



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:55 PM GMT

PDB ID : 1D8Y  
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF DNA POLYMERASE I  
KLENOW FRAGMENT WITH DNA  
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Deposited on : 1999-10-26  
Resolution : 2.08 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](mailto: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.

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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

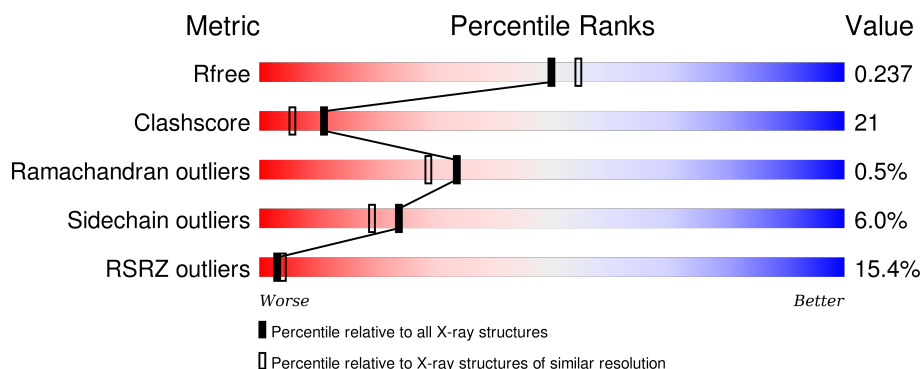
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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  $\geq 3$ , 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	B	19	
2	A	605	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5157 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 D(T)19 OLIGOMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	4	Total	C	N	O	P	0	0	1
			61	30	6	22	3			

- Molecule 2 is a protein called DNA POLYMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	601	Total	C	N	O	S	0	0	0
			4745	3005	830	894	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	MET	VAL	ENGINEERED	UNP P00582
A	355	ALA	ASP	ENGINEERED	UNP P00582
A	357	ALA	GLU	ENGINEERED	UNP P00582

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

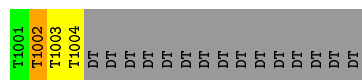
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	326	Total	O	0	0
			326	326		
5	B	9	Total	O	0	0
			9	9		

