



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3EZ5
Title : Cocystal structure of Bacillus fragment DNA polymerase I with duplex DNA
, dCTP, and zinc (closed form).
Authors : Warren, J.J.; Wu, E.Y.; Golosov, A.A.; Karplus, M.; Beese, L.S.
Deposited on : 2008-10-22
Resolution : 1.90 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

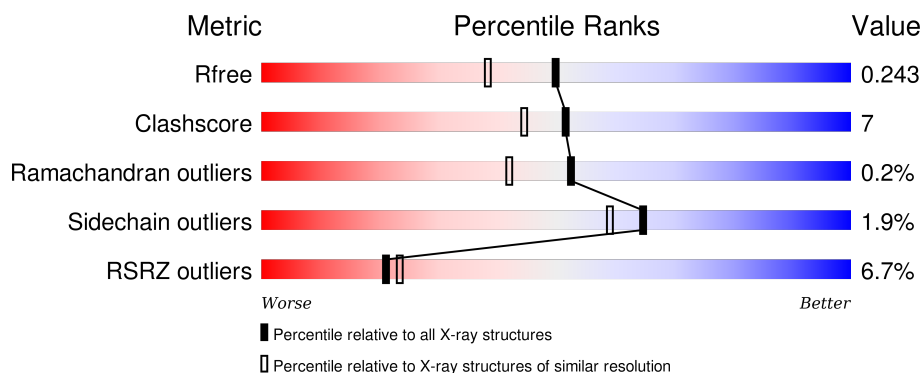
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	580	<div> <div>12%</div> <div>83%</div> <div>16%</div> </div>
1	D	580	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
2	B	9	<div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
2	E	9	<div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
3	C	12	<div> <div>8%</div> <div>50%</div> <div>42%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	12	

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	DAD	A	201	X	-	-	-
4	DAD	D	202	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10822 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	1	0
			4660	2963	811	869	17			
1	D	579	Total	C	N	O	S	0	1	0
			4652	2958	807	870	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	710	TYR	PHE	ENGINEERED	PDB 3EZ5
D	710	TYR	PHE	ENGINEERED	PDB 3EZ5

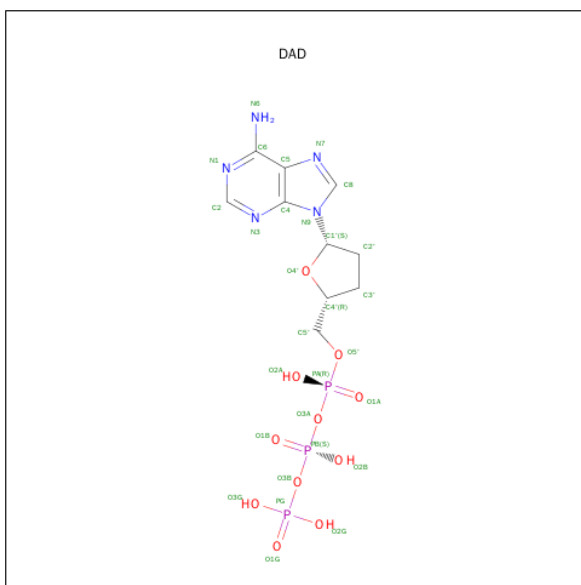
- Molecule 2 is a DNA chain called 5'-D(*DCP*DCP*DTP*DGP*DAP*DCP*DTP*DCP*D G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			

- Molecule 3 is a DNA chain called 5'-D(*DAP*DTP*DTP*DCP*DGP*DAP*DGP*DTP*DCP*DAP*DGP*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			246	118	47	70	11			
3	F	12	Total	C	N	O	P	0	0	0
			246	118	47	70	11			

- Molecule 4 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: DAD) (formula: C₁₀H₁₆N₅O₁₁P₃).

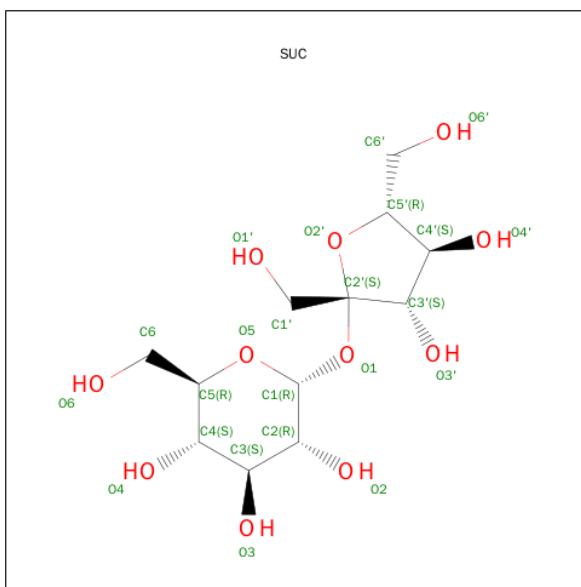


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 29	C 10	N 5	O 11	P 3	0	0
4	D	1	Total 29	C 10	N 5	O 11	P 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

