Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 10:15 am BST

PDB ID	:	8B6K
Title	:	The crystal structure of M644G variant of DNA Pol Epsilon containing dCTP in the polymerase active site
Authors	:	Parkash, V.; Johansson, E.
Deposited on	:	2022-09-27
Resolution	:	2.50 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:

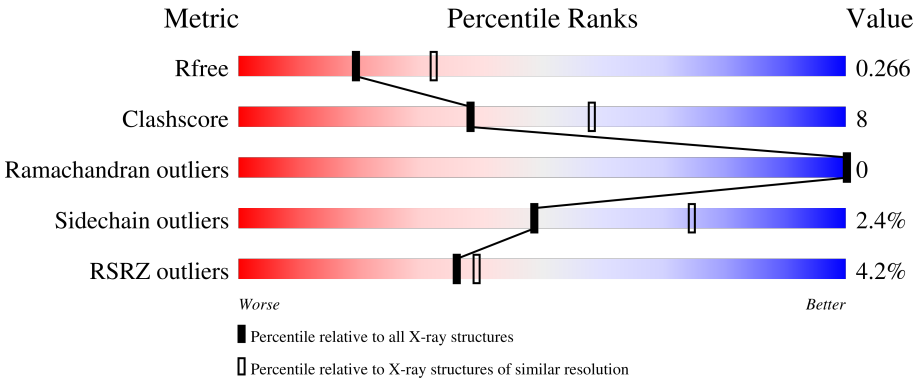
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	4% 75% 18% 7%
1	B	1191	4% 75% 18% 7%
2	C	11	64% 36%
2	P	11	64% 36%
3	D	16	56% 38% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	16	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18700 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	1108	Total	C	N	O	S	0	0	0
			8799	5650	1458	1649	42			
1	B	1108	Total	C	N	O	S	0	0	0
			8781	5630	1461	1648	42			

There are 16 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	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	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	290	ALA	ASP	engineered mutation	UNP P21951
B	292	ALA	GLU	engineered mutation	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	P	11	Total	C	N	O	P	3	0	0
			221	106	38	66	11			
2	C	11	Total	C	N	O	P	4	0	0
			221	106	38	66	11			

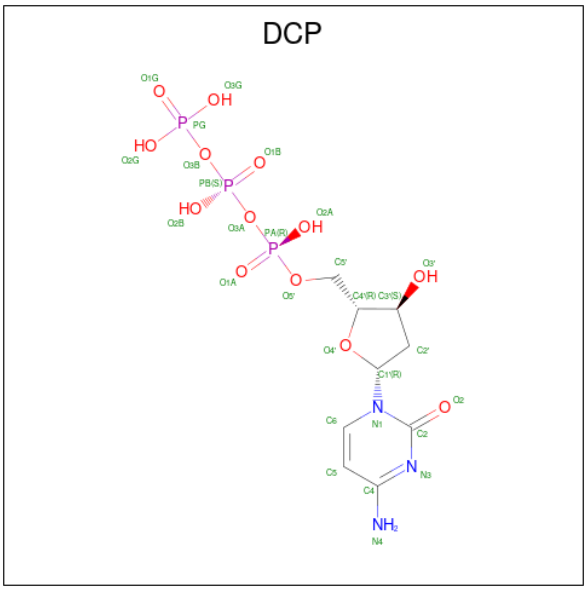
- Molecule 3 is a DNA chain called Template DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			310	147	57	91	15			
3	D	15	Total	C	N	O	P	0	0	0
			310	147	57	91	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



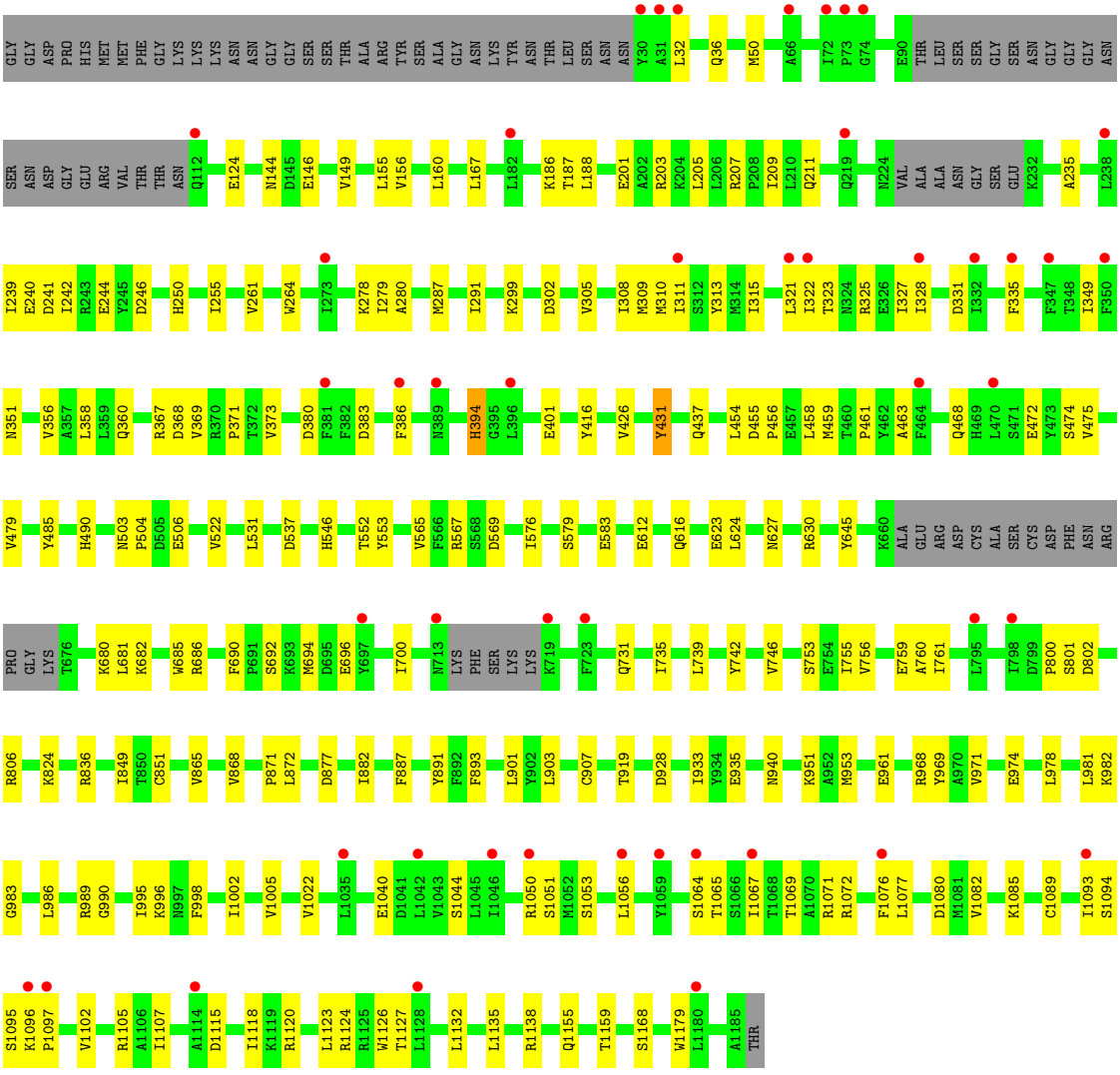
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
5	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

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.