### 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.

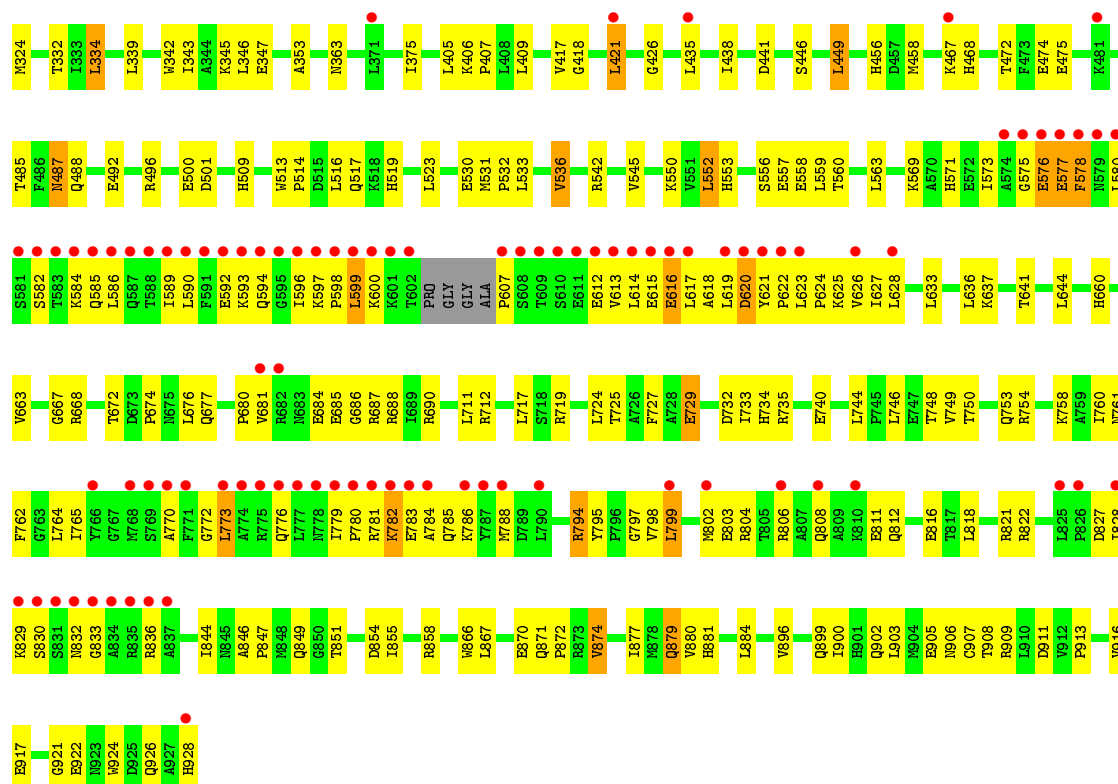
#### • Molecule 1: D(T)19 OLIGOMER

Chain B: 



#### • Molecule 2: DNA POLYMERASE I

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.88Å 101.88Å 85.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.08 33.96 – 2.08	Depositor EDS
% Data completeness (in resolution range)	84.3 (20.00-2.08) 90.3 (33.96-2.08)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.233 0.226 , 0.237	Depositor DCC
$R_{free}$ test set	4790 reflections (11.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 70.9	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47178 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 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	B	8.58	3/66 (4.5%)	1.36	1/101 (1.0%)
2	A	0.39	0/4831	0.63	1/6538 (0.0%)
All	All	1.07	3/4897 (0.1%)	0.65	2/6639 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1003	DT	C5-C7	-42.59	1.24	1.50
1	B	1004	DT	C5-C7	-41.42	1.25	1.50
1	B	1002	DT	C5-C7	-35.84	1.28	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	DT	C6-C5-C7	-6.73	118.86	122.90
2	A	607	PRO	N-CA-CB	5.70	110.14	103.30

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	B	61	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4745	0	4753	200	1
3	A	1	0	0	0	0
4	A	15	0	0	1	0
5	A	326	0	0	12	1
5	B	9	0	0	0	0
All	All	5157	0	4790	201	1

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 21.

