



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:41 am BST

PDB ID : 2WWY  
Title : Structure of human RECQ-like helicase in complex with a DNA substrate  
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Deposited on : 2009-10-30  
Resolution : 2.90 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](mailto: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 ⓘ 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

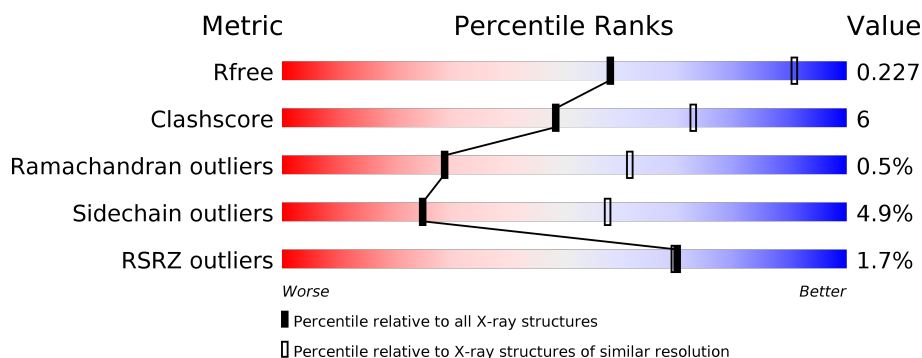
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	591	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>13%</span> <span>10%</span> </div> </div>
1	B	591	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>13%</span> <span>10%</span> </div> </div>
2	O	27	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>11%</span> <span>81%</span> </div> </div>
2	Q	27	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>19%</span> <span>41%</span> <span>15%</span> <span>26%</span> </div> </div>
2	R	27	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>4%</span> <span>7%</span> <span>89%</span> </div> </div>
2	T	27	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>11%</span> <span>41%</span> <span>11%</span> <span>15%</span> <span>33%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
3	P	13	<div><div></div><div>54%</div><div>23%</div><div>23%</div></div>
3	S	13	<div><div>23%</div><div>15%</div><div>46%</div><div>31%</div><div>8%</div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9733 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 ATP-DEPENDENT DNA HELICASE Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4122	2630	697	761	34			
1	B	530	Total	C	N	O	S	0	1	0
			4119	2627	698	759	35			

- Molecule 2 is a DNA chain called DNA OLIGO (27BP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	5	Total	C	N	O	P	0	0	1
			59	25	8	22	4			
2	Q	20	Total	C	N	O	P	0	0	0
			402	192	66	124	20			
2	R	3	Total	C	N	O	P	0	0	0
			48	20	10	15	3			
2	T	18	Total	C	N	O	P	0	0	0
			360	172	59	111	18			

- Molecule 3 is a DNA chain called 5'-D(\*DA DG DC DG DT DC DG DA DG DA DT DC DCP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			264	126	51	75	12			
3	S	12	Total	C	N	O	P	0	0	0
			245	117	48	69	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

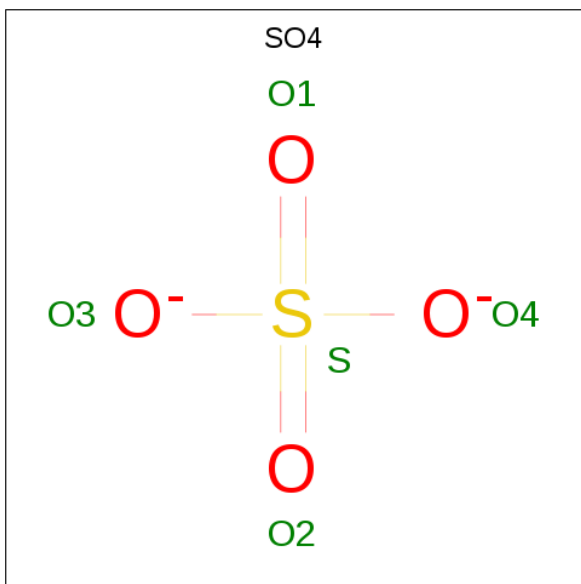
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

