Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 10:17 AM EST

PDB ID	:	2BDP
Title	:	CRYSTAL STRUCTURE OF BACILLUS DNA POLYMERASE I FRAGMENT COMPLEXED TO 9 BASE PAIRS OF DUPLEX DNA
Authors	:	Kiefer, J.R.; Mao, C.; Beese, L.S.
Deposited on	:	1997-11-17
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

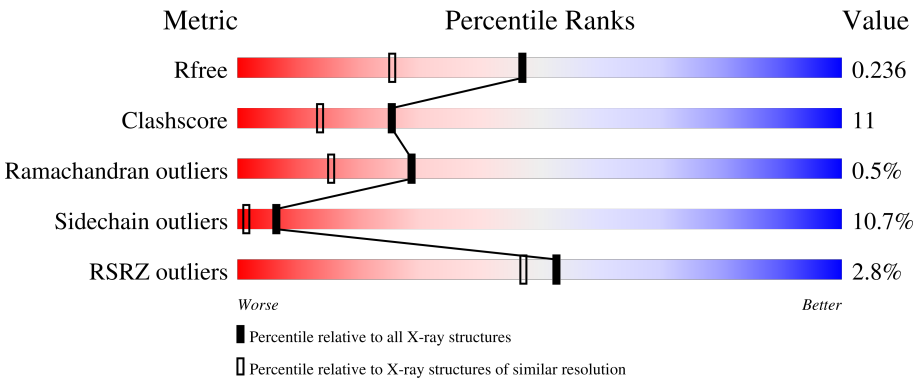
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	P	9	11% 33% 56% 11%
2	T	10	70% 30%
3	A	580	3% 78% 17% 5%

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
4	SO4	A	910	-	X	-	-
4	SO4	A	911	-	X	-	-
4	SO4	A	912	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5527 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 DNA chain called DNA (5'-D(*GP*CP*AP*TP*GP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	9	183	88	35	52	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	10	204	97	38	59	10	0	0	0

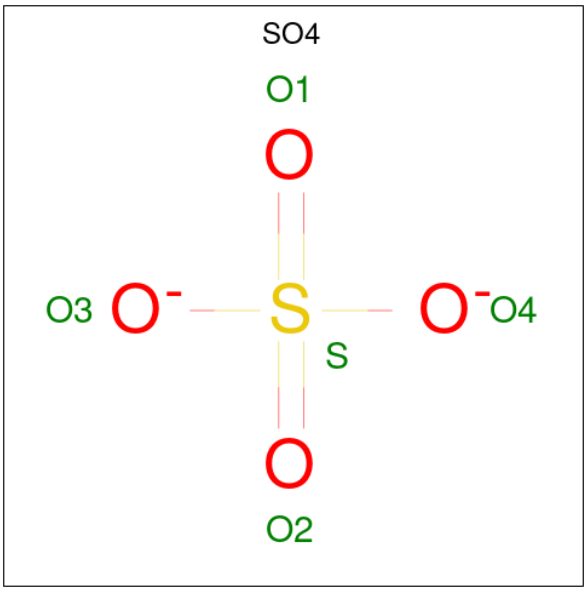
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	580	4656	2959	810	870	17	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	LYS	conflict	UNP P52026
A	411	ARG	ALA	conflict	UNP P52026
A	456	GLU	ALA	conflict	UNP P52026
A	505	LYS	GLU	conflict	UNP P52026
A	512	GLY	ARG	conflict	UNP P52026
A	550	THR	SER	conflict	UNP P52026
A	?	-	GLN	deletion	UNP P52026
A	823	HIS	ARG	conflict	UNP P52026

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

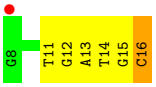
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	17	Total O 17 17	0	0
6	T	25	Total O 25 25	0	0
6	A	426	Total O 426 426	0	0

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.