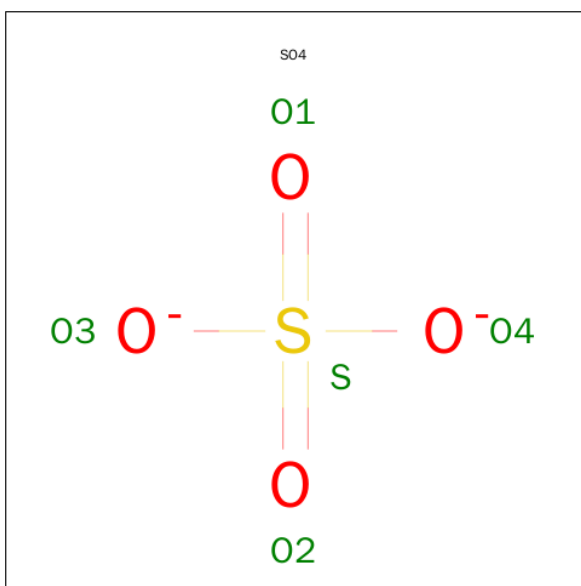
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	D	3	Total Zn 3 3	0	0

- Molecule 6 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			23	12	11		
6	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

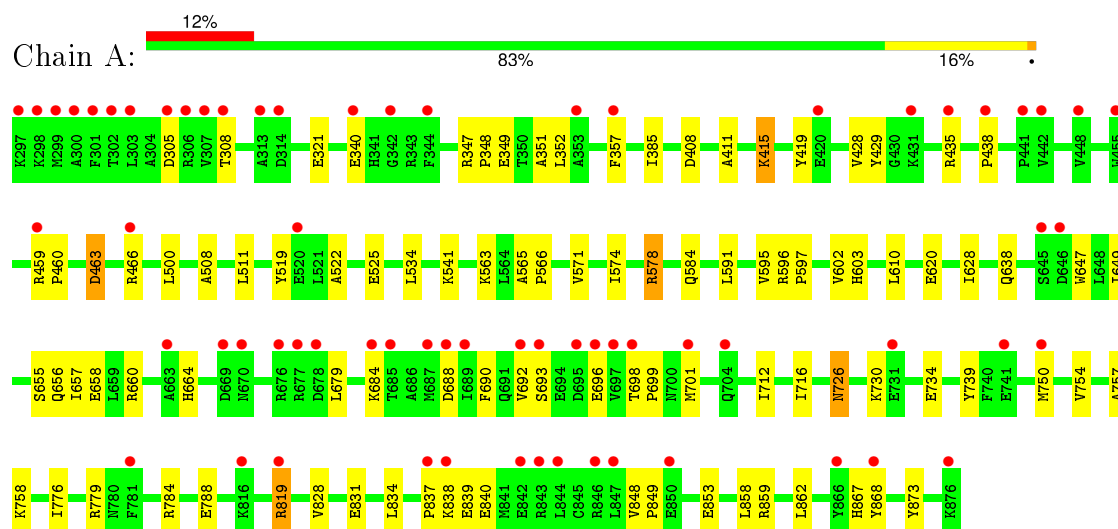
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	154	Total	O	0	0
			154	154		
8	D	290	Total	O	0	0
			290	290		
8	B	20	Total	O	0	0
			20	20		
8	C	20	Total	O	0	0
			20	20		
8	E	19	Total	O	0	0
			19	19		
8	F	37	Total	O	0	0
			37	37		

