Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 PM GMT

PDB ID	:	5KTQ
Title	:	LARGE FRAGMENT OF TAQ DNA POLYMERASE BOUND TO DCTP
Authors	:	Li, Y.; Kong, Y.; Korolev, S.; Waksman, G.
Deposited on	:	1998-09-22
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

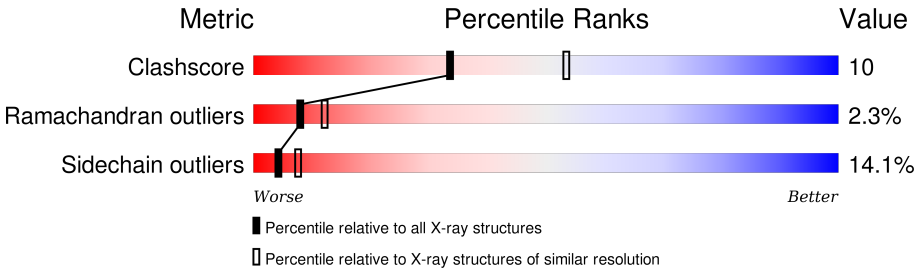
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	543	60% 28% 9%

2 Entry composition

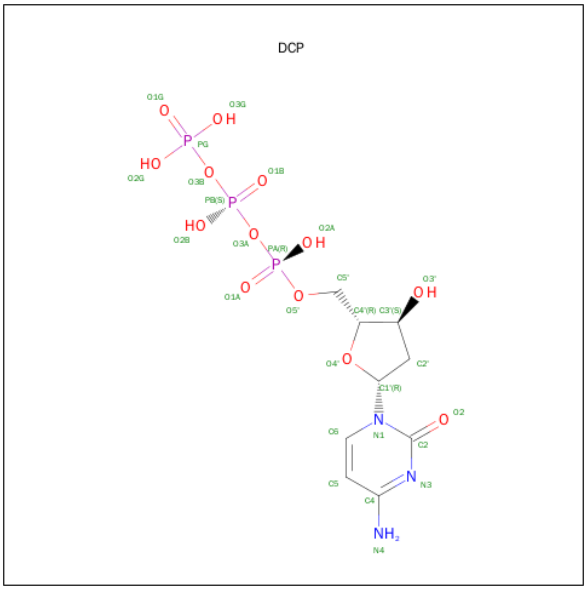
There are 2 unique types of molecules in this entry. The entry contains 4267 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4239	2698	761	767	13	0	0	0

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



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

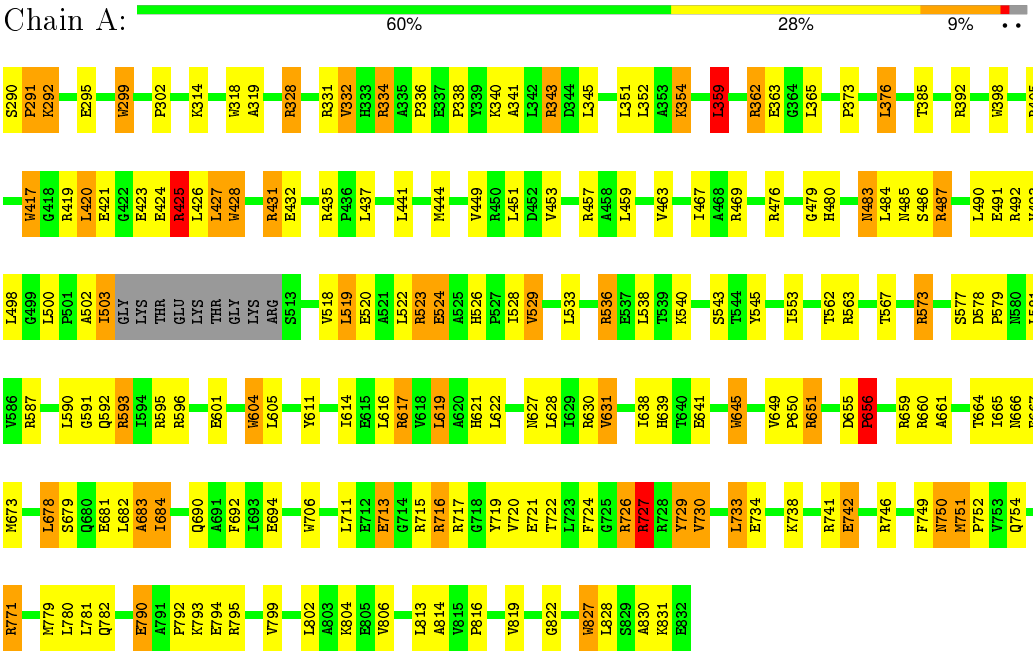
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: PROTEIN (DNA POLYMERASE I)