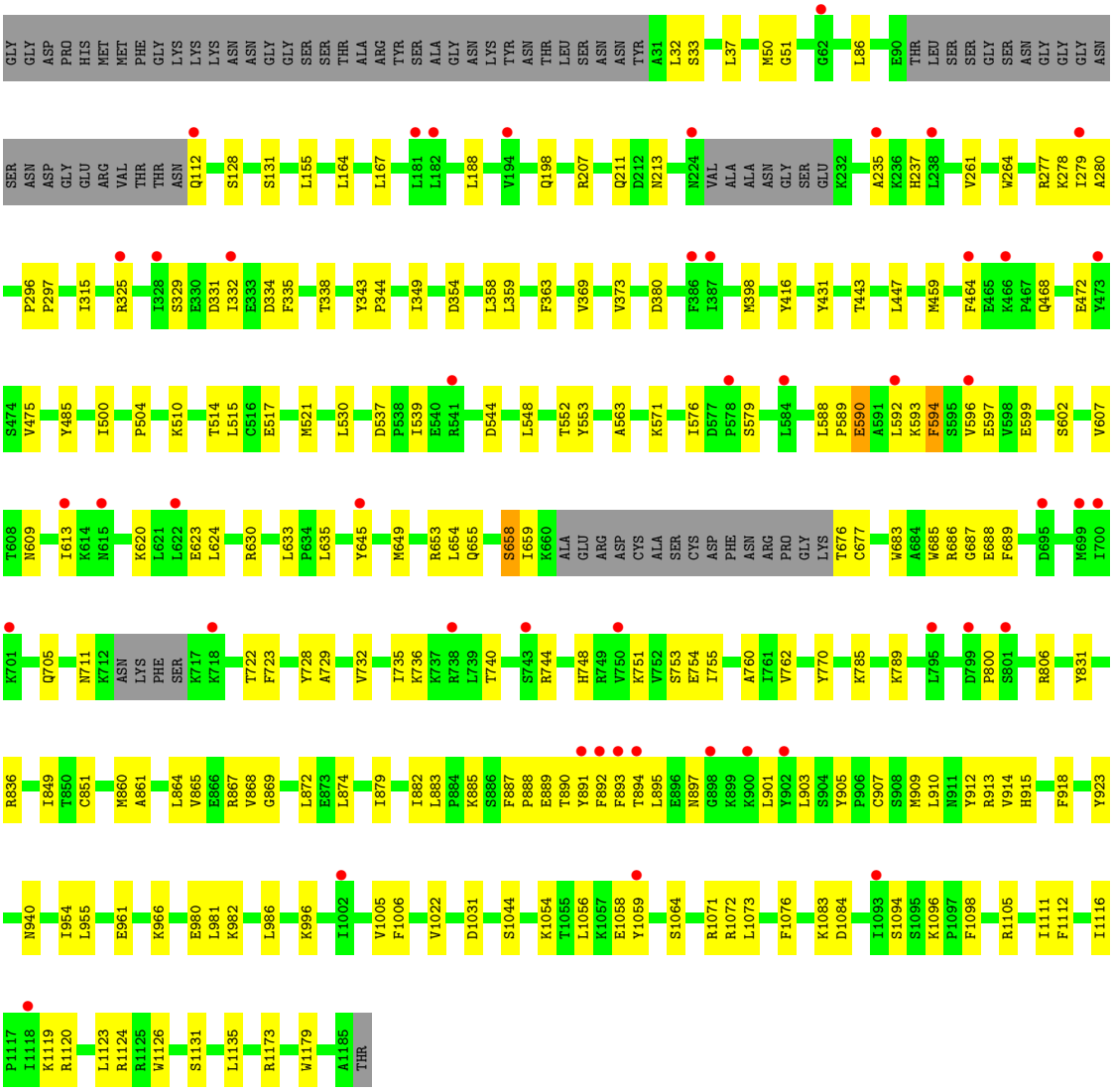
• Molecule 1: DNA polymerase epsilon catalytic subunit A

Chain A:



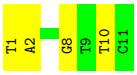
• Molecule 1: DNA polymerase epsilon catalytic subunit A

Chain B:



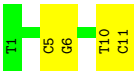
• Molecule 2: Primer DNA sequence

Chain P:



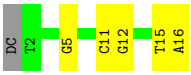
• Molecule 2: Primer DNA sequence

Chain C:



• Molecule 3: Template DNA sequence

Chain T:



• Molecule 3: Template DNA sequence

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.37Å 70.42Å 158.66Å 90.00° 112.69° 90.00°	Depositor
Resolution (Å)	86.72 – 2.50 86.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (86.72-2.50) 99.7 (86.72-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.260 0.237 , 0.266	Depositor DCC
R_{free} test set	5671 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18700	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 57.97 % 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 2.1906e-05. 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: DCP, DOC, CA

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	0.28	0/9003	0.49	0/12209
1	B	0.28	0/8983	0.48	0/12181
2	C	0.59	0/226	0.95	0/346
2	P	0.62	0/226	0.96	0/346
3	D	0.61	0/347	0.90	0/534
3	T	0.63	0/347	0.88	0/534
All	All	0.31	0/19132	0.53	0/26150

There are no bond length outliers.

There are no bond angle outliers.

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	8799	0	8472	130	0
1	B	8781	0	8439	138	0
2	C	221	0	125	2	0
2	P	221	0	125	3	0
3	D	310	0	170	6	0
3	T	310	0	170	3	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	28	0	12	2	0
5	B	28	0	12	3	0
All	All	18700	0	17525	275	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 8.