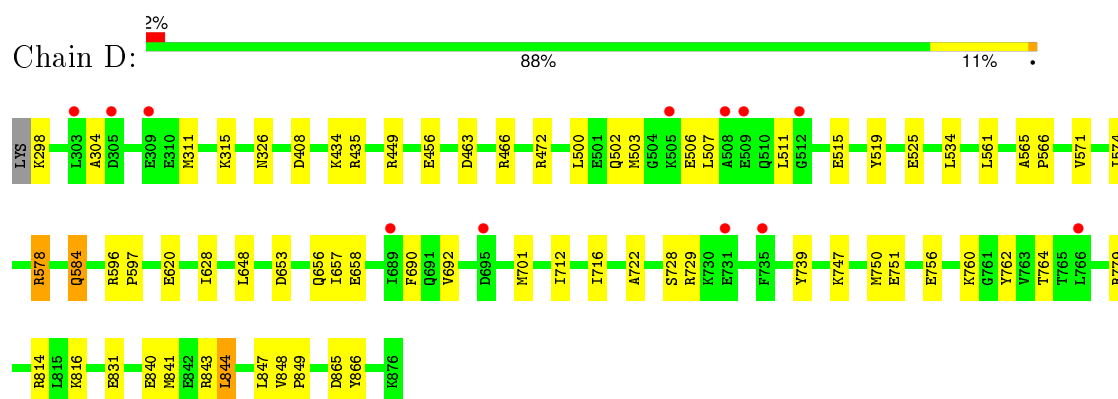
3 Residue-property plots

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.

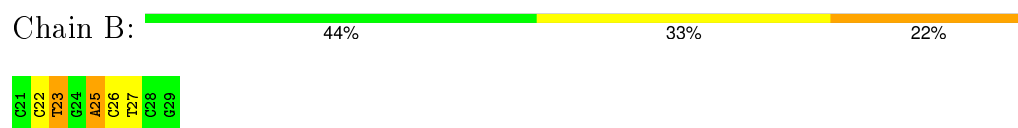
• Molecule 1: DNA polymerase I



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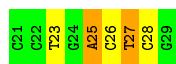


• Molecule 2: 5'-D(*DCP*DCP*DTP*DGP*DAP*DCP*DTP*DCP*DG)-3'



• Molecule 2: 5'-D(*DCP*DCP*DTP*DGP*DAP*DCP*DTP*DCP*DG)-3'

Chain E:  44% 33% 22%



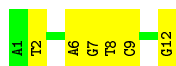
● Molecule 3: 5'-D(*DAP*DTP*DTP*DCP*DGP*DAP*DGP*DTP*DCP*DAP*DGP*DG)-3',