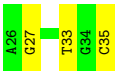
• Molecule 1: DNA (5'-D(*GP*CP*AP*TP*GP*AP*TP*GP*C)-3')

Chain P:



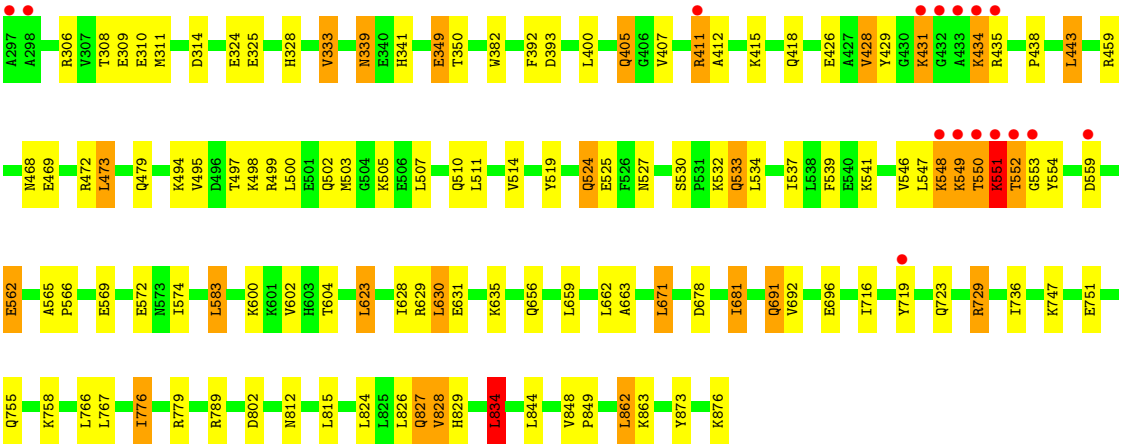
• Molecule 2: DNA (5'-D(P*AP*GP*CP*AP*TP*CP*AP*TP*GP*C)-3')

Chain T:



• Molecule 3: PROTEIN (DNA POLYMERASE I)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.24Å 93.28Å 106.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.68 – 1.65	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-1.80) 76.5 (19.68-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.65Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.241 , 0.276 0.198 , 0.236	Depositor DCC
R_{free} test set	3998 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	P	0.52	0/205	0.69	0/315
2	T	0.68	0/228	0.83	1/349 (0.3%)
3	A	0.51	0/4740	0.69	1/6405 (0.0%)
All	All	0.52	0/5173	0.70	2/7069 (0.0%)

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	P	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	834	LEU	CA-CB-CG	8.32	134.44	115.30
2	T	33	DT	C1'-O4'-C4'	-5.16	104.94	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	12	DG	Sidechain
1	P	16	DC	Sidechain

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	P	183	0	103	5	0
2	T	204	0	113	3	0
3	A	4656	0	4709	104	0
4	A	15	0	0	0	0
5	A	1	0	0	0	0
6	A	426	0	0	5	0
6	P	17	0	0	1	0
6	T	25	0	0	0	0
All	All	5527	0	4925	106	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 11.