All (275) 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:1097:PRO:HD2	1:A:1105:ARG:HG2	1.38	1.02
1:A:1096:LYS:HB2	1:A:1097:PRO:HD3	1.51	0.92
1:B:655:GLN:HG3	1:B:658:SER:HB2	1.56	0.88
1:A:1096:LYS:HB3	1:A:1127:THR:HB	1.61	0.81
1:A:919:THR:HG22	1:A:940:ASN:HD22	1.47	0.80
1:B:597:GLU:HA	1:B:602:SER:O	1.82	0.78
1:A:455:ASP:HB3	1:A:458:LEU:HD12	1.65	0.77
1:A:1094:SER:HB2	1:A:1096:LYS:HG2	1.68	0.76
1:B:800:PRO:HA	1:B:806:ARG:HD2	1.67	0.75
1:B:164:LEU:HD21	1:B:167:LEU:HD12	1.68	0.74
1:B:1120:ARG:HG2	1:B:1135:LEU:HD11	1.72	0.72
1:A:454:LEU:HD12	1:A:459:MET:HG2	1.73	0.69
1:A:315:ILE:HG21	1:A:369:VAL:HG21	1.74	0.68
1:B:613:ILE:HD13	1:B:891:TYR:HB3	1.75	0.68
1:A:953:MET:HG3	1:A:971:VAL:HG22	1.75	0.68
1:A:1097:PRO:CD	1:A:1105:ARG:HG2	2.21	0.67
1:B:37:LEU:HG	1:B:86:LEU:HD23	1.77	0.66
1:A:1056:LEU:HB3	1:A:1082:VAL:HG11	1.77	0.65
1:A:1123:LEU:O	1:A:1127:THR:HG23	1.96	0.65
1:A:456:PRO:HA	1:A:459:MET:HG3	1.78	0.65
1:B:653:ARG:HG3	1:B:923:TYR:CE2	2.31	0.65
1:B:676:THR:O	1:B:677:CYS:HB3	1.97	0.65
1:A:335:PHE:HE1	1:A:349:ILE:HD11	1.60	0.65
1:B:329:SER:HB3	1:B:464:PHE:HD1	1.63	0.64
1:B:722:THR:HG22	1:B:723:PHE:N	2.13	0.64
1:A:279:ILE:HG13	1:A:280:ALA:H	1.64	0.63
1:B:155:LEU:HD12	1:B:235:ALA:HB3	1.80	0.63
1:A:309:MET:HG2	1:A:327:ILE:HG21	1.80	0.63
1:A:250:HIS:NE2	1:A:506:GLU:OE2	2.32	0.62
1:B:588:LEU:O	1:B:592:LEU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:893:PHE:HB2	1:B:901:LEU:HB2	1.80	0.62
1:A:1064:SER:OG	1:A:1067:ILE:HG13	1.99	0.61
1:B:981:LEU:HD21	1:B:986:LEU:HD23	1.81	0.61
1:B:1031:ASP:OD2	1:B:1173:ARG:NH2	2.33	0.60
1:B:315:ILE:HD13	1:B:369:VAL:HG11	1.84	0.60
1:B:539:ILE:HD12	1:B:539:ILE:H	1.68	0.59
1:B:872:LEU:HD11	1:B:882:ILE:HG23	1.83	0.59
1:A:627:ASN:HB2	1:A:630:ARG:NH1	2.18	0.59
1:B:539:ILE:HD13	1:B:728:TYR:HE2	1.67	0.59
1:A:356:VAL:O	1:A:360:GLN:HG3	2.03	0.58
1:A:681:LEU:HB2	1:A:849:ILE:HD13	1.85	0.58
1:B:728:TYR:O	1:B:732:VAL:HG13	2.03	0.58
1:A:308:ILE:HD11	1:A:358:LEU:HD21	1.85	0.58
1:B:1120:ARG:O	1:B:1124:ARG:HG3	2.04	0.57
1:A:731:GLN:O	1:A:735:ILE:HG13	2.05	0.57
1:A:1005:VAL:HG21	1:A:1022:VAL:HG21	1.85	0.57
1:A:291:ILE:HG22	1:A:311:ILE:HG12	1.86	0.57
2:C:10:DT:H2"	2:C:11:DOC:H5'	1.85	0.57
1:A:426:VAL:HG12	1:A:437:GLN:HG2	1.87	0.56
1:B:358:LEU:HD23	1:B:359:LEU:HD23	1.87	0.56
1:B:50:MET:HG3	1:B:416:TYR:CZ	2.42	0.55
1:B:861:ALA:O	1:B:865:VAL:HG23	2.06	0.55
1:B:443:THR:HG23	1:B:447:LEU:HD12	1.87	0.55
1:A:891:TYR:HB2	1:A:903:LEU:HD23	1.87	0.55
1:A:680:LYS:HE3	1:A:761:ILE:HD11	1.89	0.55
1:A:124:GLU:OE1	1:A:278:LYS:NZ	2.30	0.55
1:A:146:GLU:HG2	1:A:187:THR:HB	1.89	0.55
1:B:1056:LEU:HD21	1:B:1071:ARG:HG3	1.89	0.55
1:A:209:ILE:HG21	1:A:239:ILE:HD12	1.90	0.54
1:B:677:CYS:O	1:B:677:CYS:SG	2.64	0.54
1:A:503:ASN:OD1	1:A:506:GLU:HG3	2.08	0.54
1:A:287:MET:HE3	1:A:371:PRO:HG3	1.90	0.54
1:A:1115:ASP:HB3	1:A:1118:ILE:CD1	2.38	0.54
1:B:207:ARG:O	1:B:211:GLN:HG3	2.08	0.53
1:B:50:MET:HG3	1:B:416:TYR:CE2	2.43	0.53
1:B:112:GLN:OE1	1:B:198:GLN:NE2	2.42	0.53
1:B:905:TYR:O	1:B:909:MET:HB3	2.09	0.53
1:B:593:LYS:HA	1:B:596:VAL:HG22	1.91	0.53
1:A:800:PRO:HA	1:A:806:ARG:HD2	1.91	0.53
1:A:1124:ARG:HG2	1:A:1132:LEU:HB3	1.91	0.53
1:A:201:GLU:O	1:A:205:LEU:HG	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ILE:HG12	1:A:624:LEU:HD22	1.92	0.52
1:B:213:ASN:HD21	1:B:237:HIS:HA	1.73	0.52
1:A:1056:LEU:HB3	1:A:1082:VAL:CG1	2.40	0.52
1:B:334:ASP:OD1	1:B:349:ILE:HG12	2.09	0.52
1:B:688:GLU:OE1	1:B:751:LYS:HD3	2.09	0.52
1:B:954:ILE:HD13	1:B:1006:PHE:CD2	2.45	0.52
1:B:910:LEU:O	1:B:914:VAL:HG23	2.10	0.52
1:A:951:LYS:HB2	1:A:974:GLU:HA	1.91	0.52
1:B:683:TRP:HB3	1:B:849:ILE:HG13	1.92	0.52
1:B:1119:LYS:HG2	1:B:1123:LEU:HD11	1.91	0.52
1:A:325:ARG:NE	1:A:331:ASP:OD1	2.29	0.51
1:B:649:MET:HA	1:B:654:LEU:HB2	1.91	0.51
1:B:705:GLN:HG3	1:B:723:PHE:CD2	2.44	0.51
1:A:485:TYR:CZ	1:A:490:HIS:HB2	2.45	0.51
1:B:732:VAL:HA	1:B:735:ILE:HD12	1.92	0.51
1:A:865:VAL:HG12	1:A:871:PRO:HD3	1.91	0.51
1:B:329:SER:HB3	1:B:464:PHE:CD1	2.45	0.51
1:A:760:ALA:HB3	1:A:849:ILE:HD11	1.92	0.51
1:A:468:GLN:O	1:A:472:GLU:HG3	2.10	0.51
1:B:468:GLN:O	1:B:472:GLU:HG3	2.11	0.51
1:B:722:THR:CG2	1:B:723:PHE:N	2.74	0.51
1:B:966:LYS:HD3	3:D:9:DC:H5"	1.94	0.50