Chain C:  8% 50% 42% 8%



● Molecule 3: 5'-D(*DAP*DTP*DTP*DCP*DGP*DAP*DGP*DTP*DCP*DAP*DGP*DG)-3',

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.55Å 108.57Å 149.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 1.90 46.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.83-1.90) 100.0 (46.83-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.211 , 0.244 0.210 , 0.243	Depositor DCC
R_{free} test set	5010 reflections (4.39%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 119138 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10822	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DAD, ZN, SUC, 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	0.44	0/4747	0.58	1/6415 (0.0%)
1	D	0.57	0/4739	0.65	1/6404 (0.0%)
2	B	1.02	0/197	1.95	7/301 (2.3%)
2	E	1.06	0/197	1.97	8/301 (2.7%)
3	C	1.07	0/276	1.71	7/425 (1.6%)
3	F	1.08	0/276	1.66	6/425 (1.4%)
All	All	0.58	0/10432	0.82	30/14271 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	DA	O4'-C4'-C3'	-9.93	100.04	106.00
3	C	2	DT	O4'-C1'-N1	9.39	114.57	108.00
3	C	8	DT	O4'-C1'-N1	-9.20	101.56	108.00
2	E	27	DT	O4'-C4'-C3'	-8.45	100.93	106.00
2	E	23	DT	O4'-C1'-N1	-8.07	102.35	108.00
3	F	2	DT	O4'-C1'-N1	8.07	113.65	108.00
2	E	23	DT	N3-C4-O4	7.25	124.25	119.90
3	F	8	DT	O4'-C1'-N1	-7.22	102.94	108.00
2	B	25	DA	O5'-P-OP2	-7.01	99.39	105.70
3	C	2	DT	C1'-O4'-C4'	-6.80	103.30	110.10
2	B	23	DT	O4'-C1'-N1	-6.67	103.33	108.00
1	A	578	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	F	12	DG	O4'-C1'-N9	6.55	112.58	108.00
3	C	3	DT	N3-C4-O4	6.50	123.80	119.90
2	E	23	DT	C5-C4-O4	-6.36	120.45	124.90
2	B	25	DA	C5'-C4'-C3'	6.28	125.40	114.10
2	B	27	DT	O4'-C4'-C3'	-6.18	102.03	104.50
3	F	7	DG	O4'-C1'-N9	-6.13	103.71	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	DG	O4'-C1'-N9	-6.00	103.80	108.00
2	B	27	DT	O4'-C1'-N1	5.87	112.11	108.00
3	F	9	DC	N1-C2-O2	-5.79	115.43	118.90
2	E	25	DA	C5'-C4'-C3'	5.77	124.48	114.10
3	C	5	DG	O4'-C4'-C3'	-5.58	102.27	104.50
2	B	23	DT	N3-C2-O2	-5.42	119.05	122.30
3	C	3	DT	C5-C4-O4	-5.37	121.14	124.90
2	E	28	DC	O4'-C4'-C3'	-5.32	102.37	104.50
3	F	6	DA	O4'-C1'-C2'	5.30	110.14	105.90
2	E	25	DA	O5'-P-OP2	-5.26	100.97	105.70
2	E	25	DA	N1-C6-N6	5.21	121.73	118.60
1	D	578	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4660	0	4720	81	0
1	D	4652	0	4709	50	0
2	B	177	0	101	3	0
2	E	177	0	101	3	0
3	C	246	0	137	3	0
3	F	246	0	137	0	0
4	A	29	0	12	2	0
4	D	29	0	12	1	0
5	A	2	0	0	0	0
5	D	3	0	0	0	0
6	A	23	0	22	2	0
6	D	23	0	22	1	0
7	A	10	0	0	1	0
7	D	5	0	0	0	0
8	A	154	0	0	5	0
8	B	20	0	0	0	0
8	C	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	290	0	0	8	0
8	E	19	0	0	0	0
8	F	37	0	0	0	0
All	All	10822	0	9973	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (138) 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:408:ASP:HB2	6:A:877:SUC:H1'	1.19	1.16
1:A:819:ARG:HG3	1:A:819:ARG:HH11	1.01	1.15
1:A:819:ARG:HG3	1:A:819:ARG:NH1	1.82	0.87
1:A:522:ALA:O	1:A:541:LYS:HE2	1.74	0.87
1:D:653[A]:ASP:OD1	1:D:831:GLU:HB2	1.75	0.86
1:A:739:TYR:HD2	8:A:917:HOH:O	1.58	0.86
1:D:750:MET:HG3	8:D:938:HOH:O	1.83	0.77