All (106) 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)
3:A:692:VAL:HB	3:A:696:GLU:HG3	1.46	0.97
3:A:411:ARG:NH1	3:A:412:ALA:HA	1.83	0.94
3:A:431:LYS:H	3:A:434:LYS:HE2	1.34	0.88
3:A:426:GLU:CD	3:A:431:LYS:HD3	2.05	0.76
3:A:758:LYS:HG3	3:A:776:ILE:HG23	1.69	0.73
3:A:328:HIS:HD2	3:A:382:TRP:HE1	1.35	0.72
3:A:549:LYS:HD3	3:A:550:THR:O	1.89	0.72
3:A:498:LYS:O	3:A:502:GLN:HG3	1.93	0.67
3:A:550:THR:HG22	3:A:553:GLY:C	2.15	0.67
3:A:569:GLU:O	3:A:572:GLU:HG2	1.95	0.66
3:A:431:LYS:O	3:A:434:LYS:HG3	1.96	0.65
3:A:550:THR:HG23	3:A:551:LYS:HG2	1.77	0.65
3:A:729:ARG:H	3:A:729:ARG:CD	2.08	0.65
3:A:495:VAL:O	3:A:600:LYS:HE3	1.97	0.65
3:A:411:ARG:HG3	3:A:412:ALA:N	2.11	0.64
3:A:507:LEU:HD21	3:A:583:LEU:HB3	1.81	0.63
3:A:729:ARG:H	3:A:729:ARG:HD2	1.64	0.63
3:A:565:ALA:HB3	3:A:566:PRO:HD3	1.81	0.61
3:A:411:ARG:NH1	3:A:415:LYS:HB2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:DC:H5	3:A:629:ARG:HH22	1.48	0.59
3:A:411:ARG:NH1	3:A:415:LYS:HD2	2.17	0.59
3:A:549:LYS:NZ	3:A:553:GLY:H	2.00	0.59
3:A:524:GLN:HG2	3:A:525:GLU:N	2.18	0.58
3:A:623:LEU:HD23	3:A:826:LEU:HD21	1.85	0.58
3:A:510:GLN:O	3:A:514:VAL:HG23	2.02	0.58
3:A:392:PHE:HA	3:A:479:GLN:HE22	1.68	0.57
3:A:663:ALA:HB2	3:A:671:LEU:HD13	1.86	0.57
3:A:530:SER:HB3	3:A:533:GLN:HB2	1.85	0.57
3:A:758:LYS:HG3	3:A:776:ILE:CG2	2.34	0.56
3:A:827:GLN:NE2	3:A:829:HIS:H	2.04	0.56
3:A:431:LYS:H	3:A:434:LYS:CE	2.12	0.56
3:A:411:ARG:CG	6:A:1299:HOH:O	2.54	0.55
3:A:494:LYS:HZ1	3:A:600:LYS:HE2	1.72	0.54
1:P:11:DT:OP1	3:A:551:LYS:HD3	2.07	0.54
3:A:550:THR:O	3:A:551:LYS:C	2.46	0.54
3:A:539:PHE:CD1	3:A:546:VAL:HG22	2.41	0.54
3:A:333:VAL:HG13	3:A:443:LEU:HD11	1.89	0.53
3:A:339:ASN:ND2	3:A:341:HIS:H	2.06	0.53
3:A:824:LEU:HD23	3:A:834:LEU:HD22	1.91	0.53
3:A:339:ASN:C	3:A:339:ASN:HD22	2.12	0.53
6:P:1123:HOH:O	3:A:630:LEU:HD22	2.08	0.52
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.46	0.51
3:A:393:ASP:H	3:A:479:GLN:NE2	2.08	0.50
3:A:534:LEU:HD11	3:A:574:ILE:HD13	1.94	0.50
3:A:310:GLU:HG2	3:A:341:HIS:CG	2.46	0.50
3:A:349:GLU:H	3:A:349:GLU:CD	2.15	0.49
3:A:411:ARG:CZ	3:A:412:ALA:HA	2.42	0.49
3:A:631:GLU:OE2	3:A:635:LYS:HE3	2.12	0.49
3:A:411:ARG:HH11	3:A:415:LYS:HB2	1.75	0.49
3:A:527:ASN:H	3:A:533:GLN:NE2	2.11	0.48
3:A:411:ARG:HG3	6:A:1299:HOH:O	2.14	0.48
3:A:499:ARG:HG3	3:A:503:MET:CE	2.44	0.48
3:A:411:ARG:NH1	3:A:415:LYS:CD	2.77	0.48
3:A:604:THR:HB	3:A:623:LEU:HD22	1.96	0.48
