Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 01:12 pm BST

PDB ID	:	8B76
Title	:	The crystal structure of M644G variant of DNA Pol Epsilon containing dTTP in the polymerase active site
Authors	:	Parkash, V.; Johansson, E.
Deposited on	:	2022-09-28
Resolution	:	2.60 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:

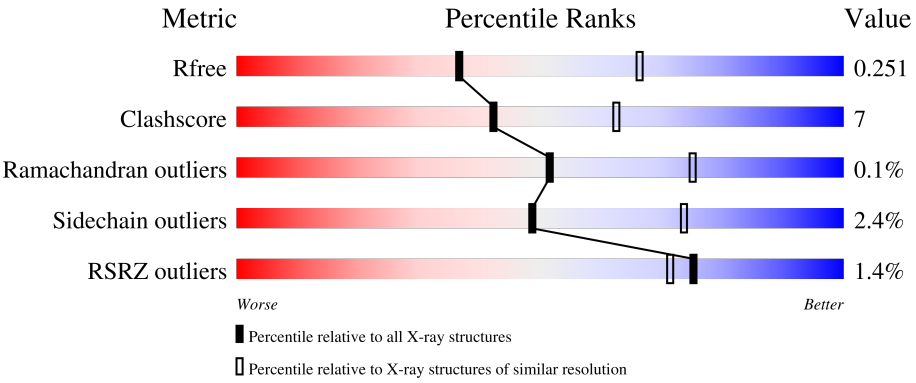
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	1191	% 76% 17% 6%
1	B	1191	% 77% 17% 6%
2	C	11	82% 18%
2	P	11	82% 18%
3	D	16	81% 12% 6%

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Mol	Chain	Length	Quality of chain
3	T	16	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18886 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
1	A	1118	Total	C	N	O	S	0	0	0
			8900	5705	1483	1669	43			
1	B	1121	Total	C	N	O	S	0	0	0
			8809	5640	1462	1665	42			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P21951
A	-3	GLY	-	expression tag	UNP P21951
A	-2	ASP	-	expression tag	UNP P21951
A	-1	PRO	-	expression tag	UNP P21951
A	0	HIS	-	expression tag	UNP P21951
A	644	GLY	MET	engineered mutation	UNP P21951
B	-4	GLY	-	expression tag	UNP P21951
B	-3	GLY	-	expression tag	UNP P21951
B	-2	ASP	-	expression tag	UNP P21951
B	-1	PRO	-	expression tag	UNP P21951
B	0	HIS	-	expression tag	UNP P21951
B	644	GLY	MET	engineered mutation	UNP P21951

- Molecule 2 is a DNA chain called Primer DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			217	106	38	63	10			
2	P	11	Total	C	N	O	P	0	0	0
			217	106	38	63	10			

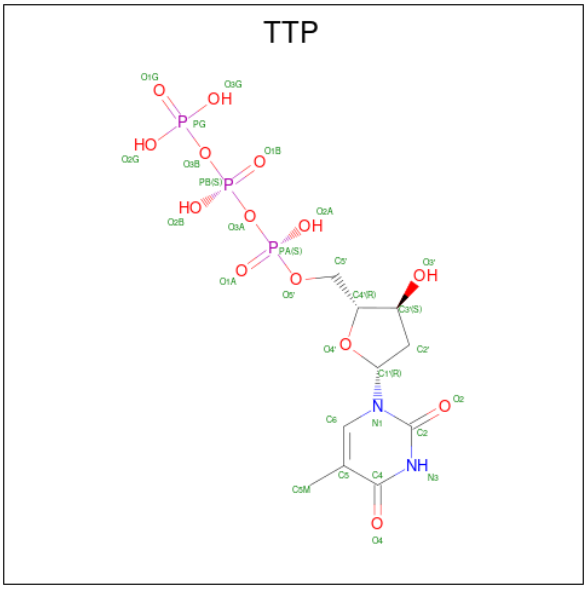
- Molecule 3 is a DNA chain called Template DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	15	Total	C	N	O	P	0	0	0
			309	147	57	90	15			
3	T	15	Total	C	N	O	P	0	0	0
			309	147	57	90	15			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

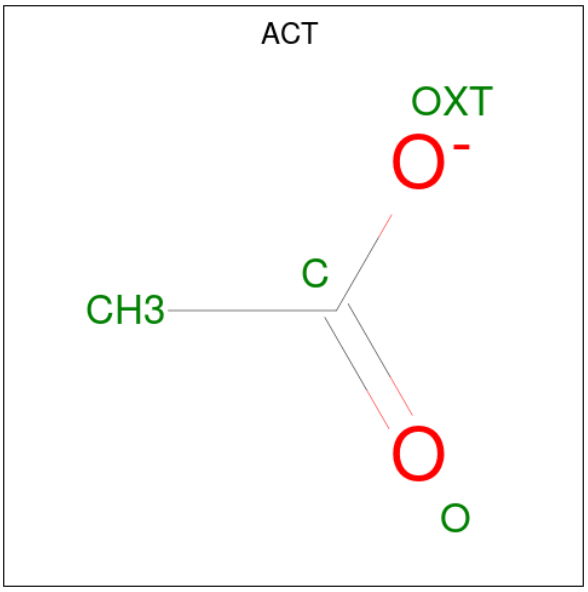
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
5	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

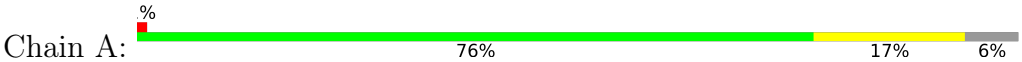
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	21	Total O 21 21	0	0
7	B	26	Total O 26 26	0	0
7	C	1	Total O 1 1	0	0
7	D	2	Total O 2 2	0	0
7	P	1	Total O 1 1	0	0
7	T	2	Total O 2 2	0	0