1:D:561:LEU:HB3	1:D:571:VAL:HG13	1.66	0.76
1:A:408:ASP:HB2	6:A:877:SUC:C1'	2.08	0.75
1:A:656:GLN:HB2	1:A:660:ARG:NH1	2.01	0.75
1:D:561:LEU:O	1:D:571:VAL:HG11	1.87	0.74
1:D:456:GLU:HG2	8:D:929:HOH:O	1.88	0.72
1:A:519:TYR:CD2	1:A:525:GLU:HG2	2.25	0.71
1:D:578:ARG:NH2	2:E:25:DA:H5"	2.05	0.70
1:A:679:LEU:HD13	1:A:684:LYS:NZ	2.06	0.70
3:C:1:DA:H2"	3:C:2:DT:O5'	1.92	0.69
1:A:739:TYR:CD2	8:A:917:HOH:O	2.39	0.69
1:D:690:PHE:CG	1:D:701:MET:HE3	2.29	0.68
1:A:819:ARG:CG	1:A:819:ARG:HH11	1.92	0.65
1:A:656:GLN:HB2	1:A:660:ARG:HH12	1.62	0.64
1:D:653[B]:ASP:OD1	1:D:865:ASP:O	2.17	0.62
1:A:656:GLN:HA	4:A:201:DAD:O1B	2.00	0.61
1:D:690:PHE:CB	1:D:701:MET:HE3	2.31	0.61
1:D:298:LYS:HB3	1:D:449:ARG:NH2	2.16	0.60
1:D:534:LEU:HD11	1:D:574:ILE:HD13	1.82	0.60
1:A:784:ARG:O	1:A:788:GLU:HG3	2.01	0.60
1:A:596[B]:ARG:NH1	8:A:920:HOH:O	2.35	0.59
1:A:828:VAL:HB	1:A:831:GLU:HG3	1.85	0.59
1:A:411:ALA:O	1:A:415:LYS:HG2	2.03	0.58
1:D:690:PHE:O	1:D:692:VAL:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.84	0.58
1:D:690:PHE:CD2	1:D:701:MET:HE3	2.38	0.58
1:A:305:ASP:HB3	1:A:347:ARG:HH12	1.68	0.57
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.85	0.57
1:A:459:ARG:HB2	1:A:460:PRO:HD3	1.86	0.57
1:A:657:ILE:HG23	1:A:658:GLU:N	2.20	0.56
1:D:656:GLN:HA	4:D:202:DAD:O1B	2.05	0.56
8:A:884:HOH:O	3:C:2:DT:H71	2.05	0.56
1:A:563:LYS:HG2	1:A:726:ASN:HD21	1.69	0.56
3:C:2:DT:H6	8:C:328:HOH:O	1.88	0.56
1:D:840:GLU:O	1:D:844:LEU:HD22	2.07	0.55
1:D:692:VAL:HG21	1:D:701:MET:HE1	1.88	0.55
1:D:712:ILE:HA	1:D:716:ILE:HG22	1.89	0.55
1:D:408:ASP:HB2	6:D:877:SUC:H1'1	1.88	0.55
1:D:739:TYR:C	1:D:739:TYR:CD2	2.81	0.53
1:A:664:HIS:CE1	1:A:859:ARG:HH11	2.25	0.53
1:A:838:LYS:HG3	1:A:839:GLU:OE2	2.08	0.53
1:D:519:TYR:CD2	1:D:525:GLU:HG2	2.43	0.53
1:A:349:GLU:H	1:A:349:GLU:CD	2.12	0.53
1:A:754:VAL:O	1:A:758:LYS:HG3	2.10	0.51
1:A:858:LEU:HD12	1:A:862:LEU:HD21	1.92	0.51
1:D:722:ALA:HB2	1:D:729:ARG:HA	1.93	0.50
1:D:304:ALA:HB2	1:D:311:MET:HE2	1.93	0.50
1:A:591:LEU:O	1:A:595:VAL:HG23	2.12	0.50
1:A:351:ALA:HB1	1:A:357:PHE:CD2	2.47	0.49
1:A:578:ARG:NH2	2:B:25:DA:H5''	2.27	0.49
1:A:839:GLU:CD	1:A:839:GLU:H	2.16	0.49
1:A:679:LEU:HD13	1:A:684:LYS:HZ1	1.76	0.49
1:D:298:LYS:NZ	8:D:961:HOH:O	2.46	0.48
1:A:690:PHE:CG	1:A:701:MET:HE3	2.49	0.48
1:A:658:GLU:CD	4:A:201:DAD:H2'1	2.34	0.48
1:D:648:LEU:HD12	1:D:841:MET:HG3	1.96	0.48
1:A:610:LEU:HD23	1:A:610:LEU:C	2.34	0.48
2:B:22:DC:H1'	2:B:23:DT:H5'	1.96	0.48
1:A:308:THR:HA	7:A:1:SO4:O4	2.14	0.48
1:A:596[B]:ARG:NH1	1:A:603:HIS:HD2	2.11	0.48
1:A:837:PRO:HG2	1:A:840:GLU:HG3	1.96	0.48
1:D:762:TYR:HE1	1:D:764:THR:CG2	2.27	0.48
1:D:298:LYS:HB3	1:D:449:ARG:HH22	1.78	0.47
1:A:508:ALA:HB2	1:A:584:GLN:HE22	1.80	0.47
1:D:456:GLU:CG	8:D:929:HOH:O	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PRO:HD2	1:A:349:GLU:OE2	2.14	0.47
1:A:500:LEU:HD21	1:A:591:LEU:HD23	1.96	0.47
1:D:584:GLN:HE21	1:D:584:GLN:HA	1.80	0.47
1:A:690:PHE:CE2	1:A:701:MET:HB3	2.50	0.47
1:D:816:LYS:HD3	1:D:816:LYS:HA	1.66	0.47
1:D:843:ARG:HD2	8:D:965:HOH:O	2.14	0.46
1:D:690:PHE:HB2	1:D:701:MET:CE	2.45	0.46
1:A:660:ARG:HG3	1:A:660:ARG:HH11	1.79	0.46
1:A:459:ARG:N	1:A:460:PRO:CD	2.79	0.46
