



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:53 PM GMT

PDB ID : 4DQR
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment E658A, DNA duplex, and rCTP (paired with dG of template) in presence of Mn²⁺
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-16
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

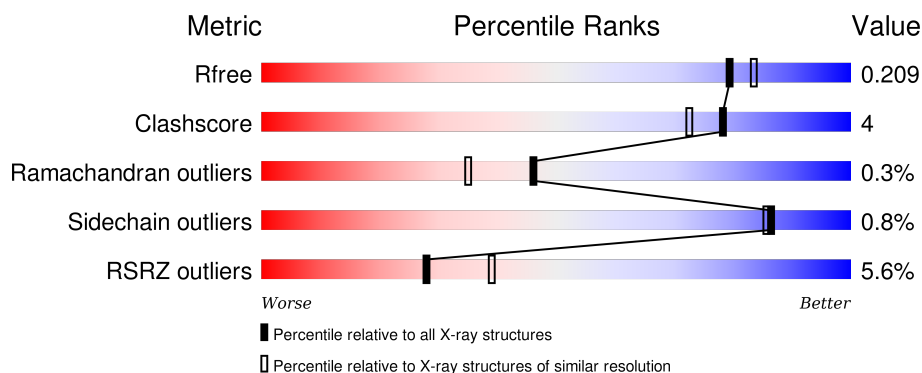
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	592	<div> <div>8%</div> <div>90%</div> <div>8%</div> </div>
1	D	592	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
2	B	9	<div> <div>11%</div> <div>67%</div> <div>33%</div> </div>
2	E	9	<div> <div>44%</div> <div>56%</div> </div>
3	C	13	<div> <div>46%</div> <div>38%</div> <div>15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	13	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MPD	A	904	-	-	-	X
7	MPD	D	904	-	-	-	X
7	MPD	D	905	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21345 atoms, of which 10147 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	H	N	O	S	0	16	0
			9514	2995	4801	822	878	18			
1	D	579	Total	C	H	N	O	S	0	23	0
			9561	3012	4823	823	885	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	658	ALA	GLU	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	ENGINEERED MUTATION	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	658	ALA	GLU	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	ENGINEERED MUTATION	UNP Q5KWC1

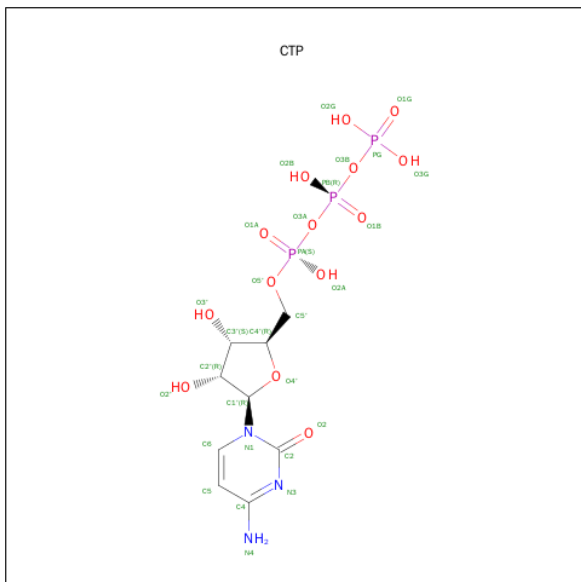
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			356	109	123	47	66	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			41	9	12	3	14	3		
4	D	1	Total	C	H	N	O	P	0	0
			41	9	12	3	14	3		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

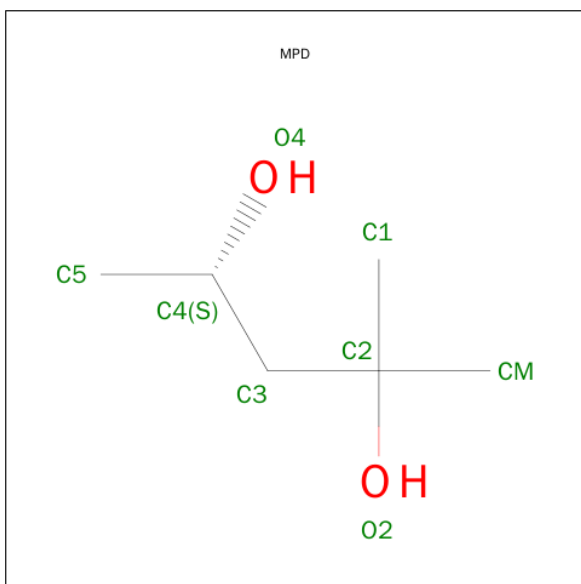
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			22	6	14	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			22	6	14	2		
7	D	1	Total	C	H	O	0	0
			22	6	14	2		