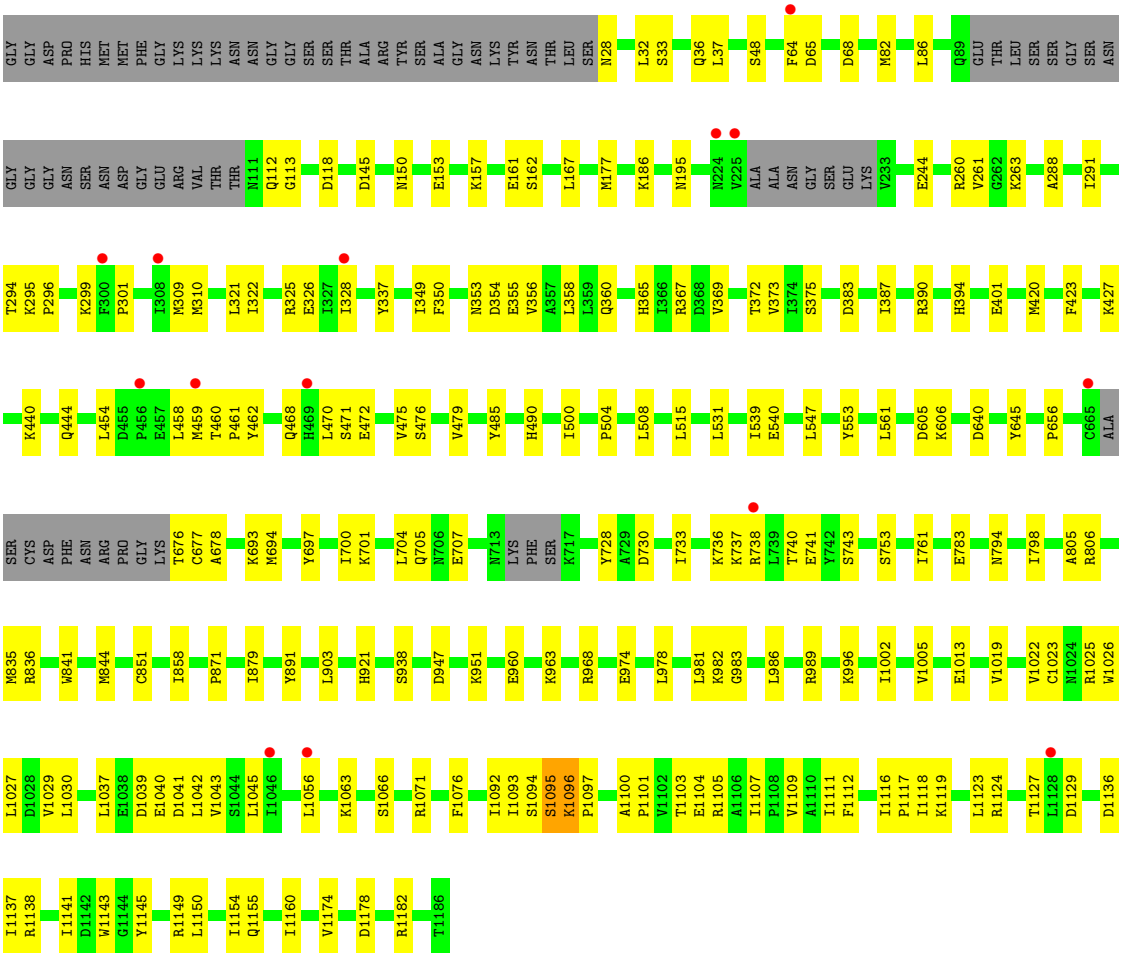
3 Residue-property plots (i)

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: DNA polymerase epsilon catalytic subunit A

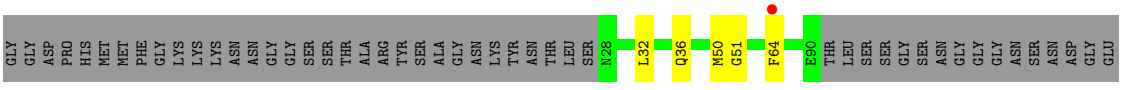
Chain A:

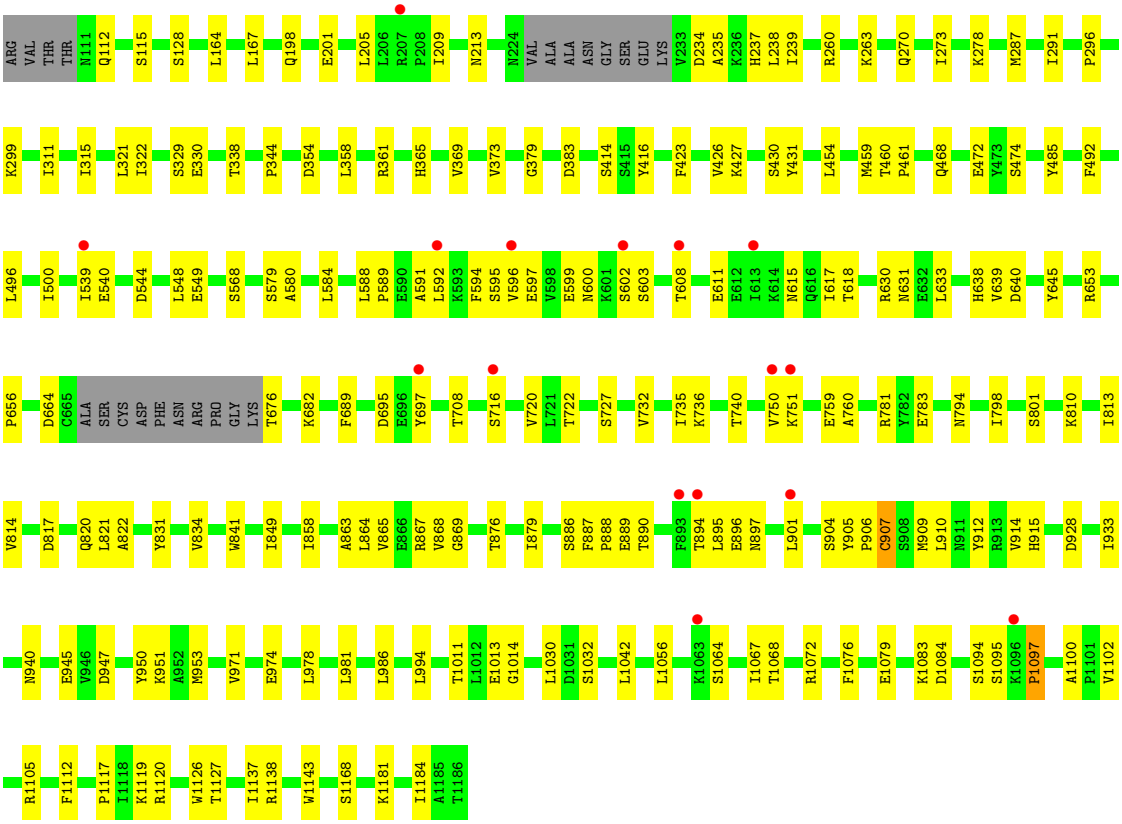




• Molecule 1: DNA polymerase epsilon catalytic subunit A

Chain B:



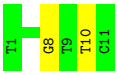


• Molecule 2: Primer DNA sequence

Chain C:

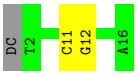
• Molecule 2: Primer DNA sequence

Chain P:



• Molecule 3: Template DNA sequence

Chain D:



• Molecule 3: Template DNA sequence

Chain T:


DC
T2
A5
G13
A16

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.16Å 69.88Å 159.05Å 90.00° 112.63° 90.00°	Depositor
Resolution (Å)	86.83 – 2.60 86.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.83-2.60) 99.4 (86.83-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.220 , 0.247 0.222 , 0.251	Depositor DCC
R_{free} test set	4813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18886	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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 64.07 % 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 8.7764e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, ACT, CA, TTP

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	0.26	0/9105	0.48	0/12338
1	B	0.28	0/9010	0.49	1/12231 (0.0%)
2	C	0.49	0/222	0.94	0/341
2	P	0.51	0/222	0.95	0/341
3	D	0.50	0/346	0.91	0/532
3	T	0.47	0/346	0.89	0/532
All	All	0.29	0/19251	0.52	1/26315 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1097	PRO	N-CA-C	-5.02	99.05	112.10

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	8900	0	8612	141	0
1	B	8809	0	8411	109	0
2	C	217	0	123	2	0
2	P	217	0	123	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	309	0	170	1	0
3	T	309	0	170	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	29	0	13	1	0
5	B	29	0	13	1	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	A	21	0	0	0	0
7	B	26	0	0	1	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	P	1	0	0	0	0
7	T	2	0	0	0	0
All	All	18886	0	17641	252	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 7.