1:D:657:ILE:HG23	1:D:658:GLU:N	2.31	0.46
1:D:747:LYS:HE2	1:D:751:GLU:OE1	2.16	0.46
1:D:750:MET:CG	8:D:938:HOH:O	2.54	0.46
1:A:849:PRO:O	1:A:853:GLU:HG3	2.16	0.45
1:A:693:SER:OG	1:A:696:GLU:HG3	2.16	0.45
1:A:595:VAL:HG22	1:A:602:VAL:HG13	1.99	0.45
1:D:463:ASP:OD2	1:D:466:ARG:NH2	2.50	0.45
1:A:415:LYS:HE2	1:A:419:TYR:O	2.16	0.45
1:D:326:ASN:HD22	1:D:620:GLU:CD	2.20	0.45
1:A:819:ARG:CG	1:A:819:ARG:NH1	2.63	0.45
1:D:866:TYR:N	1:D:866:TYR:CD2	2.85	0.45
1:A:657:ILE:HG23	1:A:658:GLU:H	1.80	0.45
1:A:647:TRP:CE2	1:A:837:PRO:HD3	2.52	0.44
1:A:730:LYS:O	1:A:734:GLU:HG3	2.16	0.44
1:A:664:HIS:CE1	1:A:859:ARG:NH1	2.85	0.44
1:A:757:ALA:HB3	1:A:776:ILE:HD13	1.99	0.44
1:A:757:ALA:CB	1:A:776:ILE:HD13	2.48	0.44
1:D:503:MET:O	1:D:507:LEU:HB2	2.18	0.44
1:A:828:VAL:HB	1:A:831:GLU:CG	2.47	0.44
1:A:595:VAL:HG22	1:A:602:VAL:CG1	2.47	0.44
1:D:565:ALA:N	1:D:566:PRO:CD	2.80	0.44
1:A:638:GLN:HG3	1:A:873:TYR:CG	2.52	0.44
1:A:664:HIS:O	1:A:859:ARG:HD2	2.18	0.43
1:A:428:VAL:HG12	1:A:438:PRO:HG3	2.00	0.43
1:A:690:PHE:CB	1:A:701:MET:HE3	2.48	0.43
1:A:834:LEU:N	1:A:834:LEU:HD12	2.33	0.43
2:E:25:DA:H2'	2:E:26:DC:C6	2.54	0.43
1:A:867:HIS:CE1	8:A:7:HOH:O	2.71	0.43
1:A:698:THR:HB	1:A:699:PRO:HD2	2.00	0.43
1:D:472:ARG:NH1	8:D:989:HOH:O	2.51	0.43
1:A:750:MET:O	1:A:754:VAL:HG23	2.19	0.43
1:A:596[B]:ARG:HH12	1:A:603:HIS:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HD3	1:A:415:LYS:HA	1.75	0.42
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.50	0.42
1:A:649:ILE:O	1:A:868:TYR:HA	2.19	0.42
1:A:463:ASP:HA	1:A:466:ARG:NH1	2.34	0.42
1:A:534:LEU:HD11	1:A:574:ILE:HD13	2.01	0.42
1:D:315:LYS:HD2	8:D:988:HOH:O	2.18	0.42
2:E:26:DC:H2'	2:E:27:DT:C6	2.55	0.42
1:A:596[B]:ARG:NH1	1:A:603:HIS:CD2	2.88	0.42
1:D:848:VAL:HB	1:D:849:PRO:HD3	2.01	0.42
1:A:596[A]:ARG:HA	1:A:597:PRO:HD3	1.82	0.42
1:A:565:ALA:HA	1:A:571:VAL:HG21	2.01	0.42
1:D:756:GLU:OE2	1:D:760:LYS:HE2	2.20	0.41
1:D:840:GLU:O	1:D:844:LEU:CD2	2.68	0.41
1:A:828:VAL:HG12	1:A:828:VAL:O	2.21	0.41
1:D:596:ARG:HA	1:D:597:PRO:HD3	1.90	0.41
2:B:25:DA:H2'	2:B:26:DC:C6	2.56	0.41
1:A:321:GLU:OE2	1:A:429:TYR:OH	2.35	0.41
1:A:712:ILE:HA	1:A:716:ILE:HG22	2.03	0.41
1:D:502:GLN:O	1:D:506:GLU:HG3	2.21	0.41
1:D:690:PHE:CD2	1:D:701:MET:CE	3.04	0.41
1:A:500:LEU:HA	1:A:500:LEU:HD12	1.94	0.40
1:A:565:ALA:N	1:A:566:PRO:CD	2.83	0.40
1:D:814:ARG:NH2	1:D:847:LEU:HD13	2.36	0.40
1:A:352:LEU:HD22	1:A:385:ILE:HD13	2.04	0.40
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.57	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	579/580 (100%)	560 (97%)	18 (3%)	1 (0%)	52	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	578/580 (100%)	566 (98%)	11 (2%)	1 (0%)	52	42
All	All	1157/1160 (100%)	1126 (97%)	29 (2%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	496/496 (100%)	485 (98%)	11 (2%)	60	53
1	D	496/496 (100%)	488 (98%)	8 (2%)	70	66
All	All	992/992 (100%)	973 (98%)	19 (2%)	65	59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	GLU
1	A	415	LYS
1	A	435	ARG
1	A	463	ASP
1	A	511	LEU
1	A	620	GLU
1	A	655	SER
1	A	688	ASP
1	A	726	ASN
1	A	779	ARG
1	A	819	ARG
1	D	434	LYS
1	D	435	ARG
1	D	500	LEU