1:B:588:LEU:N	1:B:589:PRO:CD	2.75	0.50
1:B:213:ASN:ND2	1:B:237:HIS:HA	2.26	0.50
1:B:1005:VAL:HG21	1:B:1022:VAL:HG21	1.92	0.50
1:B:279:ILE:HG13	1:B:280:ALA:H	1.76	0.50
1:A:836:ARG:HB2	3:T:5:DG:H4'	1.93	0.50
1:A:261:VAL:HG11	1:A:504:PRO:HD3	1.93	0.50
1:B:590:GLU:HB3	1:B:912:TYR:CE1	2.47	0.49
1:B:594:PHE:CE1	1:B:915:HIS:CD2	3.00	0.49
1:A:203:ARG:HH21	1:A:207:ARG:NH2	2.09	0.49
1:A:155:LEU:HD12	1:A:235:ALA:HB3	1.93	0.49
1:B:864:LEU:O	1:B:868:VAL:HG12	2.12	0.49
1:B:961:GLU:HB2	1:B:1179:TRP:CD2	2.47	0.49
1:B:659:ILE:HD13	1:B:762:VAL:HG22	1.94	0.49
1:B:553:TYR:HE2	1:B:851:CYS:HG	1.61	0.48
1:B:1054:LYS:HE2	1:B:1059:TYR:CE1	2.48	0.48
3:D:2:DT:H2'	3:D:3:DC:O4'	2.13	0.48
1:A:928:ASP:HB3	1:A:933:ILE:HD12	1.96	0.48
1:B:980:GLU:HB3	1:B:982:LYS:HE3	1.94	0.48
1:B:645:TYR:CG	5:B:1202:DCP:H2'2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:MET:HA	1:B:654:LEU:HD12	1.95	0.48
1:A:264:TRP:CE3	1:A:278:LYS:HD3	2.48	0.48
1:B:332:ILE:HB	1:B:349:ILE:HG21	1.96	0.48
1:A:50:MET:HG3	1:A:416:TYR:CZ	2.49	0.48
1:A:986:LEU:HA	1:A:996:LYS:HG2	1.96	0.48
1:B:609:ASN:ND2	1:B:894:THR:OG1	2.46	0.48
1:B:1054:LYS:HE3	1:B:1058:GLU:HB2	1.95	0.47
1:B:1116:ILE:O	1:B:1120:ARG:HG3	2.14	0.47
1:A:645:TYR:CG	5:A:1202:DCP:H2'2	2.49	0.47
1:B:510:LYS:HD2	1:B:514:THR:HG21	1.95	0.47
1:B:986:LEU:HA	1:B:996:LYS:HG2	1.97	0.47
1:A:299:LYS:HE3	1:A:1077:LEU:HD22	1.96	0.47
1:A:552:THR:HG22	1:A:553:TYR:N	2.29	0.47
1:B:1072:ARG:HB3	1:B:1126:TRP:CZ2	2.48	0.47
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.49	0.47
1:B:918:PHE:O	1:B:940:ASN:ND2	2.48	0.47
1:B:1096:LYS:HG2	1:B:1098:PHE:CE1	2.49	0.47
1:A:246:ASP:OD1	1:A:246:ASP:N	2.48	0.47
1:B:751:LYS:HE3	1:B:751:LYS:HB2	1.53	0.47
1:A:475:VAL:O	1:A:479:VAL:HG23	2.15	0.47
1:A:872:LEU:HD11	1:A:882:ILE:HG23	1.95	0.47
1:A:1072:ARG:HB3	1:A:1126:TRP:CZ2	2.50	0.47
1:B:500:ILE:HD13	1:B:515:LEU:HD22	1.97	0.47
1:A:156:VAL:HG23	1:A:167:LEU:HD11	1.97	0.47
1:A:244:GLU:HG2	1:A:531:LEU:HB2	1.97	0.47
1:A:868:VAL:HG11	1:A:887:PHE:CE1	2.50	0.47
1:A:1069:THR:HB	1:A:1089:CYS:HB3	1.97	0.47
1:B:33:SER:HB2	1:B:86:LEU:HD21	1.96	0.47
1:B:592:LEU:HD11	1:B:903:LEU:HD21	1.97	0.47
1:A:978:LEU:HD21	1:A:981:LEU:HB2	1.97	0.46
5:B:1202:DCP:H6	5:B:1202:DCP:O5'	2.16	0.46
1:B:1112:PHE:CE1	1:B:1123:LEU:HD21	2.50	0.46
1:A:1082:VAL:HG12	1:A:1082:VAL:O	2.15	0.46
1:A:685:TRP:HE3	1:A:756:VAL:HG12	1.81	0.46
1:A:696:GLU:O	1:A:700:ILE:HD12	2.15	0.46
1:B:860:MET:HE1	1:B:914:VAL:HG22	1.98	0.46
1:A:160:LEU:HD23	1:A:205:LEU:HD12	1.97	0.46
1:A:990:GLY:O	1:A:996:LYS:HE3	2.15	0.46
1:A:1120:ARG:HB2	1:A:1135:LEU:HD11	1.98	0.46
1:B:32:LEU:HD12	1:B:32:LEU:H	1.81	0.46
1:B:895:LEU:HD23	1:B:895:LEU:HA	1.82	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:GLN:HA	1:B:723:PHE:CB	2.45	0.45
1:B:459:MET:HE3	1:B:459:MET:HB3	1.84	0.45
1:A:310:MET:HB3	1:A:321:LEU:HD11	1.98	0.45
1:B:623:GLU:OE1	1:B:630:ARG:NH2	2.47	0.45
1:A:207:ARG:O	1:A:211:GLN:HG2	2.16	0.45
1:B:736:LYS:O	1:B:740:THR:HG23	2.16	0.45
1:A:203:ARG:HE	1:A:207:ARG:NH2	2.15	0.45
1:A:998:PHE:CE1	1:A:1002:ILE:HD13	2.51	0.45
1:B:594:PHE:CE2	1:B:599:GLU:HG3	2.51	0.45
1:A:968:ARG:HG3	1:A:983:GLY:HA3	1.99	0.45
1:A:1072:ARG:HD3	1:A:1126:TRP:CE2	2.52	0.45
1:A:1096:LYS:N	1:A:1096:LYS:HD2	2.32	0.45
1:A:431:TYR:OH	1:A:824:LYS:HE2	2.17	0.45
1:B:785:LYS:HB2	1:B:785:LYS:HE3	1.85	0.45
1:B:548:LEU:HD23	1:B:689:PHE:HB3	1.99	0.45
1:B:909:MET:O	1:B:913:ARG:HG3	2.16	0.45
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.81	0.45
1:A:313:TYR:HE1	1:A:322:ILE:HD12	1.82	0.45
1:B:705:GLN:HA	1:B:723:PHE:HB3	1.99	0.45
1:B:1119:LYS:O	1:B:1123:LEU:HD12	2.16	0.45
1:B:653:ARG:HG3	1:B:923:TYR:CZ	2.52	0.44
1:A:1050:ARG:NH1	1:A:1065:THR:OG1	2.50	0.44
1:A:579:SER:O	1:A:583:GLU:HG3	2.18	0.44
1:B:552:THR:OG1	3:D:7:DA:H5"	2.18	0.44
1:A:1094:SER:OG	1:A:1105:ARG:HB3	2.18	0.44
2:P:1:DT:H2"	2:P:2:DA:C8	2.53	0.44
1:A:1093:ILE:HD13	1:A:1102:VAL:HB	1.99	0.43
1:B:338:THR:HG23	1:B:344:PRO:HA	2.01	0.43
1:B:363:PHE:CZ	1:B:398:MET:HG3	2.54	0.43
1:B:633:LEU:O	1:B:885:LYS:HB2	2.17	0.43
1:A:335:PHE:CE1	1:A:349:ILE:HD11	2.47	0.43
1:A:982:LYS:HB3	2:P:10:DT:H5"	1.99	0.43
1:A:961:GLU:HB2	1:A:1179:TRP:CD2	2.54	0.43
1:B:789:LYS:HE3	1:B:789:LYS:HB2	1.72	0.43