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.40Å 137.00Å 45.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	85.0 (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.217 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4267	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.82	0/4329	1.55	64/5867 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	318	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	487	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	827	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	299	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	A	457	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	318	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	A	671	TYR	CB-CG-CD1	-7.89	116.27	121.00
1	A	398	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	299	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	593	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	398	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	706	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	604	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	417	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	827	TRP	CE2-CD2-CG	-7.32	101.44	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	645	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	362	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	645	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	359	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	428	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	519	LEU	CA-CB-CG	7.04	131.49	115.30
1	A	328	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	523	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	536	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	417	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	A	604	TRP	CD1-CG-CD2	6.73	111.69	106.30
1	A	706	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	A	331	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	487	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	392	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	494	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	617	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	716	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	543	SER	CA-CB-OG	6.01	127.43	111.20
1	A	604	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	523	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	428	TRP	CD1-CG-CD2	5.86	110.98	106.30
1	A	631	VAL	CG1-CB-CG2	-5.85	101.53	110.90
1	A	524	GLU	N-CA-C	5.85	126.79	111.00
1	A	771	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	408	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	A	656	PRO	N-CA-C	5.65	126.79	112.10
1	A	827	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	457	ARG	CD-NE-CZ	5.57	131.39	123.60
1	A	334	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	469	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	729	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	726	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	573	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	343	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	431	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	405	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	484	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	727	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	431	ARG	CB-CG-CD	-5.27	97.89	111.60
1	A	453	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	730	VAL	CG1-CB-CG2	-5.19	102.60	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	354	LYS	CA-CB-CG	5.15	124.73	113.40
1	A	419	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	299	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	A	425	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	741	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide
1	A	655	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4239	0	4273	87	0
2	A	28	0	12	1	0
All	All	4267	0	4285	87	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 10.