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Mol	Chain	Res	Type
1	D	511	LEU
1	D	584	GLN
1	D	728	SER
1	D	779	ARG
1	D	844	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	584	GLN
1	A	724	ASN
1	A	726	ASN
1	D	502	GLN
1	D	584	GLN
1	D	823	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 12 ligands modelled in this entry, 5 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
7	SO4	A	1	-	4,4,4	0.29	0	6,6,6	0.21	0
7	SO4	A	2	-	4,4,4	0.04	0	6,6,6	0.18	0
4	DAD	A	201	5	23,31,31	2.75	8 (34%)	28,48,48	2.50	9 (32%)
6	SUC	A	877	-	24,24,24	0.37	0	36,36,36	0.78	0
4	DAD	D	202	5	23,31,31	2.50	6 (26%)	28,48,48	2.18	8 (28%)
6	SUC	D	877	-	24,24,24	0.41	0	36,36,36	0.90	1 (2%)
7	SO4	D	878	-	4,4,4	0.41	0	6,6,6	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	A	1	-	-	0/0/0/0	0/0/0/0
7	SO4	A	2	-	-	0/0/0/0	0/0/0/0
4	DAD	A	201	5	2/2/5/5	0/18/31/31	0/3/3/3
6	SUC	A	877	-	-	0/12/51/51	0/2/2/2
4	DAD	D	202	5	2/2/5/5	0/18/31/31	0/3/3/3
6	SUC	D	877	-	-	0/12/51/51	0/2/2/2
7	SO4	D	878	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	DAD	PA-O1A	2.12	1.58	1.51
4	D	202	DAD	PG-O1G	2.24	1.58	1.51
4	A	201	DAD	PB-O1B	2.41	1.60	1.51
4	D	202	DAD	C5-C4	2.60	1.46	1.40
4	A	201	DAD	PG-O1G	2.75	1.60	1.51
4	A	201	DAD	C5-C4	3.19	1.47	1.40
4	D	202	DAD	PA-O2A	4.89	1.75	1.54
4	A	201	DAD	PA-O2A	5.09	1.76	1.54
4	D	202	DAD	PB-O2B	5.18	1.77	1.54
4	A	201	DAD	PB-O2B	5.23	1.77	1.54
4	D	202	DAD	PG-O2G	5.84	1.75	1.54
4	D	202	DAD	PG-O3G	6.02	1.76	1.54
4	A	201	DAD	PG-O3G	6.17	1.76	1.54
4	A	201	DAD	PG-O2G	6.86	1.79	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	DAD	N3-C2-N1	-9.18	121.86	128.89
4	D	202	DAD	N3-C2-N1	-6.67	123.79	128.89
4	A	201	DAD	C2'-C1'-N9	-5.32	101.71	112.49
4	D	202	DAD	C2'-C1'-N9	-4.65	103.07	112.49
4	D	202	DAD	C4-C5-N7	-3.10	106.63	109.48
4	A	201	DAD	PA-O3A-PB	-2.99	124.33	132.73
4	D	202	DAD	PA-O3A-PB	-2.92	124.52	132.73
4	D	202	DAD	O4'-C1'-C2'	-2.64	103.81	106.67
4	A	201	DAD	C4-C5-N7	-2.34	107.33	109.48
6	D	877	SUC	O6'-C6'-C5'	-2.16	104.20	111.33
4	D	202	DAD	PB-O3B-PG	-2.02	125.90	132.67
4	A	201	DAD	O4'-C4'-C5'	2.06	112.58	109.54
4	A	201	DAD	O2A-PA-O3A	2.15	114.83	105.09
4	A	201	DAD	C2-N1-C6	2.16	122.63	118.77
4	A	201	DAD	O2B-PB-O3B	2.38	115.90	105.09
4	A	201	DAD	O4'-C1'-N9	2.52	112.09	107.72
4	D	202	DAD	O2B-PB-O3B	2.88	118.15	105.09
4	D	202	DAD	C3'-C2'-C1'	2.94	106.00	102.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	201	DAD	C4'
4	A	201	DAD	C1'
4	D	202	DAD	C4'
4	D	202	DAD	C1'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	SO4	1	0
4	A	201	DAD	2	0
6	A	877	SUC	2	0
4	D	202	DAD	1	0
6	D	877	SUC	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 ⓘ