All (201) 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)
2:A:517:GLN:HB2	5:A:1216:HOH:O	1.38	1.21
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.43	0.96
2:A:485:THR:H	2:A:488:GLN:HE21	1.02	0.91
2:A:719:ARG:CZ	2:A:804:ARG:HH12	1.87	0.87
2:A:808:GLN:NE2	5:A:1123:HOH:O	2.08	0.86
2:A:677:GLN:HE21	2:A:881:HIS:H	1.19	0.86
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.59	0.83
2:A:519:HIS:CD2	2:A:822:ARG:HH22	1.98	0.82
2:A:586:LEU:HD13	2:A:627:ILE:HD13	1.62	0.81
2:A:472:THR:HG23	2:A:475:GLU:H	1.44	0.80
2:A:556:SER:HB2	2:A:641:THR:HG22	1.63	0.79
2:A:725:THR:O	2:A:729:GLU:HG2	1.83	0.79
2:A:746:LEU:O	2:A:749:VAL:HG12	1.85	0.75
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.52	0.74
2:A:487:ASN:HD22	2:A:487:ASN:H	1.36	0.71
2:A:719:ARG:NH1	2:A:804:ARG:HH12	1.88	0.70
2:A:615:GLU:HB3	2:A:628:LEU:CD2	2.20	0.70
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.73	0.70
2:A:687:ARG:HG2	2:A:690:ARG:HH12	1.56	0.70
2:A:663:VAL:HG23	5:A:1139:HOH:O	1.93	0.69
2:A:517:GLN:OE1	5:A:1051:HOH:O	2.10	0.68
2:A:599:LEU:O	2:A:613:VAL:HB	1.94	0.68
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.74	0.67
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.40	0.67
2:A:684:GLU:HG3	5:A:1239:HOH:O	1.93	0.67
2:A:600:LYS:CB	2:A:614:LEU:HG	2.24	0.67
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.76	0.67
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.77	0.66
2:A:446:SER:OG	2:A:456:HIS:HD2	1.79	0.66
2:A:732:ASP:OD2	2:A:735:ARG:HG3	1.96	0.66
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.25	0.66
2:A:623:LEU:O	2:A:626:VAL:HG22	1.96	0.65
2:A:908:THR:HG22	2:A:909:ARG:H	1.62	0.64
2:A:556:SER:HB2	2:A:641:THR:CG2	2.28	0.64
2:A:474:GLU:OE2	5:A:1172:HOH:O	2.15	0.63
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.02	0.63
2:A:764:LEU:HD13	2:A:798:VAL:HG11	1.80	0.63
2:A:485:THR:H	2:A:488:GLN:NE2	1.85	0.62
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.81	0.62
2:A:472:THR:HG22	2:A:475:GLU:CD	2.21	0.61
2:A:580:LEU:N	2:A:580:LEU:HD22	2.16	0.61
2:A:582:SER:HA	2:A:586:LEU:HB2	1.83	0.60
2:A:569:LYS:O	2:A:573:ILE:HG13	2.01	0.60
2:A:586:LEU:CD1	2:A:627:ILE:HD13	2.31	0.60
2:A:854:ASP:O	2:A:858:ARG:HG3	2.01	0.60
2:A:687:ARG:HA	2:A:690:ARG:NH1	2.17	0.60
2:A:802:MET:O	2:A:806:ARG:HG3	2.01	0.60
2:A:773:LEU:CD1	2:A:784:ALA:HB1	2.32	0.60