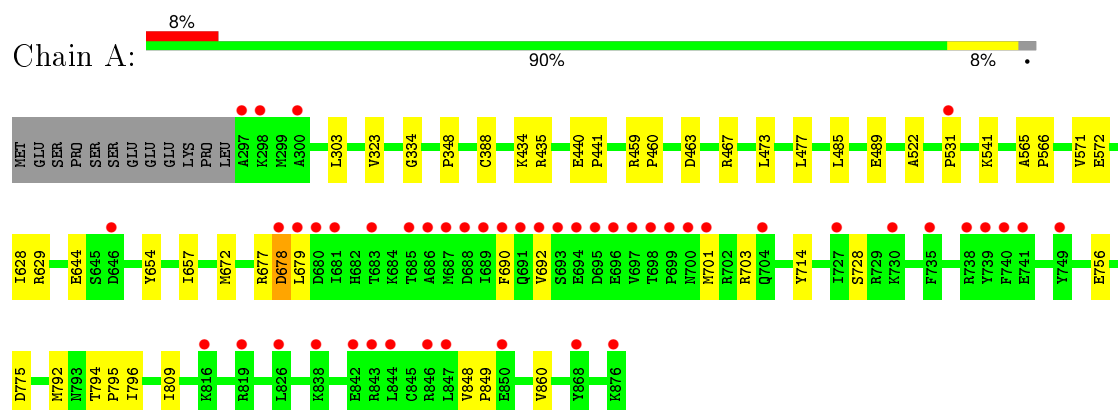
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	239	Total	O	0	0
			239	239		
8	D	447	Total	O	0	0
			447	447		
8	B	22	Total	O	0	0
			22	22		
8	C	39	Total	O	0	0
			39	39		
8	E	29	Total	O	0	0
			29	29		
8	F	45	Total	O	0	0
			45	45		

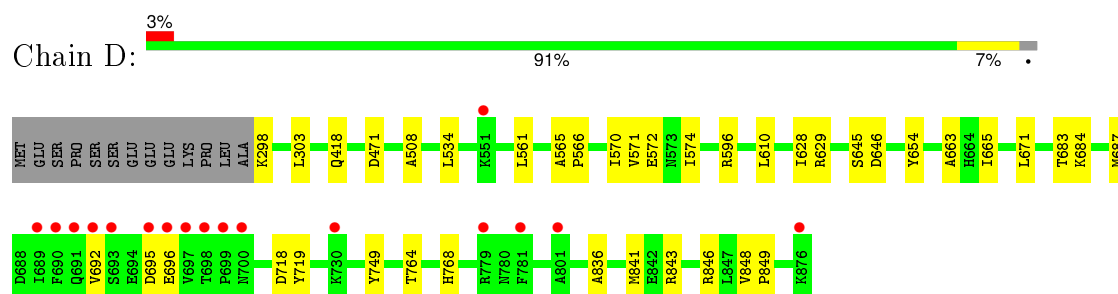
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

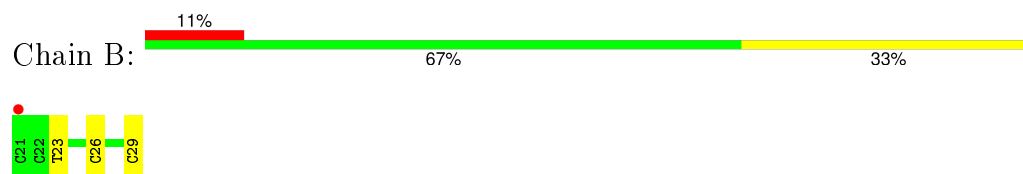
- Molecule 1: DNA polymerase



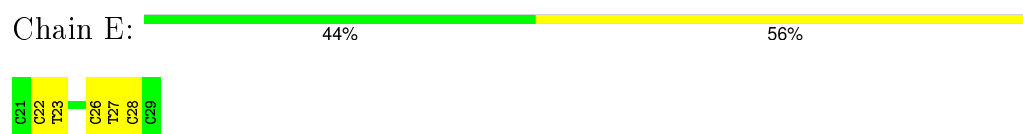
- Molecule 1: DNA polymerase



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



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



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

Chain C: 