1:A:367:ARG:NH2	1:A:401:GLU:OE1	2.51	0.43
1:A:1053:SER:O	1:A:1085:LYS:HB2	2.18	0.43
1:B:869:GLY:HA3	1:B:883:LEU:HD23	1.99	0.43
1:A:893:PHE:HB2	1:A:901:LEU:HB2	2.01	0.43
1:B:687:GLY:O	1:B:753:SER:HA	2.19	0.43
1:A:302:ASP:HB3	1:A:305:VAL:HG12	2.00	0.43
1:A:553:TYR:HE2	1:A:851:CYS:HG	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:HG11	1:B:504:PRO:HD3	2.01	0.43
1:B:576:ILE:HG23	1:B:868:VAL:HA	2.00	0.43
1:B:635:LEU:HD23	1:B:635:LEU:HA	1.85	0.43
1:B:836:ARG:HG3	3:D:5:DG:H4'	2.00	0.43
2:C:5:DC:H2"	2:C:6:DG:C8	2.54	0.43
1:A:1155:GLN:HA	1:A:1159:THR:OG1	2.19	0.43
1:B:594:PHE:HE1	1:B:915:HIS:CD2	2.37	0.43
1:A:186:LYS:HD3	1:A:188:LEU:HD21	2.01	0.42
1:B:889:GLU:HB3	1:B:890:THR:H	1.68	0.42
1:A:308:ILE:HD11	1:A:358:LEU:CD2	2.48	0.42
3:T:15:DT:H2"	3:T:16:DA:C8	2.54	0.42
1:B:744:ARG:HA	1:B:748:HIS:HA	2.01	0.42
1:A:1056:LEU:HD21	1:A:1071:ARG:HG3	2.01	0.42
1:B:579:SER:OG	1:B:867:ARG:NH2	2.52	0.42
1:B:1111:ILE:O	1:B:1119:LYS:HG3	2.19	0.42
1:A:323:THR:HB	1:A:328:ILE:HD11	2.01	0.42
1:B:329:SER:HB3	1:B:464:PHE:HA	2.02	0.42
1:B:1119:LYS:C	1:B:1123:LEU:HD12	2.40	0.42
1:A:241:ASP:OD1	1:A:242:ILE:N	2.53	0.42
1:B:325:ARG:NH1	1:B:331:ASP:OD1	2.41	0.42
1:B:623:GLU:CG	1:B:630:ARG:HH12	2.33	0.42
1:B:685:TRP:O	1:B:755:ILE:HA	2.20	0.42
1:B:892:PHE:HA	1:B:901:LEU:O	2.20	0.42
1:A:32:LEU:O	1:A:36:GLN:HG3	2.20	0.42
1:A:255:ILE:HG12	1:A:522:VAL:HG22	2.01	0.42
1:A:742:TYR:CZ	1:A:746:VAL:HG21	2.55	0.42
1:B:1096:LYS:HG2	1:B:1098:PHE:CD1	2.55	0.42
1:A:356:VAL:HG13	1:A:394:HIS:CD2	2.55	0.41
1:B:51:GLY:O	1:B:128:SER:OG	2.32	0.41
1:B:373:VAL:HG11	1:B:485:TYR:CZ	2.54	0.41
1:B:874:LEU:HD12	1:B:879:ILE:HG12	2.02	0.41
1:A:877:ASP:OD2	1:A:877:ASP:C	2.58	0.41
1:A:1115:ASP:HB3	1:A:1118:ILE:HD12	2.03	0.41
1:B:655:GLN:HB3	1:B:770:TYR:HB3	2.02	0.41
1:A:325:ARG:HD2	1:A:325:ARG:HA	1.80	0.41
1:A:989:ARG:HH21	2:P:8:DG:P	2.43	0.41
1:A:612:GLU:O	1:A:616:GLN:HG3	2.21	0.41
1:A:1096:LYS:HB2	1:A:1097:PRO:CD	2.35	0.41
1:A:1096:LYS:HG3	1:A:1127:THR:HG22	2.03	0.41
1:A:1120:ARG:HD2	1:A:1124:ARG:CZ	2.51	0.41
1:B:1073:LEU:HD23	1:B:1073:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:LYS:HG3	1:A:1127:THR:CG2	2.51	0.41
1:B:563:ALA:HA	1:B:955:LEU:HB2	2.03	0.41
1:A:144:ASN:HB3	1:A:240:GLU:HG3	2.03	0.41
1:A:146:GLU:HA	1:A:149:VAL:HG23	2.01	0.41
1:A:567:ARG:HB3	1:A:569:ASP:OD1	2.20	0.41
1:A:700:ILE:HD13	1:A:739:LEU:CD2	2.51	0.41
1:A:328:ILE:HA	1:A:463:ALA:O	2.21	0.41
1:A:458:LEU:C	1:A:461:PRO:HD2	2.41	0.41
1:A:546:HIS:HB3	1:A:690:PHE:O	2.21	0.41
1:A:686:ARG:HG3	1:A:755:ILE:HG12	2.03	0.41
1:B:335:PHE:CE2	1:B:475:VAL:HG21	2.55	0.41
1:B:645:TYR:CD2	5:B:1202:DCP:H2'2	2.56	0.41
1:B:1083:LYS:HZ2	1:B:1084:ASP:CG	2.24	0.41
1:A:279:ILE:HG13	1:A:280:ALA:N	2.32	0.41
1:A:373:VAL:HG11	1:A:485:TYR:CZ	2.55	0.41
1:A:802:ASP:O	1:A:806:ARG:HG3	2.21	0.41
1:A:1107:ILE:HG23	1:A:1126:TRP:CE3	2.56	0.41
1:B:517:GLU:O	1:B:521:MET:HG3	2.21	0.41
1:B:552:THR:OG1	1:B:553:TYR:N	2.52	0.41
1:B:620:LYS:O	1:B:624:LEU:HG	2.19	0.41
1:B:686:ARG:NH2	3:D:8:DA:OP1	2.53	0.41
1:B:686:ARG:HH22	3:D:8:DA:P	2.43	0.41
1:B:1094:SER:O	1:B:1105:ARG:HD2	2.20	0.41
1:B:887:PHE:CD1	1:B:888:PRO:HD2	2.56	0.41
1:B:447:LEU:HD23	1:B:447:LEU:HA	1.90	0.40
1:A:287:MET:HG3	1:A:315:ILE:HG13	2.02	0.40
1:B:264:TRP:CE3	1:B:278:LYS:HD3	2.56	0.40
1:B:343:TYR:CZ	1:B:447:LEU:HD22	2.57	0.40
1:B:576:ILE:HD12	1:B:576:ILE:N	2.37	0.40
1:A:323:THR:OG1	1:A:351:ASN:HA	2.21	0.40
1:A:682:LYS:HG2	1:A:759:GLU:HG3	2.04	0.40
1:A:1080:ASP:OD1	1:A:1080:ASP:N	2.47	0.40
3:T:11:DC:H2"	3:T:12:DG:C8	2.56	0.40
1:B:188:LEU:HD11	1:B:530:LEU:HD22	2.04	0.40
1:B:722:THR:HG22	1:B:723:PHE:H	1.85	0.40
1:A:645:TYR:CD2	5:A:1202:DCP:H2'2	2.55	0.40
1:B:296:PRO:HA	1:B:297:PRO:HD3	1.98	0.40
1:B:685:TRP:CH2	1:B:687:GLY:HA3	2.56	0.40
1:B:729:ALA:O	1:B:732:VAL:HG22	2.21	0.40
1:B:760:ALA:HB3	1:B:849:ILE:HD11	2.04	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	1098/1191 (92%)	1055 (96%)	43 (4%)	0	100	100
1	B	1098/1191 (92%)	1055 (96%)	43 (4%)	0	100	100
All	All	2196/2382 (92%)	2110 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	933/1064 (88%)	909 (97%)	24 (3%)	46	72
1	B	929/1064 (87%)	908 (98%)	21 (2%)	50	76
All	All	1862/2128 (88%)	1817 (98%)	45 (2%)	49	74