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	580/580 (100%)	0.73	67 (11%) 6 7	23, 41, 61, 70	0
1	D	579/580 (99%)	0.36	12 (2%) 67 70	17, 30, 48, 60	0
2	B	9/9 (100%)	-0.20	0 100 100	26, 28, 43, 54	0
2	E	9/9 (100%)	-0.25	0 100 100	20, 28, 40, 51	0
3	C	12/12 (100%)	0.21	1 (8%) 14 15	24, 30, 67, 87	0
3	F	12/12 (100%)	-0.02	0 100 100	19, 26, 56, 73	0
All	All	1201/1202 (99%)	0.52	80 (6%) 21 23	17, 35, 58, 87	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	LYS	5.2
1	A	677	ARG	4.8
1	A	819	ARG	4.7
1	A	693	SER	4.6
1	A	696	GLU	4.1
1	A	678	ASP	3.6
1	A	297	LYS	3.5
1	A	685	THR	3.5
1	A	353	ALA	3.5
1	A	306	ARG	3.3
3	C	1	DA	3.2
1	A	876	LYS	3.2
1	A	695	ASP	3.2
1	A	846	ARG	3.2
1	A	684	LYS	3.1
1	A	442	VAL	3.1
1	D	689	ILE	3.1
1	A	300	ALA	3.0
1	A	692	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	505	LYS	3.0
1	A	781	PHE	3.0
1	A	698	THR	3.0
1	A	842	GLU	2.9
1	A	431	LYS	2.9
1	A	303	LEU	2.9
1	A	868	TYR	2.9
1	A	843	ARG	2.9
1	A	466	ARG	2.8
1	A	646	ASP	2.8
1	D	512	GLY	2.8
1	D	509	GLU	2.7
1	A	301	PHE	2.7
1	A	307	VAL	2.7
1	A	847	LEU	2.7
1	A	816	LYS	2.7
1	A	459	ARG	2.6
1	A	687	MET	2.6
1	A	435	ARG	2.6
1	A	697	VAL	2.6
1	A	645	SER	2.6
1	A	689	ILE	2.5
1	A	850	GLU	2.5
1	A	342	GLY	2.5
1	D	766	LEU	2.5
1	A	441	PRO	2.5
1	A	314	ASP	2.4
1	A	837	PRO	2.4
1	D	731	GLU	2.4
1	A	344	PHE	2.4
1	A	688	ASP	2.4
1	D	735	PHE	2.4
1	A	676	ARG	2.4
1	A	838	LYS	2.4
1	A	750	MET	2.4
1	A	520	GLU	2.3
1	A	741	GLU	2.3
1	A	305	ASP	2.3
1	A	844	LEU	2.3
1	A	302	THR	2.3
1	D	695	ASP	2.2
1	D	508	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	THR	2.2
1	A	420	GLU	2.2
1	A	731	GLU	2.2
1	D	309	GLU	2.2
1	A	313	ALA	2.2
1	A	448	VAL	2.1
1	A	663	ALA	2.1
1	A	701	MET	2.1
1	A	438	PRO	2.1
1	A	866	TYR	2.1
1	A	669	ASP	2.1
1	D	305	ASP	2.1
1	A	670	ASN	2.1
1	A	704	GLN	2.1
1	A	455	TRP	2.0
1	A	340	GLU	2.0
1	A	357	PHE	2.0
1	D	303	LEU	2.0
1	A	299	MET	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 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
6	SUC	A	877	23/23	0.86	0.16	1.66	47,51,52,55	0
5	ZN	D	2	1/1	0.96	0.23	1.17	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SO4	A	2	5/5	0.97	0.14	0.58	45,45,47,47	0
6	SUC	D	877	23/23	0.93	0.12	-0.32	30,35,37,37	0
4	DAD	D	202	29/29	0.98	0.11	-0.36	16,23,30,32	0
4	DAD	A	201	29/29	0.94	0.11	-1.32	32,35,42,44	0
5	ZN	D	1	1/1	0.99	0.04	-2.91	29,29,29,29	1
5	ZN	A	4	1/1	0.99	0.08	-3.10	29,29,29,29	1
5	ZN	A	5	1/1	0.91	0.13	-	32,32,32,32	1
7	SO4	D	878	5/5	0.96	0.15	-	46,46,49,50	0
7	SO4	A	1	5/5	0.92	0.24	-	80,81,81,81	0
5	ZN	D	3	1/1	0.39	0.40	-	46,46,46,46	1

6.5 Other polymers [i](#)

There are no such residues in this entry.