2:A:559:LEU:O	2:A:563:LEU:HG	2.03	0.59
2:A:750:THR:OG1	2:A:753:GLN:HG3	2.03	0.59
2:A:733:ILE:HD12	2:A:734:HIS:N	2.19	0.58
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.85	0.58
2:A:590:LEU:HA	2:A:593:LYS:HE2	1.85	0.58
2:A:851:THR:O	2:A:855:ILE:HG13	2.04	0.58
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.86	0.58
2:A:772:GLY:O	2:A:776:GLN:HG2	2.04	0.58
2:A:458:MET:HE1	2:A:501:ASP:OD1	2.05	0.57
2:A:575:GLY:O	2:A:576:GLU:HG2	2.04	0.57
2:A:582:SER:HB3	2:A:586:LEU:HD12	1.86	0.57
2:A:735:ARG:HG2	2:A:754:ARG:HG3	1.86	0.57
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.35	0.57
2:A:735:ARG:HB3	2:A:749:VAL:HG11	1.87	0.56
2:A:519:HIS:CD2	2:A:822:ARG:NH2	2.73	0.56
2:A:744:LEU:HD12	2:A:748:THR:OG1	2.06	0.56
2:A:324:MET:HG2	5:A:1083:HOH:O	2.05	0.56
4:A:40:SO4:O2	5:A:1010:HOH:O	2.17	0.55
2:A:740:GLU:HG3	2:A:795:TYR:OH	2.06	0.55
2:A:590:LEU:HD22	2:A:624:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:492:GLU:OE1	5:A:1171:HOH:O	2.18	0.55
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.89	0.55
2:A:711:LEU:CD1	2:A:765:ILE:HD11	2.37	0.54
2:A:922:GLU:HB2	2:A:926:GLN:HE22	1.72	0.54
2:A:922:GLU:HB2	2:A:926:GLN:NE2	2.22	0.54
2:A:758:LYS:HE3	2:A:762:PHE:HE2	1.72	0.54
2:A:472:THR:HG22	2:A:475:GLU:CG	2.38	0.54
2:A:712:ARG:HD3	2:A:913:PRO:O	2.08	0.54
2:A:773:LEU:O	2:A:773:LEU:HD22	2.08	0.54
2:A:782:LYS:HD2	2:A:782:LYS:N	2.23	0.54
2:A:780:PRO:O	2:A:783:GLU:HB3	2.08	0.54
2:A:908:THR:HG22	2:A:909:ARG:N	2.22	0.53
2:A:519:HIS:HD2	2:A:822:ARG:HH22	1.50	0.53
2:A:363:ASN:HD21	2:A:426:GLY:HA3	1.74	0.53
2:A:924:TRP:O	2:A:928:HIS:HB2	2.08	0.53
2:A:553:HIS:O	2:A:557:GLU:HG2	2.08	0.53
2:A:846:ALA:HB3	2:A:847:PRO:HD3	1.91	0.53
2:A:550:LYS:NZ	2:A:550:LYS:HB2	2.23	0.53
2:A:589:ILE:O	2:A:593:LYS:HG2	2.09	0.53
2:A:487:ASN:ND2	2:A:487:ASN:H	2.05	0.53
2:A:808:GLN:O	2:A:812:GLN:HG2	2.08	0.52
2:A:781:ARG:C	2:A:783:GLU:H	2.13	0.52
2:A:615:GLU:O	2:A:618:ALA:HB3	2.10	0.52
1:B:1002:DT:O4	2:A:660:HIS:HE1	1.93	0.52
2:A:446:SER:OG	2:A:456:HIS:CD2	2.61	0.52
2:A:727:PHE:CZ	2:A:733:ILE:HG21	2.44	0.52
2:A:342:TRP:CE3	2:A:375:ILE:HD11	2.45	0.52
2:A:590:LEU:HD23	2:A:623:LEU:HD23	1.92	0.51
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.08	0.51
2:A:719:ARG:NH1	2:A:804:ARG:NH1	2.57	0.51
1:B:1002:DT:O4	2:A:660:HIS:CE1	2.64	0.51