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

Mol	Chain	Res	Type
1	A	368	ASP
1	A	380	ASP
1	A	383	ASP
1	A	386	PHE
1	A	394	HIS
1	A	431	TYR
1	A	474	SER
1	A	537	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	565	VAL
1	A	623	GLU
1	A	692	SER
1	A	694	MET
1	A	753	SER
1	A	801	SER
1	A	907	CYS
1	A	935	GLU
1	A	995	ILE
1	A	1040	GLU
1	A	1044	SER
1	A	1051	SER
1	A	1076	PHE
1	A	1095	SER
1	A	1138	ARG
1	A	1168	SER
1	B	131	SER
1	B	277	ARG
1	B	354	ASP
1	B	380	ASP
1	B	431	TYR
1	B	537	ASP
1	B	544	ASP
1	B	571	LYS
1	B	590	GLU
1	B	594	PHE
1	B	607	VAL
1	B	658	SER
1	B	711	ASN
1	B	754	GLU
1	B	831	TYR
1	B	897	ASN
1	B	907	CYS
1	B	1044	SER
1	B	1064	SER
1	B	1076	PHE
1	B	1131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	GLN
1	B	198	GLN
1	B	213	ASN
1	B	922	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	C	11	2,3	16,19,20	0.40	0	20,26,29	0.32	0
2	DOC	P	11	2,3	16,19,20	0.41	0	20,26,29	0.35	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	C	11	2,3	-	2/7/18/19	0/2/2/2
2	DOC	P	11	2,3	-	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	O4'-C4'-C5'-O5'
2	P	11	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
5	DCP	B	1202	4	25,29,29	0.58	0	37,45,45	0.56	0
5	DCP	A	1202	4	25,29,29	0.61	0	37,45,45	0.57	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	DCP	B	1202	4	-	4/22/34/34	0/2/2/2
5	DCP	A	1202	4	-	1/22/34/34	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1202	DCP	PB-O3B-PG-O2G
5	B	1202	DCP	PB-O3B-PG-O3G
5	B	1202	DCP	PA-O3A-PB-O2B
5	B	1202	DCP	PA-O3A-PB-O1B
5	B	1202	DCP	PB-O3B-PG-O2G