All (252) 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:367:ARG:HH12	1:A:401:GLU:HG3	1.50	0.77
1:B:810:LYS:HA	1:B:813:ILE:HD12	1.67	0.75
1:A:693:LYS:HD2	1:A:694:MET:H	1.50	0.75
1:A:1094:SER:HB3	1:A:1107:ILE:HD12	1.71	0.73
1:A:454:LEU:HD23	1:A:459:MET:HG3	1.71	0.73
1:A:1097:PRO:HD2	1:A:1105:ARG:HG2	1.73	0.69
1:B:260:ARG:HB2	1:B:263:LYS:HD2	1.74	0.69
1:A:33:SER:O	1:A:37:LEU:N	2.20	0.69
1:B:608:THR:HG1	1:B:894:THR:HG1	1.34	0.67
1:A:1092:ILE:HG23	1:A:1109:VAL:HG12	1.76	0.66
1:B:953:MET:HG3	1:B:971:VAL:HG22	1.74	0.66
1:B:234:ASP:OD1	1:B:235:ALA:N	2.29	0.65
1:A:1042:LEU:HD11	1:A:1143:TRP:HH2	1.62	0.64
1:A:37:LEU:HD21	1:A:113:GLY:HA3	1.80	0.63
1:B:1137:ILE:HD12	1:B:1137:ILE:H	1.64	0.63
1:A:704:LEU:HD11	1:A:738:ARG:HG3	1.79	0.63
1:A:1116:ILE:HD12	1:A:1116:ILE:H	1.64	0.63
1:A:458:LEU:HD22	1:A:462:TYR:HE1	1.63	0.63
1:B:1013:GLU:N	1:B:1013:GLU:OE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:PRO:O	1:B:1120:ARG:HG2	1.99	0.62
1:B:1097:PRO:HG3	1:B:1127:THR:HA	1.82	0.62
2:C:10:DT:H2"	2:C:11:DOC:H5'	1.82	0.61
1:B:539:ILE:HD12	1:B:539:ILE:H	1.65	0.61
1:A:704:LEU:HA	1:A:707:GLU:HG3	1.82	0.61
1:B:978:LEU:HD21	1:B:981:LEU:HB2	1.83	0.61
1:A:153:GLU:HG2	1:A:167:LEU:HD21	1.83	0.61
1:A:459:MET:HG2	1:A:470:LEU:HD11	1.83	0.60
1:A:37:LEU:HD23	1:A:86:LEU:HB3	1.85	0.59
1:B:209:ILE:HG21	1:B:239:ILE:HD12	1.84	0.59
1:A:539:ILE:H	1:A:539:ILE:HD12	1.68	0.59
1:A:1137:ILE:HD12	1:A:1137:ILE:H	1.66	0.59
1:B:732:VAL:HA	1:B:735:ILE:HD12	1.85	0.59
1:B:1011:THR:HG23	1:B:1014:GLY:H	1.68	0.58
1:B:630:ARG:HH12	1:B:886:SER:HB2	1.68	0.58
1:A:310:MET:HE1	1:A:471:SER:HA	1.84	0.58
1:B:910:LEU:O	1:B:914:VAL:HG23	2.04	0.57
1:B:750:VAL:HG12	1:B:751:LYS:HG3	1.85	0.57
1:B:584:LEU:HD11	1:B:864:LEU:HD11	1.87	0.57
1:A:693:LYS:NZ	1:A:694:MET:HB2	2.19	0.57
1:B:112:GLN:OE1	1:B:198:GLN:NE2	2.37	0.56
1:A:356:VAL:O	1:A:360:GLN:HG3	2.05	0.56
1:A:540:GLU:HB2	1:A:547:LEU:HD11	1.87	0.56
1:A:553:TYR:HE2	1:A:851:CYS:HG	1.53	0.56
1:B:864:LEU:O	1:B:868:VAL:HG12	2.04	0.56
1:A:656:PRO:HG2	1:A:841:TRP:HB3	1.88	0.56
1:B:682:LYS:HG2	1:B:759:GLU:HG3	1.86	0.56
1:B:611:GLU:O	1:B:615:ASN:N	2.29	0.56
1:A:28:ASN:O	1:A:32:LEU:N	2.27	0.56
1:B:468:GLN:O	1:B:472:GLU:HG3	2.06	0.56
1:B:426:VAL:HA	1:B:430:SER:HB3	1.88	0.55
1:A:475:VAL:O	1:A:479:VAL:HG13	2.06	0.55
1:B:904:SER:O	1:B:907:CYS:N	2.40	0.55
1:B:1079:GLU:OE2	1:B:1079:GLU:N	2.28	0.55
1:B:51:GLY:O	1:B:128:SER:OG	2.25	0.54
1:B:588:LEU:O	1:B:592:LEU:HB2	2.07	0.54
1:B:895:LEU:HB3	1:B:897:ASN:OD1	2.07	0.54
1:B:1072:ARG:HB3	1:B:1126:TRP:CZ2	2.42	0.54
1:A:1013:GLU:OE1	1:A:1013:GLU:N	2.40	0.54
1:B:794:ASN:O	1:B:798:ILE:HD12	2.08	0.53
1:B:549:GLU:OE1	1:B:751:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:TRP:HZ3	1:A:1045:LEU:HD21	1.74	0.53
1:B:656:PRO:HG2	1:B:841:TRP:HB3	1.90	0.52
1:A:730:ASP:HA	1:A:733:ILE:HD12	1.91	0.52
1:A:891:TYR:HB2	1:A:903:LEU:HD23	1.90	0.52
1:A:354:ASP:OD1	1:A:354:ASP:N	2.38	0.52
1:A:458:LEU:HD22	1:A:462:TYR:CE1	2.45	0.52
3:D:11:DC:H2"	3:D:12:DG:C8	2.45	0.51
1:A:321:LEU:HB3	1:A:349:ILE:HD13	1.92	0.51
1:B:580:ALA:HB2	1:B:867:ARG:HE	1.76	0.51
1:A:539:ILE:HD13	1:A:728:TYR:HE2	1.75	0.51
1:A:693:LYS:HZ2	1:A:694:MET:HB2	1.76	0.51
1:A:921:HIS:ND1	1:A:938:SER:OG	2.39	0.51
1:A:440:LYS:O	1:A:444:GLN:HG3	2.11	0.51
1:B:423:PHE:CE2	1:B:427:LYS:HD2	2.46	0.51
1:A:737:LYS:O	1:A:740:THR:OG1	2.28	0.51
1:A:177:MET:HE1	1:A:186:LYS:HB2	1.92	0.50
1:B:600:ASN:HB3	1:B:901:LEU:HD13	1.93	0.50
1:A:291:ILE:HG21	1:A:387:ILE:HD11	1.94	0.50
1:B:904:SER:O	1:B:905:TYR:C	2.50	0.50
1:A:468:GLN:O	1:A:472:GLU:HG3	2.11	0.50
1:A:1101:PRO:HB2	1:A:1104:GLU:HG3	1.93	0.50
1:A:693:LYS:CD	1:A:694:MET:H	2.22	0.49
1:A:858:ILE:HD11	1:A:879:ILE:HG13	1.94	0.49
1:B:296:PRO:HB2	1:B:299:LYS:HB2	1.94	0.49
1:A:1118:ILE:H	1:A:1118:ILE:HD12	1.77	0.49
1:B:905:TYR:O	1:B:909:MET:HG3	2.11	0.49
1:A:989:ARG:HH21	2:P:8:DG:P	2.36	0.49
1:A:1124:ARG:HA	1:A:1127:THR:HG22	1.93	0.49
1:A:1178:ASP:O	1:A:1182:ARG:HG3	2.13	0.49
1:B:213:ASN:ND2	1:B:237:HIS:HA	2.28	0.49
1:B:781:ARG:NH2	1:B:820:GLN:OE1	2.46	0.49
1:A:1040:GLU:O	1:A:1043:VAL:HG22	2.13	0.48
1:B:951:LYS:HB2	1:B:974:GLU:HA	1.94	0.48
1:B:1181:LYS:O	1:B:1184:ILE:HG13	2.13	0.48
1:A:112:GLN:HG2	1:A:195:ASN:HD21	1.78	0.48
1:A:1145:TYR:OH	1:A:1149:ARG:NH1	2.46	0.48
1:B:338:THR:HG23	1:B:344:PRO:HA	1.94	0.48
1:A:693:LYS:HD2	1:A:694:MET:N	2.25	0.48
1:B:379:GLY:HA2	1:B:383:ASP:HB2	1.96	0.48
1:A:1150:LEU:O	1:A:1154:ILE:HG13	2.13	0.48
1:B:708:THR:HB	1:B:720:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:ALA:O	1:B:867:ARG:HG3	2.13	0.47
1:B:287:MET:HG3	1:B:315:ILE:HG12	1.97	0.47
1:A:1023:CYS:HB3	1:A:1154:ILE:HD13	1.94	0.47
1:B:994:LEU:HD21	1:B:1030:LEU:HD11	1.95	0.47
1:A:1026:TRP:CZ3	1:A:1045:LEU:HD21	2.50	0.47
1:A:1116:ILE:N	1:A:1117:PRO:HD2	2.29	0.47
1:A:1127:THR:HG23	1:A:1129:ASP:H	1.78	0.47
1:B:638:HIS:HB3	1:B:947:ASP:HB2	1.96	0.47
1:B:865:VAL:O	1:B:869:GLY:N	2.41	0.47
1:B:887:PHE:CD1	1:B:888:PRO:HD2	2.50	0.47
1:B:354:ASP:OD1	1:B:354:ASP:N	2.46	0.47
1:B:64:PHE:CE1	1:B:273:ILE:HD11	2.50	0.47
1:A:1095:SER:O	1:A:1096:LYS:C	2.53	0.47
1:B:321:LEU:HD12	1:B:322:ILE:N	2.29	0.47
1:B:1068:THR:O	1:B:1072:ARG:HG3	2.15	0.47
1:A:295:LYS:NZ	1:A:299:LYS:H	2.13	0.46
1:B:608:THR:OG1	1:B:894:THR:OG1	2.21	0.46
1:A:1094:SER:O	1:A:1105:ARG:HB3	2.16	0.46
1:B:579:SER:OG	1:B:867:ARG:NH2	2.47	0.46
1:B:864:LEU:HD21	1:B:909:MET:HE3	1.96	0.46
1:A:798:ILE:HD13	1:A:805:ALA:HB1	1.97	0.46
1:B:736:LYS:O	1:B:740:THR:OG1	2.31	0.46
1:B:947:ASP:HB3	1:B:950:TYR:OH	2.15	0.46
1:A:539:ILE:HD13	1:A:728:TYR:CE2	2.50	0.46
1:B:454:LEU:HD23	1:B:459:MET:HG2	1.97	0.46
1:B:645:TYR:CG	5:B:1304:TTP:H2'1	2.51	0.46
1:B:1097:PRO:O	1:B:1100:ALA:HB3	2.15	0.46
1:B:278:LYS:HE3	1:B:278:LYS:HB3	1.83	0.46