2:A:677:GLN:HE21	2:A:881:HIS:N	1.98	0.51
2:A:458:MET:CE	2:A:501:ASP:OD1	2.59	0.51
2:A:406:LYS:HB3	2:A:407:PRO:HD3	1.93	0.50
2:A:343:ILE:O	2:A:347:GLU:HG3	2.12	0.50
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.93	0.49
2:A:533:LEU:HD12	2:A:536:VAL:HG21	1.93	0.49
2:A:556:SER:CA	2:A:641:THR:HG21	2.42	0.49
2:A:773:LEU:HD12	2:A:784:ALA:HB1	1.94	0.49
2:A:818:LEU:HD22	2:A:851:THR:HG21	1.93	0.49
2:A:620:ASP:OD1	2:A:621:TYR:HD1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:830:SER:C	2:A:832:ASN:H	2.16	0.49
2:A:680:PRO:HB2	2:A:686:GLY:HA3	1.95	0.48
2:A:531:MET:HB2	2:A:532:PRO:HD3	1.95	0.48
2:A:784:ALA:O	2:A:788:MET:HG3	2.13	0.48
2:A:808:GLN:HA	2:A:811:GLU:HB3	1.94	0.48
2:A:615:GLU:HA	2:A:618:ALA:HB2	1.95	0.48
2:A:773:LEU:HD13	2:A:784:ALA:HB1	1.93	0.48
2:A:485:THR:N	2:A:488:GLN:HE21	1.87	0.48
2:A:472:THR:HG23	2:A:475:GLU:N	2.20	0.48
2:A:342:TRP:CZ3	2:A:375:ILE:HD11	2.49	0.47
2:A:571:HIS:CE1	2:A:577:GLU:HG3	2.49	0.47
2:A:550:LYS:HB2	2:A:550:LYS:HZ2	1.76	0.47
2:A:667:GLY:HA3	2:A:821:ARG:NE	2.29	0.47
2:A:586:LEU:HD22	2:A:627:ILE:HD11	1.97	0.47
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.80	0.47
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.96	0.47
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.45	0.47
2:A:614:LEU:O	2:A:624:PRO:HB2	2.16	0.46
2:A:550:LYS:NZ	2:A:550:LYS:CB	2.78	0.46
2:A:530:GLU:OE2	2:A:821:ARG:NH2	2.47	0.46
2:A:674:PRO:HG2	2:A:676:LEU:CD1	2.45	0.46
2:A:760:ILE:O	2:A:764:LEU:HG	2.15	0.46
2:A:719:ARG:CZ	2:A:804:ARG:NH1	2.68	0.46
2:A:660:HIS:CE1	2:A:672:THR:HG1	2.34	0.46
2:A:353:ALA:HA	2:A:417:VAL:O	2.16	0.46
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.98	0.46
2:A:797:GLY:CA	5:A:1186:HOH:O	2.63	0.45
2:A:513:TRP:HB3	2:A:514:PRO:HD3	1.97	0.45
2:A:866:TRP:CE2	2:A:899:GLN:HG2	2.50	0.45
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.98	0.45
2:A:578:PHE:HE2	2:A:586:LEU:HD23	1.81	0.45
2:A:585:GLN:O	2:A:589:ILE:HG12	2.16	0.45
2:A:580:LEU:N	2:A:580:LEU:CD2	2.79	0.45
2:A:896:VAL:O	2:A:900:ILE:HG12	2.16	0.45
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.47	0.45
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.98	0.45
2:A:797:GLY:HA3	5:A:1186:HOH:O	2.16	0.45
2:A:590:LEU:O	2:A:593:LYS:HG2	2.17	0.45
2:A:870:GLU:HB3	2:A:872:PRO:HD3	1.99	0.45
2:A:802:MET:CE	2:A:844:ILE:HD13	2.47	0.45