All (87) 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:596:ARG:HE	1:A:828:LEU:HD23	1.49	0.77
1:A:449:VAL:HG12	1:A:780:LEU:HD13	1.69	0.72
1:A:500:LEU:O	1:A:503:ILE:HB	1.89	0.71
1:A:673:MET:SD	1:A:678:LEU:HD12	2.29	0.71
1:A:722:THR:HG22	1:A:724:PHE:H	1.56	0.70
1:A:780:LEU:HD11	1:A:790:GLU:HG3	1.74	0.68
1:A:585:PRO:O	1:A:591:GLY:HA3	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HG	1:A:441:LEU:HD13	1.76	0.67
1:A:664:THR:HG21	1:A:682:LEU:HG	1.79	0.64
1:A:420:LEU:HD23	1:A:427:LEU:HD22	1.80	0.62
1:A:768:LEU:HG	1:A:806:VAL:HG11	1.82	0.60
1:A:581:LEU:HD11	1:A:781:LEU:HD22	1.84	0.59
1:A:523:ARG:HA	1:A:529:VAL:HG23	1.85	0.59
1:A:545:TYR:OH	1:A:583:ASN:HB2	2.04	0.58
1:A:423:GLU:HG2	1:A:426:LEU:HD12	1.87	0.57
1:A:621:HIS:HD2	1:A:814:ALA:H	1.52	0.57
1:A:605:LEU:HG	1:A:793:LYS:HG2	1.88	0.56
1:A:299:TRP:HB2	1:A:334:ARG:O	2.06	0.56
1:A:592:GLN:HB2	1:A:828:LEU:HD13	1.88	0.56
1:A:730:VAL:HG12	1:A:733:LEU:HB2	1.88	0.55
1:A:661:ALA:O	1:A:665:ILE:HG12	2.07	0.54
1:A:385:THR:HG22	1:A:567:THR:O	2.08	0.54
1:A:495:PHE:CG	1:A:503:ILE:HG13	2.43	0.53
1:A:502:ALA:C	1:A:503:ILE:HD13	2.29	0.53
1:A:711:LEU:O	1:A:715:ARG:HB2	2.08	0.53
1:A:742:GLU:O	1:A:746:ARG:HG2	2.08	0.53
1:A:314:LYS:HB2	1:A:319:ALA:HB2	1.89	0.53
1:A:492:ARG:O	1:A:496:ASP:HB2	2.09	0.53
1:A:595:ARG:O	1:A:827:TRP:HB3	2.09	0.53
1:A:483:ASN:HD22	1:A:485:ASN:H	1.57	0.52
1:A:722:THR:HG21	1:A:759:ASP:OD2	2.09	0.52
1:A:376:LEU:HD12	1:A:420:LEU:HD13	1.90	0.51
1:A:528:ILE:HG23	1:A:529:VAL:HG13	1.92	0.51
1:A:751:MET:HB3	1:A:752:PRO:HD3	1.92	0.51
1:A:750:ASN:HB3	1:A:754:GLN:HE21	1.76	0.51
1:A:487:ARG:HH22	1:A:536:ARG:NH2	2.09	0.50
1:A:621:HIS:CD2	1:A:814:ALA:H	2.28	0.50
1:A:463:VAL:HG13	1:A:538:LEU:HD22	1.93	0.50
1:A:563:ARG:HB2	1:A:577:SER:HB2	1.94	0.49
1:A:639:HIS:HE2	1:A:667:PHE:HE1	1.58	0.49
1:A:292:LYS:HB2	1:A:292:LYS:NZ	2.27	0.49
1:A:804:LYS:HA	1:A:819:VAL:HG21	1.94	0.49
1:A:649:VAL:HB	1:A:651:ARG:O	2.13	0.49
1:A:421:GLU:HA	1:A:427:LEU:HD23	1.95	0.48
1:A:684:ILE:HD13	1:A:692:PHE:HE1	1.78	0.47
1:A:771:ARG:HB3	1:A:802:LEU:HD21	1.97	0.46
1:A:463:VAL:O	1:A:467:ILE:HG13	2.15	0.46
1:A:359:LEU:O	1:A:362:ARG:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLU:O	1:A:717:ARG:HG2	2.14	0.46
1:A:617:ARG:HD3	1:A:816:PRO:O	2.15	0.46
1:A:794:GLU:CD	1:A:794:GLU:H	2.19	0.46
1:A:679:SER:O	1:A:683:ALA:HA	2.15	0.46
1:A:601:GLU:HB3	1:A:604:TRP:CD1	2.51	0.46
1:A:302:PRO:HG2	1:A:328:ARG:HD3	1.98	0.46
1:A:627:ASN:O	1:A:631:VAL:HG23	2.15	0.46
1:A:822:GLY:HA3	1:A:830:ALA:O	2.17	0.45
1:A:828:LEU:O	1:A:831:LYS:HB3	2.15	0.45
1:A:479:GLY:O	1:A:480:HIS:HD2	2.00	0.45
1:A:417:TRP:HH2	1:A:427:LEU:HD11	1.81	0.45
1:A:487:ARG:O	1:A:491:GLU:HG2	2.17	0.45
1:A:417:TRP:CH2	1:A:427:LEU:HD11	2.52	0.45
1:A:363:GLU:O	1:A:365:LEU:HD13	2.17	0.45
1:A:639:HIS:CD2	1:A:666:ASN:HD22	2.34	0.44
1:A:639:HIS:HE1	2:A:901:DCP:O2B	2.01	0.44
1:A:444:MET:HG2	1:A:779:MET:O	2.18	0.44
1:A:596:ARG:NE	1:A:828:LEU:HD23	2.26	0.44
1:A:338:PRO:O	1:A:341:ALA:HB3	2.18	0.44
1:A:495:PHE:CE2	1:A:503:ILE:HD11	2.52	0.43
1:A:425:ARG:HD3	1:A:724:PHE:O	2.18	0.43
1:A:604:TRP:HA	1:A:792:PRO:HA	2.00	0.43
1:A:292:LYS:O	1:A:295:GLU:HB3	2.18	0.43
1:A:493:VAL:HA	1:A:497:GLU:HB2	2.00	0.43
1:A:619:LEU:HD13	1:A:628:LEU:HD21	2.00	0.42
1:A:719:TYR:HB3	1:A:729:TYR:CD1	2.54	0.42
1:A:351:LEU:HG	1:A:373:PRO:HG2	2.02	0.42
1:A:495:PHE:N	1:A:495:PHE:CD2	2.88	0.41
1:A:431:ARG:HH11	1:A:431:ARG:HD2	1.70	0.41
1:A:428:TRP:CE3	1:A:432:GLU:HG3	2.55	0.41
1:A:616:LEU:HD13	1:A:638:ILE:HG12	2.02	0.41
1:A:291:PRO:HD2	1:A:332:VAL:CG2	2.51	0.41
1:A:611:TYR:HB3	1:A:614:ILE:HB	2.02	0.41
1:A:498:LEU:HD13	1:A:526:HIS:NE2	2.36	0.41
1:A:661:ALA:HA	1:A:682:LEU:HD21	2.03	0.40
1:A:795:ARG:O	1:A:799:VAL:HG23	2.20	0.40
1:A:451:LEU:HD12	1:A:553:ILE:HD11	2.03	0.40
1:A:720:VAL:O	1:A:727:ARG:HA	2.21	0.40
1:A:721:GLU:HA	1:A:726:ARG:O	2.21	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	530/543 (98%)	474 (89%)	44 (8%)	12 (2%)	8 12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO
1	A	656	PRO
1	A	733	LEU
1	A	519	LEU
1	A	650	PRO
1	A	683	ALA
1	A	670	LEU
1	A	672	GLY
1	A	734	GLU
1	A	336	PRO
1	A	524	GLU
1	A	529	VAL