1:A:1136:ASP:OD1	1:A:1138:ARG:N	2.36	0.46
1:B:496:LEU:HG	1:B:500:ILE:HD12	1.97	0.46
1:B:591:ALA:HA	1:B:912:TYR:CD1	2.51	0.46
1:B:1042:LEU:HD11	1:B:1143:TRP:HH2	1.80	0.46
1:A:1005:VAL:HG21	1:A:1022:VAL:HG21	1.98	0.45
1:A:960:GLU:HG2	1:A:963:LYS:HG3	1.98	0.45
1:A:1155:GLN:HB3	1:A:1160:ILE:HD12	1.97	0.45
1:B:810:LYS:O	1:B:814:VAL:HG23	2.17	0.45
1:B:928:ASP:HB3	1:B:933:ILE:HB	1.97	0.45
1:A:261:VAL:HG11	1:A:504:PRO:HD3	1.98	0.45
1:A:459:MET:HG2	1:A:470:LEU:CD1	2.46	0.45
1:A:1097:PRO:HB2	1:A:1100:ALA:HB3	1.99	0.45
1:A:561:LEU:HD13	1:A:871:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:LEU:HD11	1:A:1174:VAL:HG23	1.97	0.45
1:B:1094:SER:O	1:B:1105:ARG:HD2	2.16	0.45
1:A:458:LEU:C	1:A:461:PRO:HD2	2.37	0.45
1:B:858:ILE:HD11	1:B:879:ILE:HG13	1.98	0.45
1:A:947:ASP:OD1	1:A:947:ASP:N	2.49	0.45
1:A:1112:PHE:CD1	1:A:1137:ILE:HG13	2.52	0.45
1:B:568:SER:OG	1:B:951:LYS:HA	2.17	0.45
1:A:1101:PRO:HD2	1:A:1104:GLU:OE1	2.17	0.45
1:A:356:VAL:HG23	1:A:394:HIS:HB3	1.99	0.44
1:A:701:LYS:O	1:A:705:GLN:HG3	2.17	0.44
1:A:1112:PHE:HA	1:A:1119:LYS:HD3	1.99	0.44
1:B:597:GLU:HA	1:B:602:SER:O	2.17	0.44
1:A:309:MET:HB2	1:A:310:MET:HG2	1.98	0.44
1:A:678:ALA:HB1	1:A:761:ILE:HG23	1.99	0.44
1:B:365:HIS:O	1:B:369:VAL:HG22	2.16	0.44
1:B:905:TYR:N	1:B:906:PRO:HD2	2.32	0.44
1:A:157:LYS:O	1:A:161:GLU:HG2	2.18	0.44
1:A:676:THR:OG1	1:A:677:CYS:N	2.50	0.44
1:A:32:LEU:O	1:A:36:GLN:HG3	2.18	0.44
1:A:326:GLU:HG3	1:A:353:ASN:O	2.17	0.44
1:A:365:HIS:O	1:A:369:VAL:HG22	2.17	0.44
1:B:981:LEU:HD21	1:B:986:LEU:HD23	2.00	0.44
1:A:485:TYR:CE2	1:A:490:HIS:HB2	2.53	0.44
1:A:1037:LEU:HD22	1:A:1041:ASP:HB2	1.98	0.44
1:A:291:ILE:O	1:A:291:ILE:HG13	2.17	0.44
1:B:291:ILE:HG22	1:B:311:ILE:HG12	2.00	0.44
1:B:817:ASP:O	1:B:820:GLN:HG3	2.17	0.44
1:A:978:LEU:HD21	1:A:981:LEU:HB2	2.00	0.44
1:A:1039:ASP:O	1:A:1043:VAL:HG13	2.17	0.44
1:B:1112:PHE:CD2	1:B:1137:ILE:HG13	2.53	0.44
1:A:1030:LEU:HD23	1:A:1030:LEU:HA	1.79	0.43
1:A:32:LEU:O	1:A:32:LEU:HD12	2.17	0.43
1:A:321:LEU:HD12	1:A:322:ILE:N	2.34	0.43
1:B:617:ILE:HG12	1:B:888:PRO:HB3	2.01	0.43
1:A:373:VAL:HG11	1:A:485:TYR:CZ	2.54	0.43
1:B:568:SER:O	1:B:633:LEU:HD22	2.18	0.43
1:B:1102:VAL:HG23	7:B:1423:HOH:O	2.19	0.43
1:A:295:LYS:HB2	1:A:301:PRO:HG3	2.00	0.43
1:B:889:GLU:HB3	1:B:890:THR:H	1.65	0.43
1:B:1112:PHE:HA	1:B:1119:LYS:HD3	2.01	0.43
1:A:325:ARG:NE	1:A:328:ILE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD21	1:A:986:LEU:HD23	2.01	0.43
1:B:64:PHE:CE1	1:B:270:GLN:HB3	2.54	0.43
1:B:235:ALA:HA	1:B:238:LEU:CD1	2.49	0.43
1:B:639:VAL:HA	1:B:945:GLU:O	2.19	0.43
1:A:367:ARG:NH1	1:A:401:GLU:HG3	2.25	0.43
1:A:645:TYR:CG	5:A:1204:TTP:H2'1	2.54	0.43
1:A:736:LYS:O	1:A:740:THR:HG23	2.19	0.43
1:A:982:LYS:HB3	2:P:10:DT:H5"	2.00	0.43
1:A:458:LEU:HB3	1:A:462:TYR:CD1	2.53	0.43
1:A:355:GLU:OE2	1:A:390:ARG:HD2	2.18	0.42
1:A:1097:PRO:HD3	1:A:1127:THR:HA	2.00	0.42
1:A:1002:ILE:HD11	1:A:1019:VAL:HG13	2.00	0.42
1:A:694:MET:O	1:A:697:TYR:N	2.52	0.42
1:A:260:ARG:HB2	1:A:263:LYS:HD2	2.01	0.42
1:A:835:MET:SD	1:A:844:MET:HA	2.59	0.42
1:B:460:THR:HB	1:B:461:PRO:HD3	2.02	0.42
1:A:737:LYS:O	1:A:741:GLU:HG3	2.20	0.42
1:A:794:ASN:O	1:A:798:ILE:HG13	2.19	0.42
1:A:1093:ILE:HD13	1:A:1093:ILE:HA	1.84	0.42
1:A:986:LEU:HA	1:A:996:LYS:HG2	2.01	0.42
1:B:373:VAL:HG11	1:B:485:TYR:CZ	2.54	0.42
1:B:813:ILE:O	1:B:817:ASP:HB2	2.19	0.42
1:B:905:TYR:N	1:B:906:PRO:CD	2.83	0.42
1:B:1083:LYS:HG3	1:B:1084:ASP:N	2.35	0.42
1:A:968:ARG:HG3	1:A:983:GLY:HA3	2.01	0.42
1:A:1123:LEU:O	1:A:1127:THR:HG22	2.20	0.42
1:A:951:LYS:HB2	1:A:974:GLU:HA	2.00	0.41
1:A:1025:ARG:O	1:A:1029:VAL:HG23	2.20	0.41
1:A:1103:THR:HG23	3:T:13:DG:O3'	2.20	0.41
1:B:201:GLU:O	1:B:205:LEU:HG	2.20	0.41
1:A:296:PRO:HG2	1:A:299:LYS:CB	2.50	0.41
1:A:294:THR:HA	1:A:309:MET:HE3	2.00	0.41
1:A:485:TYR:CZ	1:A:490:HIS:HB2	2.55	0.41
1:A:1111:ILE:O	1:A:1119:LYS:HG3	2.20	0.41
1:B:32:LEU:O	1:B:36:GLN:HG3	2.21	0.41
1:B:596:VAL:O	1:B:602:SER:N	2.53	0.41
1:A:244:GLU:HG2	1:A:531:LEU:HB2	2.02	0.41
1:A:337:TYR:CE2	1:A:476:SER:HA	2.54	0.41
1:A:288:ALA:HA	1:A:375:SER:O	2.21	0.41
1:A:1026:TRP:HB3	1:A:1150:LEU:HD21	2.01	0.41
1:A:1136:ASP:OD1	1:A:1137:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:LEU:HD23	1:B:689:PHE:HB3	2.01	0.41
1:A:700:ILE:O	1:A:704:LEU:HD13	2.20	0.41
1:B:915:HIS:HE1	1:B:940:ASN:O	2.04	0.41
1:B:492:PHE:CZ	1:B:822:ALA:HB1	2.55	0.41
1:A:82:MET:HA	1:A:118:ASP:O	2.20	0.41
1:B:431:TYR:HD2	1:B:821:LEU:HB3	1.85	0.41
1:A:500:ILE:HD13	1:A:515:LEU:HD22	2.03	0.41
1:A:700:ILE:HD12	1:A:700:ILE:H	1.86	0.41
1:A:798:ILE:HB	1:A:806:ARG:HD2	2.02	0.41
1:A:1137:ILE:HG22	1:A:1141:ILE:HD11	2.02	0.41
1:B:876:THR:CB	2:C:11:DOC:H2"	2.51	0.41
1:B:1056:LEU:HD11	1:B:1067:ILE:HG23	2.02	0.41
1:A:606:LYS:HA	1:A:606:LYS:HD3	1.84	0.41
1:A:322:ILE:HA	1:A:350:PHE:O	2.21	0.40
1:A:322:ILE:HB	1:A:358:LEU:HD12	2.02	0.40
1:A:423:PHE:CE2	1:A:427:LYS:HD3	2.56	0.40
1:B:594:PHE:CE1	1:B:599:GLU:HG3	2.56	0.40
1:A:1056:LEU:HD21	1:A:1071:ARG:HG3	2.03	0.40
1:B:760:ALA:HB3	1:B:849:ILE:HD11	2.02	0.40
1:B:831:TYR:O	1:B:834:VAL:HG22	2.20	0.40
1:A:68:ASP:OD1	1:A:68:ASP:N	2.54	0.40
1:A:420:MET:HE1	1:A:508:LEU:HB2	2.04	0.40
1:A:836:ARG:HB2	3:T:5:DA:H4'	2.04	0.40
1:B:50:MET:HG3	1:B:416:TYR:CZ	2.56	0.40
1:A:309:MET:HE2	1:A:460:THR:HA	2.03	0.40
1:B:164:LEU:HD21	1:B:167:LEU:HB2	2.02	0.40
1:B:329:SER:OG	1:B:330:GLU:HG3	2.22	0.40
1:B:697:TYR:CE2	1:B:735:ILE:HG21	2.57	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	1108/1191 (93%)	1066 (96%)	41 (4%)	1 (0%)	51 75
1	B	1113/1191 (94%)	1070 (96%)	41 (4%)	2 (0%)	47 71
All	All	2221/2382 (93%)	2136 (96%)	82 (4%)	3 (0%)	51 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1096	LYS
1	B	664	ASP
1	B	589	PRO