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

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 108.85Å 149.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.79 – 1.95 37.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.1 (36.79-1.95) 94.1 (37.36-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.166 , 0.198 0.179 , 0.209	Depositor DCC
R_{free} test set	4479 reflections (4.43%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 105644 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21345	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DOC, MPD, MN, CTP, SO4

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	0.47	0/4854	0.57	0/6558
1	D	0.61	0/4911	0.67	0/6637
2	B	0.99	0/173	1.73	3/264 (1.1%)
2	E	1.14	1/173 (0.6%)	1.81	5/264 (1.9%)
3	C	0.96	0/262	1.49	2/404 (0.5%)
3	F	1.06	0/283	1.72	8/437 (1.8%)
All	All	0.60	1/10656 (0.0%)	0.79	18/14564 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	26	DC	C3'-O3'	-5.11	1.37	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	DC	O4'-C1'-N1	9.64	114.75	108.00
3	F	8	DT	O4'-C1'-N1	-9.06	101.66	108.00
2	B	23	DT	O4'-C1'-N1	-9.06	101.66	108.00
2	E	23	DT	O4'-C1'-N1	-9.05	101.66	108.00
2	E	22	DC	O4'-C1'-N1	-7.93	102.45	108.00
2	E	26	DC	O4'-C1'-N1	6.93	112.85	108.00
3	C	8	DT	O4'-C1'-N1	-6.44	103.49	108.00
3	F	4	DG	O4'-C1'-N9	6.38	112.47	108.00
3	F	4	DG	C4-C5-N7	-6.12	108.35	110.80
3	F	8	DT	C4-C5-C7	5.66	122.39	119.00
2	E	27	DT	O4'-C4'-C3'	-5.50	102.30	104.50
3	F	9	DC	O4'-C1'-C2'	5.45	110.26	105.90
3	C	5	DG	O4'-C4'-C3'	-5.40	102.34	104.50
3	F	10	DA	O4'-C1'-N9	-5.37	104.24	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	DT	O4'-C1'-N1	5.30	111.71	108.00
3	F	4	DG	O5'-P-OP2	-5.30	100.93	105.70
2	E	26	DC	O4'-C1'-C2'	5.08	109.96	105.90
2	B	26	DC	O4'-C4'-C3'	5.04	109.03	106.00

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	4713	4801	4726	35	0
1	D	4738	4823	4711	29	0
2	B	174	100	103	1	0
2	E	174	100	103	1	0
3	C	233	123	124	2	0
3	F	251	134	136	5	0
4	A	29	12	12	0	0
4	D	29	12	12	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	A	8	14	14	0	0
7	D	16	28	28	2	0
8	A	239	0	0	12	0
8	B	22	0	0	0	0
8	C	39	0	0	1	0
8	D	447	0	0	13	0
8	E	29	0	0	0	0
8	F	45	0	0	5	0
All	All	11198	10147	9969	74	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 4.