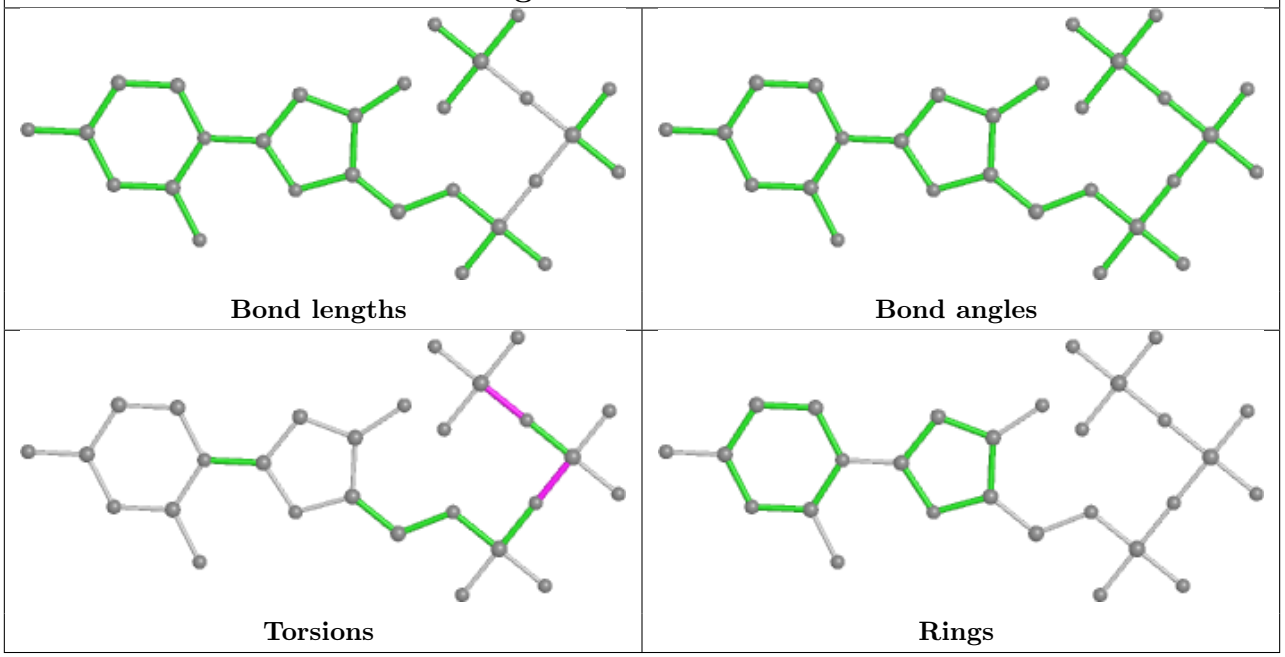
There are no ring outliers.

2 monomers are involved in 5 short contacts:

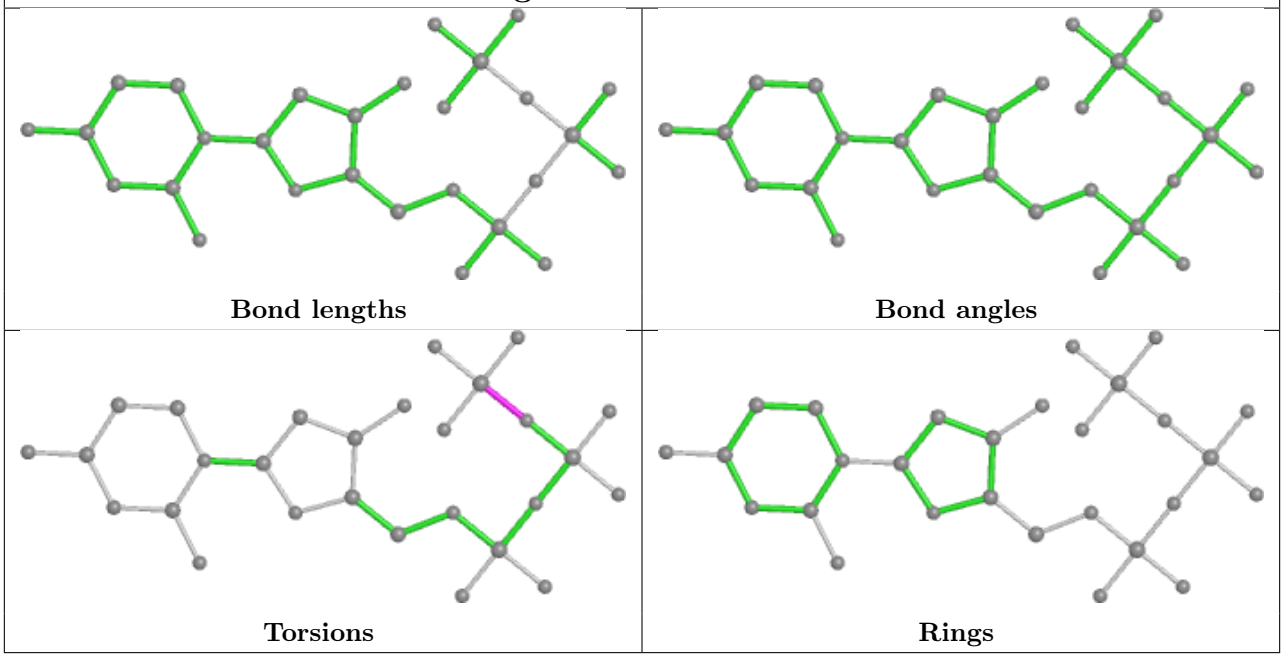
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1202	DCP	3	0
5	A	1202	DCP	2	0

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 DCP B 1202



Ligand DCP A 1202



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, 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	1108/1191 (93%)	0.35	47 (4%) 36 39	26, 58, 91, 114	0
1	B	1108/1191 (93%)	0.43	48 (4%) 35 38	29, 60, 96, 126	0
2	C	10/11 (90%)	0.06	0 100 100	37, 46, 69, 70	1 (10%)
2	P	10/11 (90%)	0.20	0 100 100	36, 46, 67, 74	1 (10%)
3	D	15/16 (93%)	0.06	0 100 100	29, 46, 84, 97	0
3	T	15/16 (93%)	0.14	0 100 100	29, 54, 81, 95	0
All	All	2266/2436 (93%)	0.38	95 (4%) 36 39	26, 59, 93, 126	2 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	6.8
1	A	31	ALA	5.9
1	A	464	PHE	5.5
1	B	700	ILE	5.4
1	B	464	PHE	5.0
1	A	66	ALA	4.9
1	A	1056	LEU	4.7
1	A	332	ILE	4.7
1	B	224	ASN	4.5
1	B	112	GLN	4.2
1	B	902	TYR	3.9
1	B	743	SER	3.6
1	A	238	LEU	3.5
1	A	723	PHE	3.5
1	B	795	LEU	3.3
1	A	328	ILE	3.3
1	A	1128	LEU	3.2
1	A	322	ILE	3.2
1	B	699	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1096	LYS	3.1
1	A	1114	ALA	3.1
1	B	596	VAL	3.1
1	A	1046	ILE	3.0
1	A	719	LYS	3.0
1	B	592	LEU	3.0
1	A	1059	TYR	3.0
1	B	1093	ILE	2.9
1	A	1050	ARG	2.9
1	A	1042	LEU	2.9
1	A	112	GLN	2.9
1	B	894	THR	2.9
1	A	74	GLY	2.9
1	A	1180	LEU	2.9
1	B	613	ILE	2.8
1	B	328	ILE	2.8
1	A	795	LEU	2.8
1	B	645	TYR	2.8
1	B	235	ALA	2.7
1	A	30	TYR	2.7
1	A	273	ILE	2.7
1	A	1067	ILE	2.6
1	A	311	ILE	2.6
1	A	321	LEU	2.6
1	A	386	PHE	2.6
1	B	801	SER	2.6
1	B	898	GLY	2.6
1	B	325	ARG	2.5
1	B	892	PHE	2.5
1	A	713	ASN	2.5
1	B	62	GLY	2.5
1	B	473	TYR	2.4
1	B	799	ASP	2.4
1	B	386	PHE	2.4
1	B	541	ARG	2.4
1	B	615	ASN	2.4
1	A	1064	SER	2.4
1	B	738	ARG	2.4
1	A	389	ASN	2.4
1	B	279	ILE	2.4
1	B	695	ASP	2.3
1	A	1035	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	893	PHE	2.3
1	A	396	LEU	2.3
1	A	73	PRO	2.3
1	A	470	LEU	2.3
1	B	387	ILE	2.3
1	B	238	LEU	2.3
1	B	1002	ILE	2.2
1	B	622	LEU	2.2
1	A	1097	PRO	2.2
1	B	194	VAL	2.2
1	A	219	GLN	2.2
1	B	891	TYR	2.2
1	B	750	VAL	2.2
1	A	1093	ILE	2.2
1	A	182	LEU	2.2
1	B	1059	TYR	2.2
1	B	701	LYS	2.2
1	B	181	LEU	2.2
1	B	584	LEU	2.2
1	B	718	LYS	2.2
1	B	1118	ILE	2.2
1	A	1076	PHE	2.2
1	B	466	LYS	2.1
1	B	332	ILE	2.1
1	B	900	LYS	2.1
1	A	72	ILE	2.1
1	B	578	PRO	2.1
1	A	347	PHE	2.1
1	A	335	PHE	2.1
1	A	350	PHE	2.1
1	A	381	PHE	2.1
1	A	798	ILE	2.0
1	B	182	LEU	2.0
1	A	697	TYR	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	0.96	0.20	27,31,45,47	0
2	DOC	C	11	18/19	0.97	0.18	33,37,48,51	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