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	953/1066 (89%)	936 (98%)	17 (2%)	59 80
1	B	928/1066 (87%)	900 (97%)	28 (3%)	41 67
All	All	1881/2132 (88%)	1836 (98%)	45 (2%)	49 74

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	64	PHE
1	A	65	ASP
1	A	145	ASP
1	A	150	ASN
1	A	162	SER
1	A	372	THR
1	A	383	ASP
1	A	605	ASP
1	A	640	ASP
1	A	743	SER
1	A	753	SER
1	A	783	GLU

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Mol	Chain	Res	Type
1	A	1063	LYS
1	A	1066	SER
1	A	1076	PHE
1	A	1095	SER
1	B	115	SER
1	B	358	LEU
1	B	361	ARG
1	B	414	SER
1	B	474	SER
1	B	540	GLU
1	B	544	ASP
1	B	595	SER
1	B	603	SER
1	B	618	THR
1	B	631	ASN
1	B	640	ASP
1	B	653	ARG
1	B	676	THR
1	B	695	ASP
1	B	716	SER
1	B	722	THR
1	B	727	SER
1	B	783	GLU
1	B	801	SER
1	B	896	GLU
1	B	907	CYS
1	B	1032	SER
1	B	1064	SER
1	B	1076	PHE
1	B	1095	SER
1	B	1138	ARG
1	B	1168	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	112	GLN
1	B	198	GLN
1	B	250	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	0.40	0	20,26,29	0.36	0
2	DOC	C	11	3,2	16,19,20	0.40	0	20,26,29	0.31	0

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	DOC	C3'-C4'-C5'-O5'
2	C	11	DOC	O4'-C4'-C5'-O5'
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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	DOC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	ACT	A	1205	4	3,3,3	1.26	0	3,3,3	1.35	0
5	TTP	B	1304	4	26,30,30	0.55	0	39,47,47	0.55	0
6	ACT	B	1305	4	3,3,3	1.31	0	3,3,3	1.31	0
5	TTP	A	1204	4	26,30,30	0.57	0	39,47,47	0.54	0

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
5	TTP	B	1304	4	-	5/22/34/34	0/2/2/2
5	TTP	A	1204	4	-	2/22/34/34	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

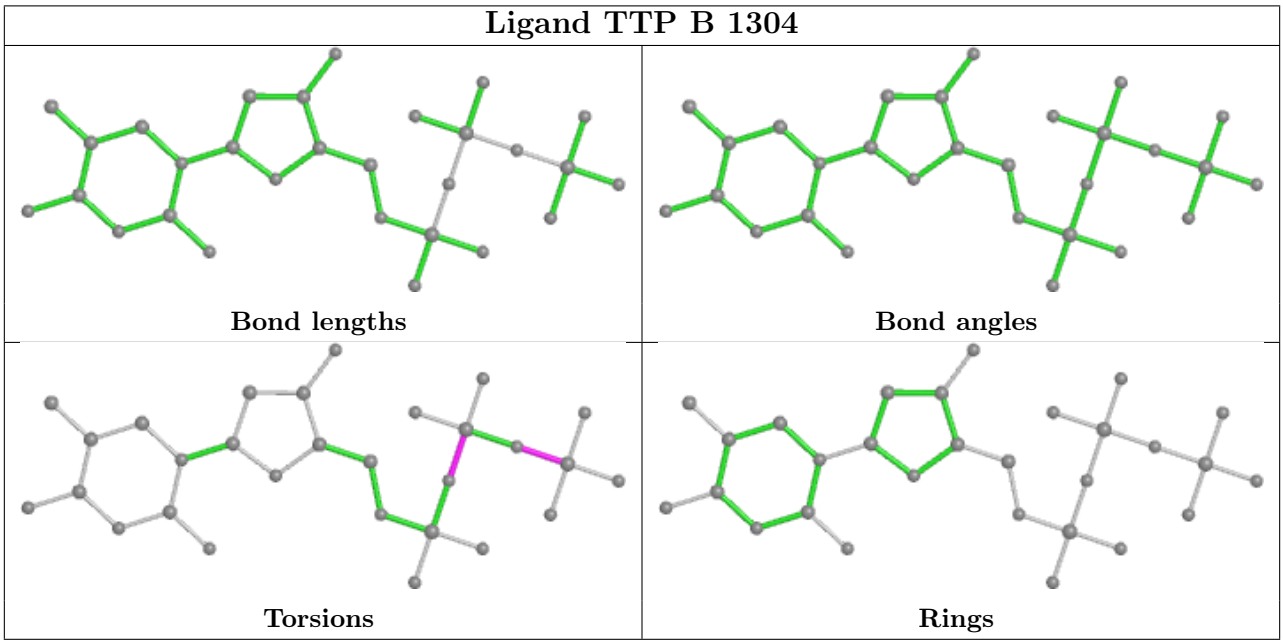
Mol	Chain	Res	Type	Atoms
5	B	1304	TTP	PB-O3B-PG-O1G
5	A	1204	TTP	PB-O3B-PG-O3G
5	B	1304	TTP	PA-O3A-PB-O1B
5	B	1304	TTP	PB-O3B-PG-O2G
5	B	1304	TTP	PB-O3B-PG-O3G
5	A	1204	TTP	PB-O3A-PA-O2A
5	B	1304	TTP	PA-O3A-PB-O2B