3:A:339:ASN:HD22	3:A:341:HIS:H	1.62	0.48
3:A:411:ARG:CG	3:A:412:ALA:N	2.77	0.48
3:A:400:LEU:HD22	3:A:473:LEU:HD13	1.96	0.47
3:A:328:HIS:CD2	3:A:382:TRP:HE1	2.25	0.47
3:A:418:GLN:HA	6:A:1302:HOH:O	2.13	0.47
3:A:767:LEU:HG	3:A:802:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.95	0.47
3:A:494:LYS:HZ3	3:A:600:LYS:HE3	1.79	0.46
3:A:691:GLN:HG3	6:A:1415:HOH:O	2.14	0.46
3:A:308:THR:HG23	3:A:311:MET:CE	2.46	0.46
3:A:497:THR:OG1	3:A:600:LYS:HD2	2.16	0.46
3:A:405:GLN:HB3	3:A:407:VAL:HG23	1.97	0.46
2:T:27:DG:OP1	3:A:789:ARG:NH1	2.46	0.46
3:A:494:LYS:NZ	3:A:600:LYS:CE	2.79	0.46
1:P:15:DG:H2'	1:P:16:DC:C6	2.51	0.45
3:A:426:GLU:OE1	3:A:431:LYS:HD3	2.16	0.45
3:A:552:THR:HG23	3:A:552:THR:O	2.16	0.45
3:A:530:SER:CB	3:A:533:GLN:HB2	2.46	0.45
2:T:35:DC:H5"	3:A:532:LYS:CD	2.47	0.45
3:A:429:TYR:O	3:A:435:ARG:HA	2.17	0.44
3:A:431:LYS:HB3	3:A:434:LYS:HZ3	1.82	0.44
3:A:310:GLU:HG2	3:A:341:HIS:CB	2.48	0.44
3:A:473:LEU:HG	3:A:767:LEU:O	2.17	0.44
3:A:559:ASP:HA	3:A:562:GLU:OE1	2.17	0.44
3:A:873:TYR:O	3:A:876:LYS:HD3	2.18	0.43
3:A:499:ARG:HG3	3:A:503:MET:HE3	2.00	0.43
3:A:524:GLN:HE22	3:A:537:ILE:HD11	1.83	0.43
3:A:308:THR:HG23	3:A:311:MET:HE1	2.00	0.43
3:A:862:LEU:HD12	3:A:862:LEU:HA	1.88	0.43
1:P:13:DA:H2'	1:P:14:DT:C6	2.54	0.43
3:A:747:LYS:O	3:A:751:GLU:HG3	2.19	0.43
3:A:431:LYS:HB3	3:A:431:LYS:NZ	2.34	0.42
3:A:324:GLU:HG2	6:A:1055:HOH:O	2.19	0.42
3:A:502:GLN:O	3:A:505:LYS:HB3	2.19	0.42
3:A:828:VAL:O	3:A:828:VAL:HG22	2.18	0.42
3:A:411:ARG:HD2	3:A:411:ARG:C	2.40	0.42
3:A:550:THR:HG22	3:A:553:GLY:O	2.19	0.42
3:A:549:LYS:HE3	3:A:552:THR:HA	2.00	0.42
3:A:494:LYS:HZ1	3:A:600:LYS:CE	2.33	0.41
3:A:431:LYS:CB	3:A:434:LYS:NZ	2.84	0.41
3:A:656:GLN:CD	3:A:681:ILE:HD11	2.41	0.41
3:A:468:ASN:O	3:A:469:GLU:HB2	2.21	0.41
3:A:339:ASN:HD22	3:A:341:HIS:N	2.18	0.41
3:A:623:LEU:HD12	3:A:623:LEU:HA	1.92	0.41
3:A:681:ILE:H	3:A:681:ILE:HG13	1.58	0.41
3:A:678:ASP:OD2	3:A:863:LYS:HE3	2.21	0.41
3:A:428:VAL:HG23	3:A:438:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:35:DC:H5"	3:A:532:LYS:HD2	2.03	0.40
1:P:15:DG:OP1	3:A:629:ARG:HD2	2.21	0.40
3:A:551:LYS:CG	3:A:552:THR:H	2.35	0.40
3:A:565:ALA:N	3:A:566:PRO:CD	2.85	0.40
3:A:716:ILE:HG12	3:A:736:ILE:HG12	2.02	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
3	A	578/580 (100%)	561 (97%)	14 (2%)	3 (0%)	29 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	551	LYS
3	A	548	LYS
3	A	628	ILE