All (74) 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:388:CYS:SG	8:A:1194:HOH:O	2.13	1.06
3:C:11:DG:OP1	8:C:123:HOH:O	1.91	0.88
1:D:764[B]:THR:HG21	8:D:1304:HOH:O	1.77	0.84
1:A:792:MET:SD	8:A:1215:HOH:O	2.38	0.82
3:F:12:DG:N3	8:F:143:HOH:O	2.11	0.82
1:D:654:TYR:O	8:D:1090:HOH:O	1.99	0.81
3:F:11:DG:OP2	8:F:122:HOH:O	2.03	0.76
1:A:323:VAL:O	1:A:435:ARG:NH2	2.24	0.71
7:D:904:MPD:HM2	8:D:1059:HOH:O	1.89	0.71
1:D:843:ARG:HD2	8:D:1101:HOH:O	1.92	0.69
1:D:418:GLN:OE1	8:D:1329:HOH:O	2.10	0.69
1:D:683:THR:HG22	1:D:687:MET:HE3	1.75	0.69
1:D:684:LYS:NZ	8:D:1303:HOH:O	2.27	0.68
1:A:434:LYS:NZ	8:A:1223:HOH:O	2.21	0.68
4:D:901:CTP:O2G	8:D:1158:HOH:O	2.13	0.67
1:A:672:MET:HG3	1:A:860:VAL:HG12	1.76	0.66
1:A:434:LYS:CE	8:A:1223:HOH:O	2.44	0.65
1:D:846:ARG:NH1	8:D:1306:HOH:O	2.08	0.65
1:D:683:THR:HG22	1:D:687:MET:CE	2.27	0.64
1:A:672:MET:HG3	1:A:860:VAL:CG1	2.29	0.62
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.30	0.62
1:A:756:GLU:OE1	8:A:1147:HOH:O	2.17	0.58
1:D:508:ALA:O	8:D:1316:HOH:O	2.17	0.58
1:A:477:LEU:HD12	1:A:809:ILE:HD12	1.86	0.57
1:A:565:ALA:HA	1:A:571:VAL:HG21	1.87	0.56
1:A:629:ARG:HH22	2:B:29:DOC:H5	1.69	0.56
1:A:714:TYR:HE1	1:A:796:ILE:HD12	1.70	0.56
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.90	0.54
1:A:629:ARG:HD3	1:A:703:ARG:CZ	2.38	0.53
1:A:531:PRO:HD2	8:A:1219:HOH:O	2.09	0.53
3:F:12:DG:C4'	8:F:121:HOH:O	2.57	0.52
3:F:12:DG:H1'	8:F:143:HOH:O	2.09	0.52
1:D:596:ARG:HD2	8:D:1438:HOH:O	2.10	0.52
1:D:610[B]:LEU:HD12	8:D:1188:HOH:O	2.10	0.51
1:D:692:VAL:HB	1:D:696:GLU:HB2	1.94	0.49
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.94	0.48
1:A:434:LYS:HD2	8:A:1223:HOH:O	2.13	0.48
1:D:561:LEU:O	1:D:571:VAL:HG11	2.14	0.48
1:D:570:ILE:O	1:D:574[B]:ILE:HG12	2.13	0.48
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.96	0.48
1:D:629:ARG:HD3	2:E:28:DC:P	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ASP:O	1:A:467[B]:ARG:HG3	2.14	0.47
1:D:565:ALA:N	1:D:566:PRO:CD	2.78	0.47
1:D:561:LEU:HB3	1:D:571:VAL:HG13	1.97	0.46
1:D:565:ALA:N	1:D:566:PRO:HD2	2.30	0.46
1:D:665:ILE:HG22	1:D:749[A]:TYR:CE1	2.51	0.45
1:D:663:ALA:HB2	1:D:671:LEU:HG	1.98	0.45
1:D:534:LEU:HD11	1:D:574[A]:ILE:HD13	1.98	0.45
1:A:565:ALA:N	1:A:566:PRO:HD2	2.33	0.44
1:A:654:TYR:HB3	1:A:657:ILE:HB	1.99	0.44
1:A:334:GLY:HA2	1:A:348:PRO:HD3	1.99	0.44
1:D:836:ALA:HB3	1:D:841:MET:CE	2.47	0.44
3:C:9:DC:H2'	3:C:10:DA:C8	2.52	0.44
1:D:764[B]:THR:CG2	1:D:768:HIS:HA	2.48	0.44
1:A:531:PRO:N	8:A:1219:HOH:O	2.49	0.44
3:F:12:DG:H4'	8:F:121:HOH:O	2.18	0.44
7:D:905:MPD:O2	8:D:1193:HOH:O	2.20	0.44
1:D:848:VAL:HB	1:D:849:PRO:HD3	2.00	0.43
1:A:677:ARG:HD2	1:A:679:LEU:HD21	1.99	0.43
1:D:596:ARG:CG	8:D:1438:HOH:O	2.66	0.43
1:D:764[B]:THR:HG22	1:D:768:HIS:HA	1.99	0.43
1:A:690:PHE:O	1:A:692:VAL:HG13	2.19	0.43
1:A:522:ALA:O	1:A:541:LYS:HE2	2.19	0.43
1:A:775:ASP:HB2	8:A:1055:HOH:O	2.19	0.43
1:A:531:PRO:CD	8:A:1219:HOH:O	2.67	0.42
1:D:645:SER:O	1:D:646:ASP:HB2	2.20	0.42
1:A:440:GLU:HB3	1:A:441:PRO:HD3	2.01	0.42
1:D:718:ASP:OD2	1:D:719:TYR:N	2.52	0.42
1:A:572:GLU:HB2	8:A:1158:HOH:O	2.20	0.41
1:A:485:LEU:O	1:A:489:GLU:HG3	2.19	0.41
1:A:794:THR:N	1:A:795:PRO:CD	2.83	0.41
1:D:471:ASP:N	1:D:471:ASP:OD1	2.52	0.41
1:A:467[B]:ARG:HD2	8:A:1101:HOH:O	2.21	0.41
1:A:473:LEU:HD12	1:A:477:LEU:HD23	2.03	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	594/592 (100%)	583 (98%)	9 (2%)	2 (0%)	46	35
1	D	600/592 (101%)	585 (98%)	14 (2%)	1 (0%)	52	43
All	All	1194/1184 (101%)	1168 (98%)	23 (2%)	3 (0%)	46	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	678	ASP
1	D	628	ILE
1	A	628	ILE