There are no ring outliers.

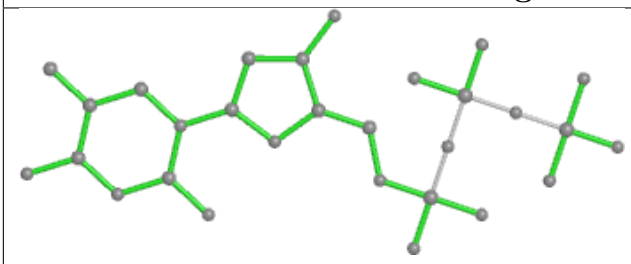
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1304	TTP	1	0
5	A	1204	TTP	1	0

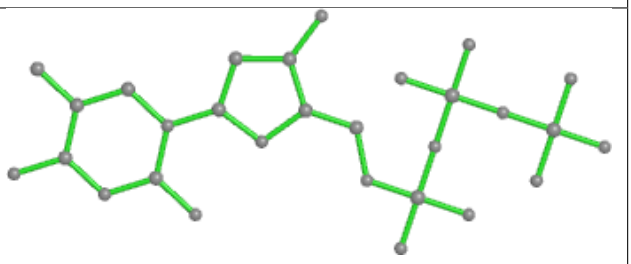
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



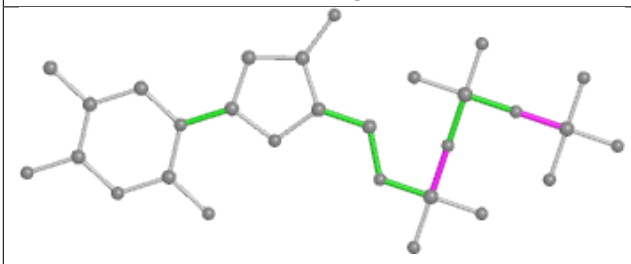
Ligand TTP A 1204



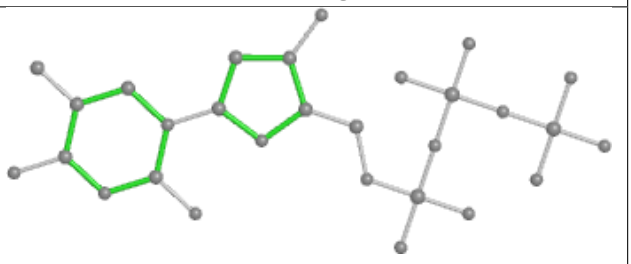
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	1118/1191 (93%)	0.02	14 (1%) 77 73	32, 63, 91, 108	0
1	B	1121/1191 (94%)	0.05	17 (1%) 73 70	33, 65, 97, 114	0
2	C	10/11 (90%)	-0.28	0 100 100	38, 52, 69, 70	0
2	P	10/11 (90%)	-0.31	0 100 100	39, 53, 69, 71	0
3	D	15/16 (93%)	-0.25	0 100 100	35, 50, 69, 87	0
3	T	15/16 (93%)	-0.24	0 100 100	35, 49, 82, 88	0
All	All	2289/2436 (93%)	0.03	31 (1%) 75 71	32, 64, 94, 114	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	596	VAL	4.9
1	B	716	SER	4.1
1	B	602	SER	3.8
1	B	613	ILE	3.3
1	B	894	THR	3.0
1	B	592	LEU	2.9
1	B	539	ILE	2.9
1	B	893	PHE	2.8
1	B	1063	LYS	2.8
1	A	64	PHE	2.7
1	A	308	ILE	2.6
1	B	697	TYR	2.6
1	A	469	HIS	2.6
1	A	328	ILE	2.5
1	A	1046	ILE	2.4
1	A	459	MET	2.4
1	B	901	LEU	2.4
1	A	225	VAL	2.4
1	A	300	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1128	LEU	2.3
1	B	608	THR	2.3
1	B	64	PHE	2.3
1	A	456	PRO	2.3
1	B	207	ARG	2.3
1	A	224	ASN	2.2
1	A	738	ARG	2.2
1	B	750	VAL	2.1
1	A	665	CYS	2.1
1	A	1056	LEU	2.1
1	B	1096	LYS	2.1
1	B	751	LYS	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, 95^{th} 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	0.16	28,36,52,53	0
2	DOC	C	11	18/19	0.99	0.17	24,38,49,52	0

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, 95^{th} 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	CA	A	1202	1/1	0.64	0.18	81,81,81,81	0
4	CA	A	1201	1/1	0.67	0.10	85,85,85,85	0
6	ACT	A	1205	4/4	0.83	0.17	66,82,83,91	0
4	CA	B	1303	1/1	0.84	0.12	72,72,72,72	0