2:A:613:VAL:O	2:A:617:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:560:THR:OG1	2:A:637:LYS:HE3	2.17	0.44
2:A:808:GLN:CG	5:A:1123:HOH:O	2.65	0.44
2:A:830:SER:C	2:A:832:ASN:N	2.70	0.44
2:A:545:VAL:HG23	2:A:877:ILE:HD12	2.00	0.44
2:A:734:HIS:HD2	2:A:761:ASN:HD22	1.65	0.44
2:A:468:HIS:HE1	2:A:500:GLU:OE2	2.00	0.43
2:A:467:LYS:HD2	2:A:467:LYS:N	2.33	0.43
2:A:324:MET:HE2	2:A:496:ARG:NH2	2.33	0.43
2:A:832:ASN:OD1	2:A:833:GLY:N	2.51	0.43
2:A:866:TRP:CZ2	2:A:899:GLN:HG2	2.53	0.43
2:A:596:ILE:HG22	2:A:598:PRO:HD2	2.00	0.43
2:A:578:PHE:N	2:A:578:PHE:CD1	2.86	0.43
2:A:770:ALA:HA	2:A:788:MET:SD	2.58	0.43
2:A:902:GLN:O	2:A:906:ASN:HB2	2.19	0.43
2:A:781:ARG:O	2:A:782:LYS:HB2	2.19	0.43
2:A:618:ALA:HB1	2:A:625:LYS:HG3	2.01	0.43
2:A:911:ASP:N	2:A:911:ASP:OD1	2.52	0.43
2:A:816:GLU:HA	2:A:821:ARG:O	2.18	0.43
2:A:623:LEU:N	2:A:624:PRO:HD2	2.33	0.43
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.18	0.43
2:A:558:GLU:OE2	2:A:688:ARG:NH1	2.48	0.43
2:A:345:LYS:HE3	2:A:375:ILE:CD1	2.49	0.43
2:A:586:LEU:HD22	2:A:627:ILE:CD1	2.49	0.42
2:A:552:LEU:O	2:A:641:THR:HG23	2.19	0.42
2:A:418:GLY:O	2:A:441:ASP:HA	2.19	0.42
2:A:417:VAL:HG11	2:A:509:HIS:HB2	2.02	0.42
2:A:613:VAL:HA	2:A:616:GLU:HB2	2.01	0.41
2:A:827:ASP:O	2:A:836:ARG:HG3	2.20	0.41
2:A:619:LEU:HD22	2:A:619:LEU:N	2.35	0.41
2:A:783:GLU:O	2:A:786:LYS:HB3	2.20	0.41
2:A:621:TYR:HA	2:A:622:PRO:HD2	1.91	0.41
2:A:779:ILE:HD12	2:A:783:GLU:HG3	2.02	0.41
2:A:617:LEU:HB2	2:A:624:PRO:HG3	2.02	0.41
2:A:727:PHE:CE1	2:A:733:ILE:HG21	2.55	0.41
2:A:615:GLU:HA	2:A:618:ALA:CB	2.50	0.41
2:A:593:LYS:O	2:A:594:GLN:HB3	2.21	0.41
2:A:577:GLU:O	2:A:578:PHE:HB3	2.20	0.41
2:A:733:ILE:HG13	2:A:733:ILE:H	1.68	0.41
2:A:905:GLU:HB3	2:A:916:VAL:HG23	2.02	0.41
2:A:624:PRO:HA	2:A:627:ILE:HD12	2.02	0.41
2:A:590:LEU:CD2	2:A:624:PRO:HD3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:575:GLY:O	2:A:576:GLU:CG	2.69	0.41
2:A:903:LEU:O	2:A:907:CYS:HB2	2.21	0.41
2:A:879:GLN:HG2	2:A:884:LEU:HD23	2.03	0.40
2:A:799:LEU:HD22	2:A:803:GLU:HG3	2.03	0.40
2:A:523:LEU:C	2:A:523:LEU:HD13	2.42	0.40
2:A:798:VAL:O	2:A:802:MET:HG3	2.21	0.40
2:A:802:MET:HE3	2:A:844:ILE:HD13	2.03	0.40
2:A:711:LEU:HA	2:A:711:LEU:HD12	1.84	0.40
2:A:449:LEU:HA	2:A:449:LEU:HD12	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:719:ARG:NH1	5:A:1138:HOH:O[2_764]	2.19	0.01