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	508/506 (100%)	504 (99%)	4 (1%)	86	85
1	D	517/506 (102%)	513 (99%)	4 (1%)	86	85
All	All	1025/1012 (101%)	1017 (99%)	8 (1%)	86	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	644	GLU
1	A	678	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	728	SER
1	D	298	LYS
1	D	303	LEU
1	D	572	GLU
1	D	695	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	709	ASN

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	B	29	3,2	11,19,20	0.90	0	14,26,29	1.09	1 (7%)
2	DOC	E	29	3,2	11,19,20	0.92	1 (9%)	14,26,29	1.06	1 (7%)

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	B	29	3,2	-	0/3/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/3/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DOC	C6-C5	-2.15	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	C2-N3-C4	2.71	119.44	115.61
2	B	29	DOC	C2-N3-C4	3.03	119.89	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	29	DOC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	CTP	A	901	5	21,30,30	1.47	2 (9%)	31,47,47	1.47	6 (19%)
6	SO4	A	903	-	4,4,4	0.15	0	6,6,6	0.16	0
7	MPD	A	904	-	6,7,7	0.32	0	7,10,10	0.89	0
4	CTP	D	901	5	21,30,30	1.50	3 (14%)	31,47,47	1.23	4 (12%)
6	SO4	D	903	-	4,4,4	0.59	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MPD	D	904	-	6,7,7	0.29	0	7,10,10	0.64	0
7	MPD	D	905	-	6,7,7	0.51	0	7,10,10	0.42	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
4	CTP	A	901	5	-	0/18/38/38	0/2/2/2
6	SO4	A	903	-	-	0/0/0/0	0/0/0/0
7	MPD	A	904	-	-	0/5/5/5	0/0/0/0
4	CTP	D	901	5	-	0/18/38/38	0/2/2/2
6	SO4	D	903	-	-	0/0/0/0	0/0/0/0
7	MPD	D	904	-	-	0/5/5/5	0/0/0/0
7	MPD	D	905	-	-	0/5/5/5	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	CTP	PB-O2B	-2.04	1.46	1.54
4	D	901	CTP	C4-N4	2.50	1.42	1.35
4	D	901	CTP	C6-N1	2.55	1.39	1.35
4	A	901	CTP	C4-N4	2.56	1.42	1.35
4	A	901	CTP	C6-N1	4.01	1.41	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	CTP	PB-O3A-PA	-3.00	124.29	132.73
4	D	901	CTP	PB-O3A-PA	-2.26	126.38	132.73
4	A	901	CTP	O2G-PG-O1G	-2.16	103.61	110.58
4	D	901	CTP	O2G-PG-O3B	2.13	114.75	105.09
4	A	901	CTP	C2-N3-C4	2.19	118.71	115.61
4	A	901	CTP	O2G-PG-O3B	2.29	115.47	105.09
4	D	901	CTP	C2-N3-C4	2.59	119.27	115.61
4	D	901	CTP	O2A-PA-O3A	2.70	117.33	105.09
4	A	901	CTP	O2B-PB-O3B	2.93	118.37	105.09
4	A	901	CTP	O4'-C1'-N1	3.28	115.00	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	CTP	1	0
7	D	904	MPD	1	0
7	D	905	MPD	1	0