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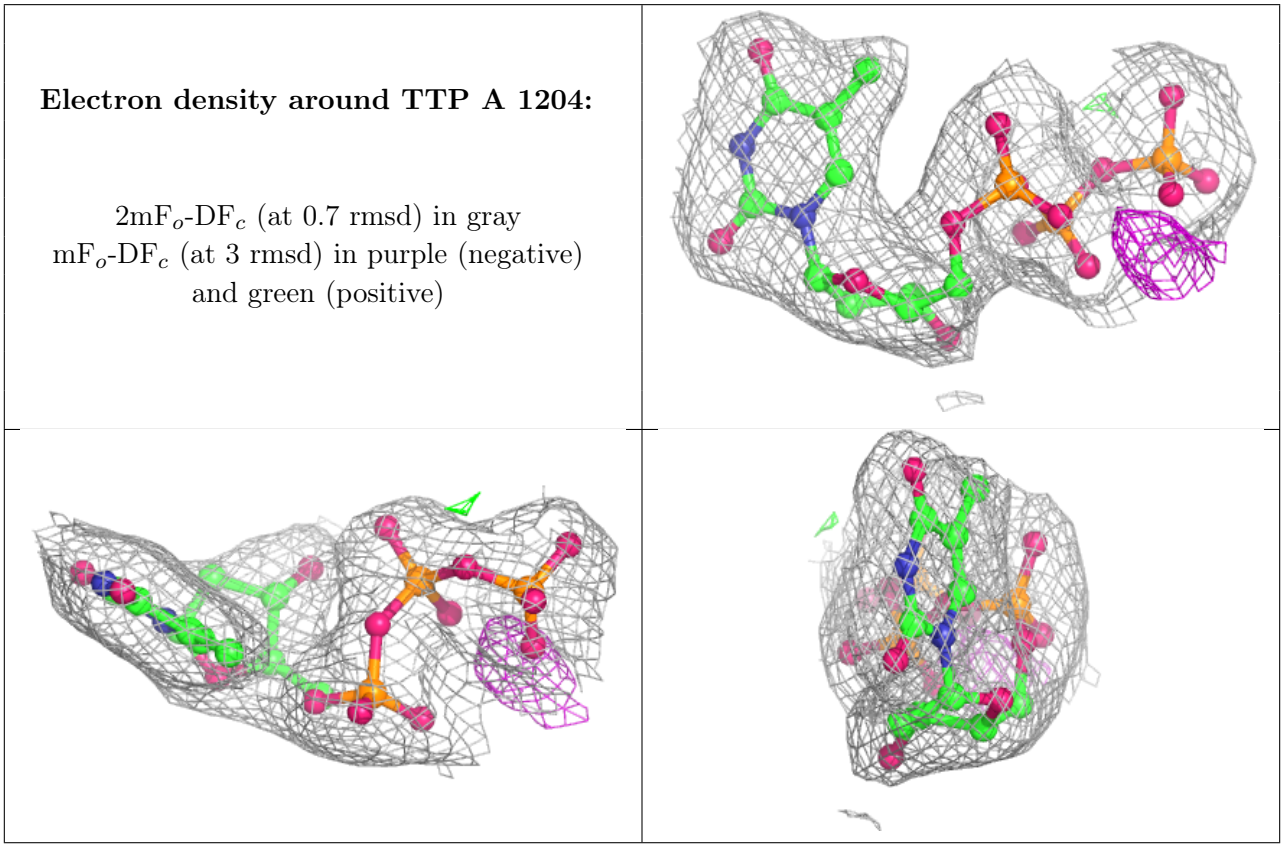
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	1302	1/1	0.92	0.08	84,84,84,84	0
4	CA	A	1203	1/1	0.93	0.07	48,48,48,48	0
6	ACT	B	1305	4/4	0.94	0.20	72,76,84,85	0
4	CA	B	1301	1/1	0.96	0.09	46,46,46,46	0
5	TTP	A	1204	29/29	0.97	0.16	29,39,47,59	0
5	TTP	B	1304	29/29	0.97	0.16	33,39,53,58	0

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.

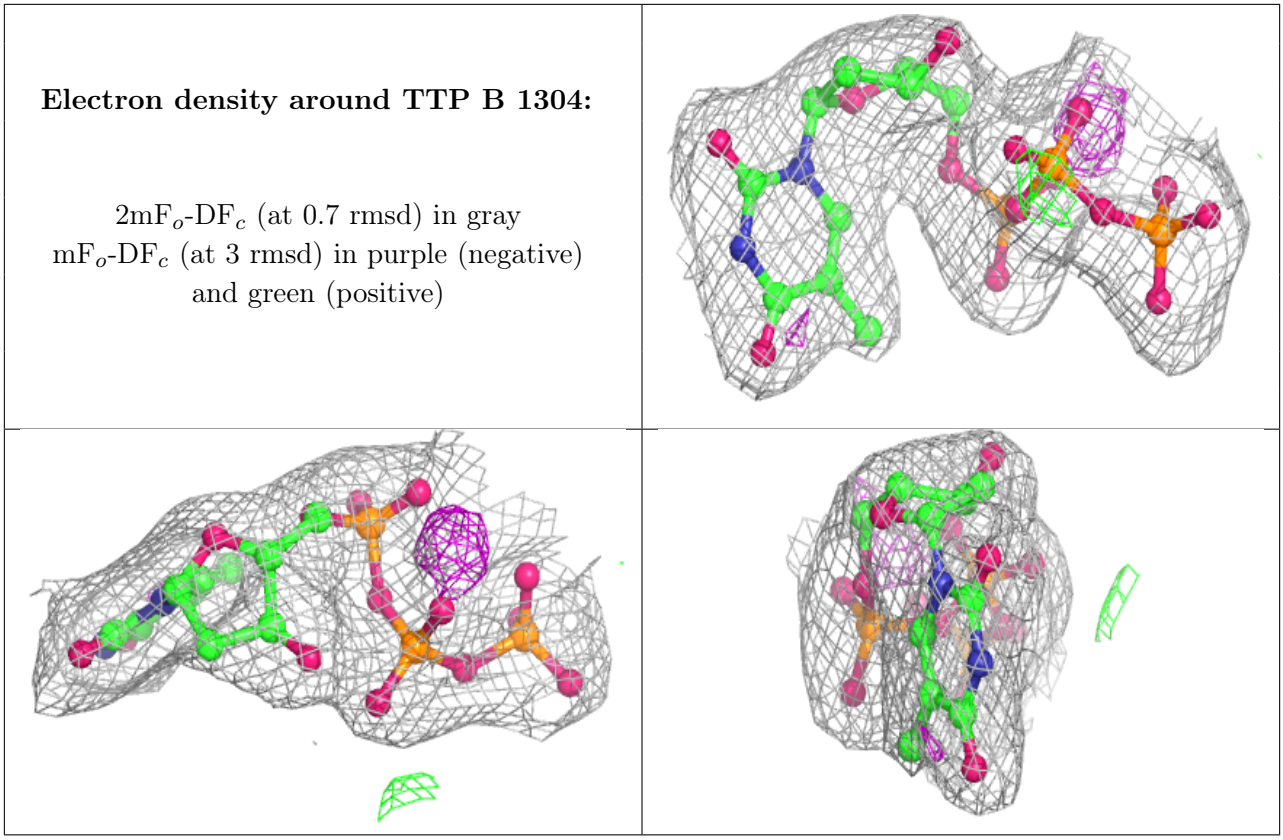
Electron density around TTP A 1204:

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



Electron density around TTP B 1304:

$2mF_o$-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.