU	2.2
1	A	1089	CYS	2.2
1	A	1146	TYR	2.2
1	A	349	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	677	CYS	2.2
1	A	1097	PRO	2.2
1	A	307	GLN	2.1
1	A	902	TYR	2.1
1	A	463	ALA	2.1
1	A	1135	LEU	2.1
1	A	1039	ASP	2.1
1	A	1093	ILE	2.1
1	A	676	THR	2.1
1	A	1127	THR	2.1
1	A	588	LEU	2.1
1	A	895	LEU	2.1
1	A	350	PHE	2.1
1	A	1123	LEU	2.1
1	A	1053	SER	2.0
1	A	919	THR	2.0
1	A	279	ILE	2.0
1	A	1076	PHE	2.0
1	A	391	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	DOC	P	11	18/19	0.97	0.09	12,28,46,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

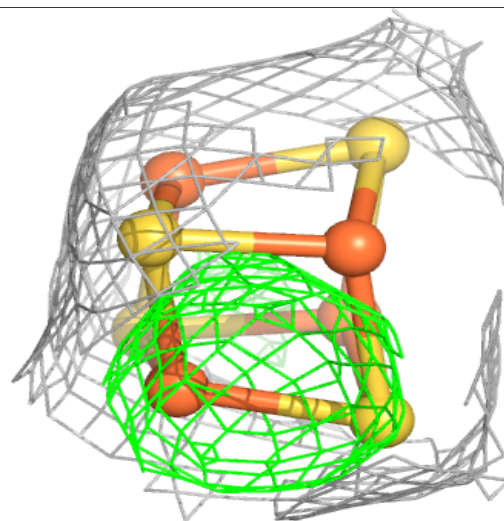
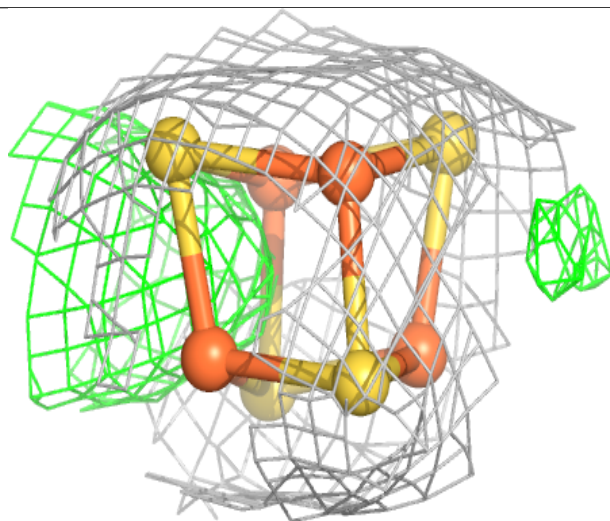
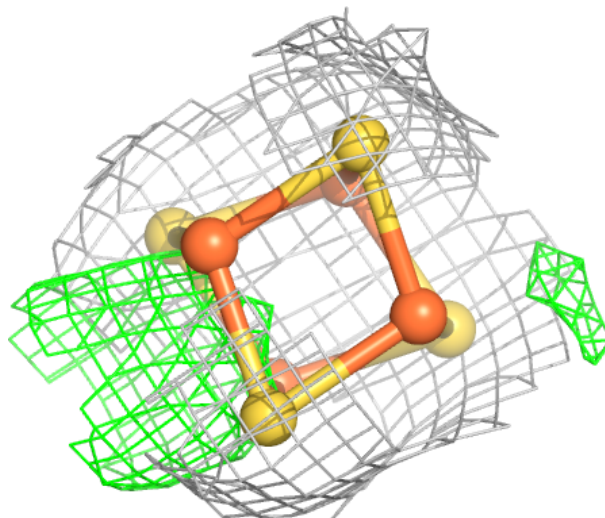
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

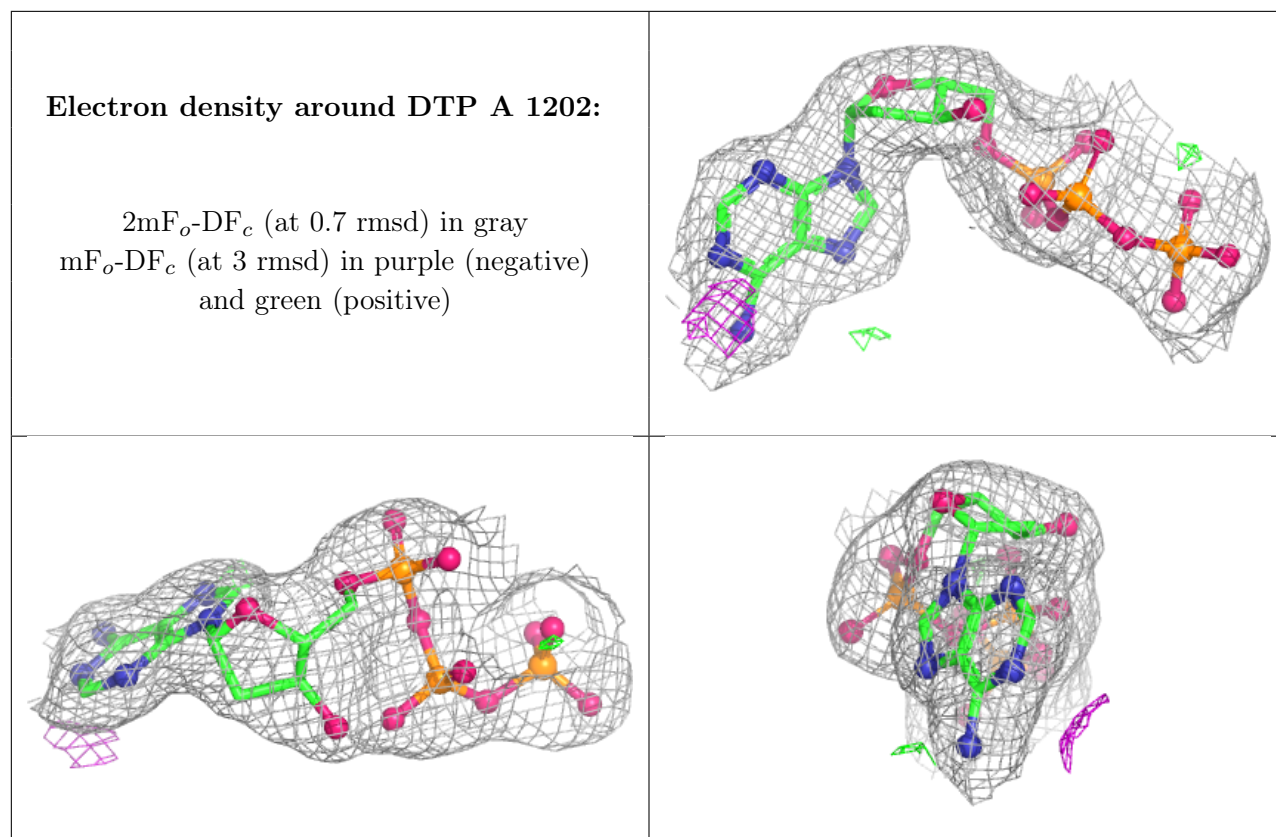
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	1203	1/1	0.92	0.07	44,44,44,44	0
4	SF4	A	1201	8/8	0.93	0.09	53,73,85,87	8
5	DTP	A	1202	30/30	0.97	0.06	18,30,44,49	0

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 SF4 A 1201:

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.