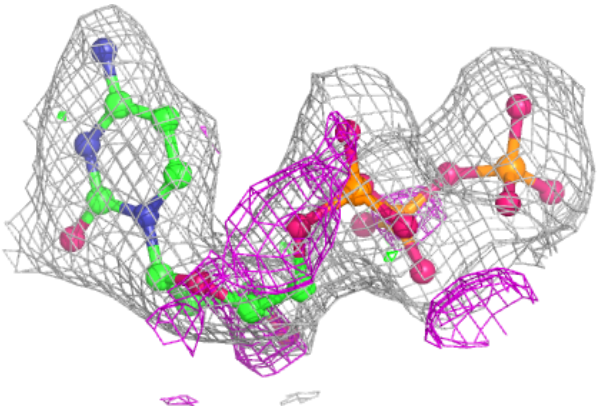
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

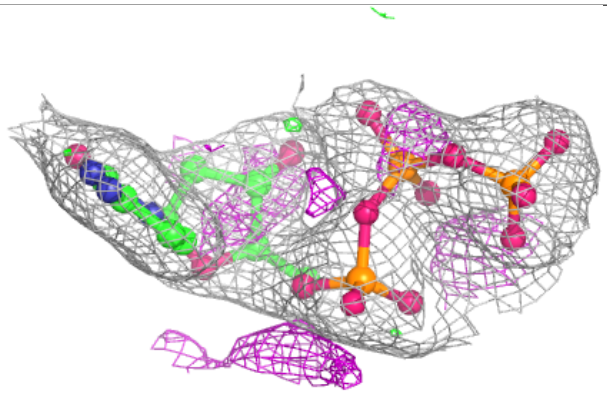
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	1201	1/1	0.89	0.08	44,44,44,44	0
4	CA	B	1201	1/1	0.93	0.15	50,50,50,50	0
5	DCP	A	1202	28/28	0.97	0.16	19,32,43,50	0
5	DCP	B	1202	28/28	0.97	0.15	23,35,41,51	0

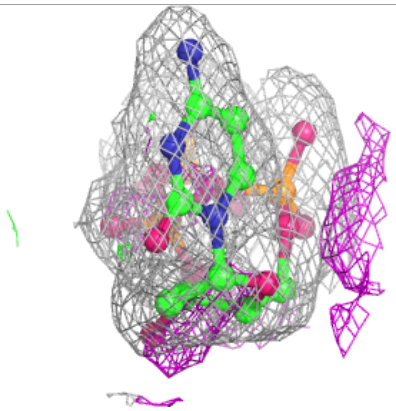
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DCP A 1202:

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

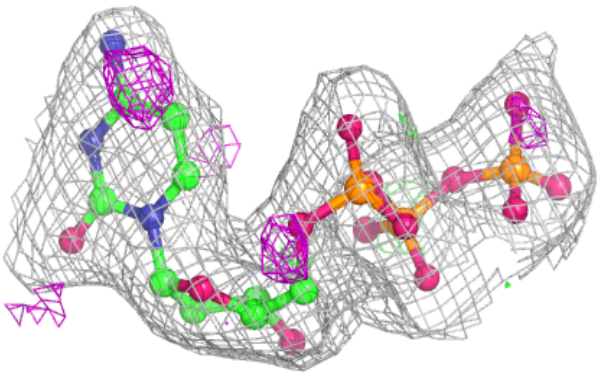


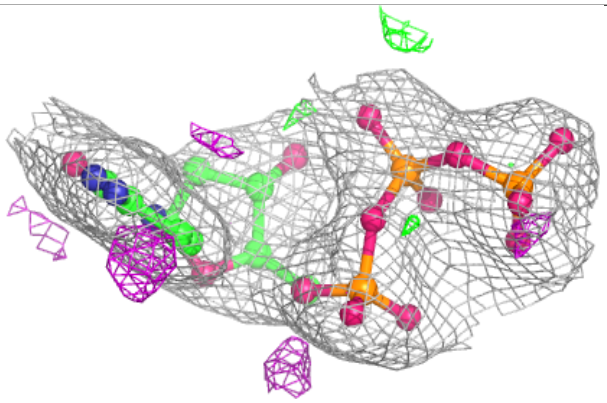


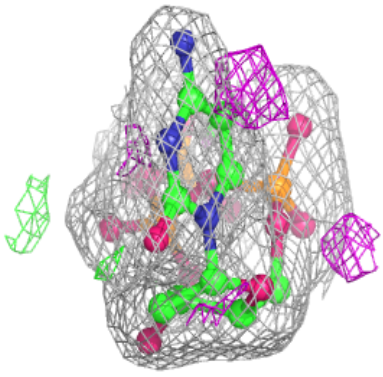


Electron density around DCP B 1202:

$2mF_o$-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.