## 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
2	A	597/605 (99%)	555 (93%)	39 (6%)	3 (0%)	34 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	576	GLU
2	A	597	LYS
2	A	599	LEU

### 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	
2	A	498/508 (98%)	468 (94%)	30 (6%)	24	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	334	LEU
2	A	339	LEU
2	A	346	LEU
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	435	LEU
2	A	449	LEU
2	A	487	ASN
2	A	536	VAL
2	A	552	LEU
2	A	577	GLU
2	A	578	PHE
2	A	584	LYS
2	A	592	GLU
2	A	616	GLU
2	A	620	ASP
2	A	636	LEU
2	A	644	LEU
2	A	724	LEU
2	A	729	GLU
2	A	773	LEU
2	A	782	LYS
2	A	794	ARG
2	A	799	LEU
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	879	GLN
2	A	917	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	363	ASN
2	A	456	HIS
2	A	468	HIS
2	A	487	ASN
2	A	488	GLN
2	A	519	HIS
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	734	HIS
2	A	776	GLN
2	A	812	GLN
2	A	849	GLN
2	A	879	GLN
2	A	899	GLN
2	A	928	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 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	38	-	4,4,4	0.15	0	6,6,6	0.34	0
4	SO4	A	40	-	4,4,4	0.21	0	6,6,6	0.38	0
4	SO4	A	94	-	4,4,4	0.28	0	6,6,6	0.22	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	SO4	A	38	-	-	0/0/0/0	0/0/0/0
4	SO4	A	40	-	-	0/0/0/0	0/0/0/0
4	SO4	A	94	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
4	A	40	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	4/19 (21%)	-0.18	0	100 100	25, 26, 39, 46	0
2	A	601/605 (99%)	0.99	93 (15%)	3 4	12, 30, 70, 70	0
All	All	605/624 (96%)	0.98	93 (15%)	3 4	12, 30, 70, 70	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	609	THR	15.5
2	A	582	SER	13.2
2	A	596	ILE	13.1
2	A	590	LEU	13.0
2	A	598	PRO	12.5
2	A	608	SER	12.4
2	A	586	LEU	12.3
2	A	591	PHE	11.9
2	A	581	SER	11.3
2	A	610	SER	11.1
2	A	607	PRO	10.7
2	A	613	VAL	9.9
2	A	583	THR	8.9
2	A	611	GLU	8.5
2	A	595	GLY	8.2
2	A	784	ALA	8.2
2	A	599	LEU	8.2
2	A	587	GLN	7.4
2	A	594	GLN	7.2
2	A	597	LYS	7.1
2	A	588	THR	7.1
2	A	589	ILE	7.1
2	A	775	ARG	7.0
2	A	771	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
2	A	834	ALA	6.5
2	A	621	TYR	6.1
2	A	602	THR	5.9
2	A	601	LYS	5.9
2	A	781	ARG	5.8
2	A	831	SER	5.8
2	A	835	ARG	5.6
2	A	614	LEU	5.6
2	A	592	GLU	5.5
2	A	833	GLY	5.4
2	A	584	LYS	5.3
2	A	620	ASP	5.2
2	A	782	LYS	5.2
2	A	681	VAL	5.1
2	A	600	LYS	5.1
2	A	576	GLU	5.0
2	A	832	ASN	4.9
2	A	780	PRO	4.8
2	A	617	LEU	4.8
2	A	779	ILE	4.5
2	A	829	LYS	4.5
2	A	579	ASN	4.2
2	A	836	ARG	4.2
2	A	777	LEU	4.1
2	A	928	HIS	4.1
2	A	585	GLN	4.1
2	A	830	SER	4.0
2	A	580	LEU	4.0
2	A	787	TYR	3.9
2	A	616	GLU	3.8
2	A	778	ASN	3.8
2	A	575	GLY	3.8
2	A	786	LYS	3.7
2	A	612	GLU	3.7
2	A	783	GLU	3.7
2	A	593	LYS	3.5
2	A	770	ALA	3.4
2	A	828	ILE	3.3
2	A	682	ARG	3.3
2	A	766	TYR	3.2
2	A	615	GLU	3.0
2	A	837	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	577	GLU	3.0
2	A	619	LEU	2.9
2	A	808	GLN	2.9
2	A	574	ALA	2.9
2	A	826	PRO	2.7
2	A	810	LYS	2.7
2	A	774	ALA	2.7
2	A	768	MET	2.6
2	A	481	LYS	2.6
2	A	435	LEU	2.5
2	A	769	SER	2.5
2	A	467	LYS	2.4
2	A	623	LEU	2.4
2	A	578	PHE	2.3
2	A	790	LEU	2.3
2	A	421	LEU	2.3
2	A	773	LEU	2.3
2	A	626	VAL	2.3
2	A	788	MET	2.2
2	A	371	LEU	2.2
2	A	802	MET	2.1
2	A	628	LEU	2.1
2	A	825	LEU	2.1
2	A	799	LEU	2.1
2	A	622	PRO	2.1
2	A	776	GLN	2.1
2	A	806	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	A	38	5/5	0.86	0.15	-0.07	69,69,70,70	0
4	SO4	A	40	5/5	0.85	0.20	-	67,67,69,69	0
4	SO4	A	94	5/5	0.85	0.27	-	68,68,70,70	0
3	ZN	A	3	1/1	0.90	0.08	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.