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	433/444 (98%)	372 (86%)	61 (14%)	4 7

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	A	332	VAL
1	A	340	LYS
1	A	343	ARG
1	A	345	LEU
1	A	352	LEU
1	A	354	LYS
1	A	359	LEU
1	A	376	LEU
1	A	408	LEU
1	A	411	ARG
1	A	420	LEU
1	A	424	GLU
1	A	425	ARG
1	A	427	LEU
1	A	435	ARG
1	A	459	LEU
1	A	476	ARG
1	A	483	ASN
1	A	486	SER
1	A	490	LEU
1	A	497	GLU
1	A	503	ILE
1	A	518	VAL
1	A	520	GLU
1	A	522	LEU
1	A	533	LEU
1	A	540	LYS
1	A	562	THR
1	A	573	ARG
1	A	578	ASP
1	A	579	PRO
1	A	582	GLN
1	A	587	ARG
1	A	590	LEU
1	A	593	ARG
1	A	619	LEU
1	A	622	LEU
1	A	630	ARG
1	A	641	GLU
1	A	645	TRP
1	A	651	ARG
1	A	656	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	659	ARG
1	A	660	ARG
1	A	678	LEU
1	A	681	GLU
1	A	684	ILE
1	A	690	GLN
1	A	694	GLU
1	A	713	GLU
1	A	716	ARG
1	A	727	ARG
1	A	738	LYS
1	A	742	GLU
1	A	749	PHE
1	A	750	ASN
1	A	751	MET
1	A	782	GLN
1	A	790	GLU
1	A	813	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	HIS
1	A	483	ASN
1	A	566	GLN
1	A	582	GLN
1	A	621	HIS
1	A	666	ASN
1	A	690	GLN
1	A	754	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DCP	A	901	-	21,29,29	0.92	0	33,45,45	1.51	5 (15%)

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	DCP	A	901	-	-	0/18/34/34	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	DCP	C4'-O4'-C1'	-3.46	100.72	109.47
2	A	901	DCP	PB-O3A-PA	-2.13	126.74	132.73
2	A	901	DCP	C2'-C1'-N1	2.51	120.26	114.16
2	A	901	DCP	O4'-C1'-N1	2.95	112.82	107.72
2	A	901	DCP	C2-N3-C4	3.90	121.12	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	A	901	DCP	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.