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
3	A	496/496 (100%)	443 (89%)	53 (11%)	6 1

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	306	ARG
3	A	309	GLU
3	A	314	ASP
3	A	325	GLU
3	A	333	VAL
3	A	339	ASN
3	A	349	GLU
3	A	350	THR
3	A	405	GLN
3	A	411	ARG
3	A	428	VAL
3	A	431	LYS
3	A	434	LYS
3	A	443	LEU
3	A	459	ARG
3	A	472	ARG
3	A	473	LEU
3	A	500	LEU
3	A	511	LEU
3	A	524	GLN
3	A	533	GLN
3	A	541	LYS
3	A	547	LEU
3	A	548	LYS
3	A	549	LYS
3	A	550	THR
3	A	551	LYS
3	A	552	THR
3	A	554	TYR
3	A	562	GLU
3	A	583	LEU
3	A	602	VAL
3	A	623	LEU
3	A	630	LEU
3	A	659	LEU
3	A	662	LEU
3	A	671	LEU
3	A	681	ILE
3	A	691	GLN
3	A	719	TYR
3	A	723	GLN
3	A	729	ARG

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Mol	Chain	Res	Type
3	A	755	GLN
3	A	766	LEU
3	A	776	ILE
3	A	779	ARG
3	A	812	ASN
3	A	815	LEU
3	A	827	GLN
3	A	828	VAL
3	A	834	LEU
3	A	844	LEU
3	A	862	LEU

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

Mol	Chain	Res	Type
3	A	328	HIS
3	A	339	ASN
3	A	479	GLN
3	A	543	GLN
3	A	724	ASN
3	A	812	ASN
3	A	827	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	SO4	A	912	-	4,4,4	2.37	4 (100%)	6,6,6	0.22	0
4	SO4	A	910	-	4,4,4	2.38	4 (100%)	6,6,6	0.15	0
4	SO4	A	911	-	4,4,4	2.45	4 (100%)	6,6,6	0.17	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	911	SO4	O4-S	2.57	1.69	1.47
4	A	912	SO4	O4-S	2.56	1.69	1.47
4	A	910	SO4	O4-S	2.54	1.68	1.47
4	A	911	SO4	O3-S	2.45	1.68	1.47
4	A	912	SO4	O3-S	2.39	1.67	1.47
4	A	911	SO4	O2-S	2.39	1.59	1.46
4	A	910	SO4	O2-S	2.39	1.58	1.46
4	A	911	SO4	O1-S	2.38	1.58	1.46
4	A	910	SO4	O3-S	2.36	1.67	1.47
4	A	912	SO4	O1-S	2.26	1.58	1.46
4	A	912	SO4	O2-S	2.26	1.58	1.46
4	A	910	SO4	O1-S	2.22	1.58	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	P	9/9 (100%)	-0.01	1 (11%) 5 4	14, 20, 47, 48	0
2	T	10/10 (100%)	-0.58	0 100 100	12, 20, 37, 40	0
3	A	580/580 (100%)	-0.20	16 (2%) 53 47	9, 18, 40, 55	0
All	All	599/599 (100%)	-0.20	17 (2%) 53 47	9, 18, 40, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	552	THR	8.6
3	A	553	GLY	8.0
3	A	433	ALA	6.8
3	A	550	THR	6.8
3	A	434	LYS	6.2
3	A	549	LYS	5.2
3	A	719	TYR	5.1
3	A	551	LYS	4.6
3	A	431	LYS	4.2
3	A	298	ALA	3.8
3	A	297	ALA	3.1
3	A	559	ASP	2.9
1	P	8	DG	2.9
3	A	548	LYS	2.7
3	A	432	GLY	2.5
3	A	411	ARG	2.1
3	A	435	ARG	2.0

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

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	910	5/5	0.96	0.15	33,34,35,35	5
4	SO4	A	912	5/5	0.96	0.14	40,40,41,43	0
4	SO4	A	911	5/5	0.98	0.09	33,33,34,34	5
5	MG	A	950	1/1	0.99	0.07	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.