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	580/592 (97%)	0.49	48 (8%) 14 22	19, 42, 77, 109	0
1	D	579/592 (97%)	0.05	17 (2%) 55 65	13, 24, 51, 77	0
2	B	8/9 (88%)	0.22	1 (12%) 5 9	25, 29, 52, 70	0
2	E	8/9 (88%)	-0.06	0 100 100	20, 26, 46, 61	0
3	C	11/13 (84%)	-0.30	0 100 100	22, 29, 55, 78	0
3	F	12/13 (92%)	0.09	1 (8%) 14 22	18, 26, 69, 79	0
All	All	1198/1228 (97%)	0.26	67 (5%) 28 39	13, 33, 69, 109	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	LYS	6.4
1	A	297	ALA	6.1
1	A	689	ILE	5.8
1	A	698	THR	5.7
1	A	699	PRO	5.7
1	A	697	VAL	5.7
1	A	690	PHE	5.7
1	A	693	SER	5.6
1	A	687	MET	5.5
1	A	679	LEU	5.3
1	A	696	GLU	5.0
1	A	692	VAL	5.0
1	A	701	MET	4.9
1	A	691	GLN	4.6
1	D	691	GLN	4.2
1	A	681	ILE	4.2
1	A	695	ASP	4.1
1	A	876	LYS	4.0
1	A	688	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	735	PHE	3.8
1	A	700	ASN	3.8
1	A	740	PHE	3.7
1	A	678	ASP	3.6
1	A	819	ARG	3.6
1	D	698	THR	3.5
1	A	842	GLU	3.5
1	D	692	VAL	3.4
1	D	696	GLU	3.4
1	D	876	LYS	3.3
1	D	697	VAL	3.2
1	D	690	PHE	3.2
1	D	689	ILE	3.2
1	A	683	THR	3.2
1	A	749	TYR	3.1
1	A	300	ALA	3.0
1	D	699	PRO	2.9
3	F	1	DA	2.8
1	A	868	TYR	2.8
1	A	846	ARG	2.7
1	D	693	SER	2.6
1	A	844	LEU	2.6
1	D	779	ARG	2.6
1	A	704	GLN	2.6
1	A	850	GLU	2.5
1	D	695	ASP	2.5
1	A	686	ALA	2.5
1	A	843	ARG	2.5
1	A	694	GLU	2.5
1	D	730	LYS	2.5
1	A	739	TYR	2.5
1	A	738	ARG	2.4
1	D	700	ASN	2.4
1	A	685	THR	2.4
1	A	646	ASP	2.4
1	A	847	LEU	2.3
1	D	551	LYS	2.3
1	D	781	PHE	2.2
1	A	727	ILE	2.2
1	A	531	PRO	2.2
1	A	826	LEU	2.1
1	D	801	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	741	GLU	2.1
1	A	680	ASP	2.1
1	A	816	LYS	2.0
1	A	838	LYS	2.0
2	B	21	DC	2.0
1	A	730	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	DOC	E	29	18/19	0.98	0.15	-	16,20,26,26	0
2	DOC	B	29	18/19	0.98	0.16	-	23,29,35,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	MPD	D	905	8/8	0.92	0.20	5.48	31,48,58,58	0
7	MPD	A	904	8/8	0.95	0.16	4.17	26,37,46,50	0
7	MPD	D	904	8/8	0.93	0.16	2.05	24,40,53,57	0
4	CTP	D	901	29/29	0.99	0.12	-0.27	17,22,27,31	0
6	SO4	A	903	5/5	0.97	0.11	-0.33	52,52,58,61	0
6	SO4	D	903	5/5	0.99	0.09	-0.40	31,35,37,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CTP	A	901	29/29	0.95	0.12	-0.49	25,35,59,66	0
5	MN	A	902	1/1	0.91	0.14	-0.74	59,59,59,59	0
5	MN	D	902	1/1	0.99	0.11	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.