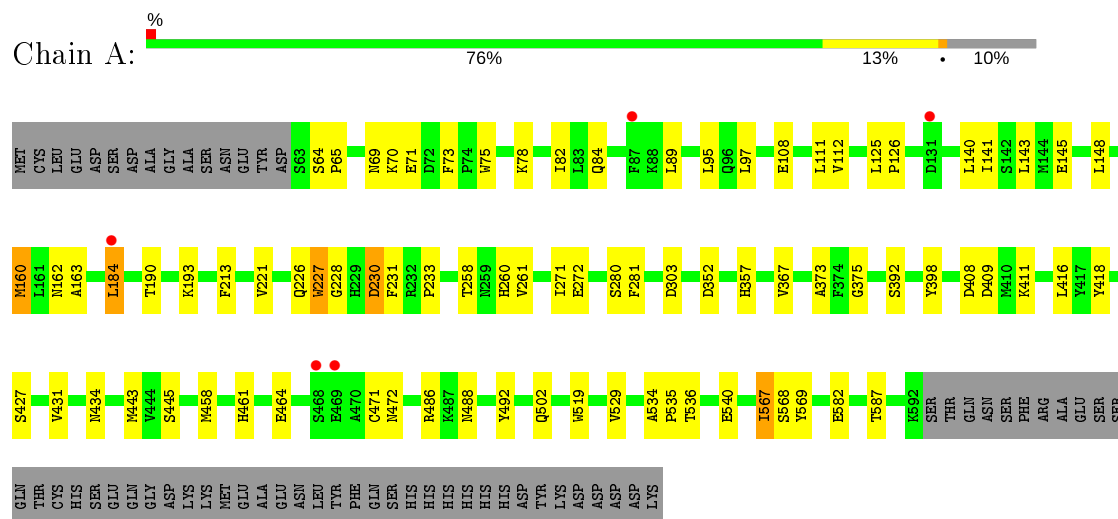
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	54	Total	O	0	0
			54	54		
7	B	23	Total	O	0	0
			23	23		
7	P	3	Total	O	0	0
			3	3		
7	Q	4	Total	O	0	0
			4	4		

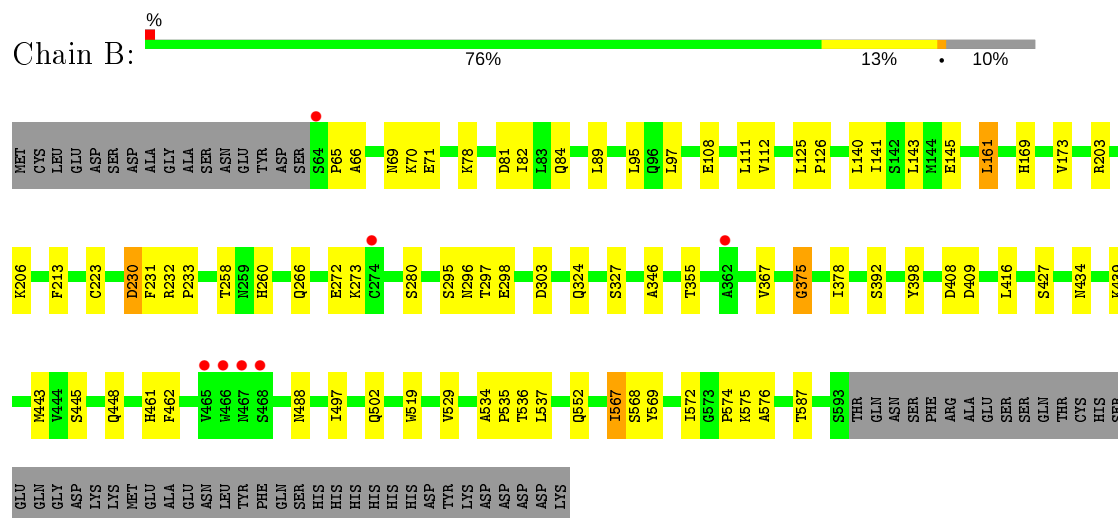
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ATP-DEPENDENT DNA HELICASE Q1

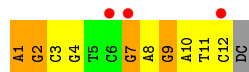


#### • Molecule 1: ATP-DEPENDENT DNA HELICASE Q1



#### • Molecule 2: DNA OLIGO (27BP)







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.33Å 174.22Å 100.23Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	43.38 – 2.90 48.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.38-2.90) 99.6 (48.09-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.198 , 0.236 0.190 , 0.227	Depositor DCC
$R_{free}$ test set	2217 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.333 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: ZN, SO4, EDO

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	0.62	0/4205	0.68	0/5690
1	B	0.55	0/4206	0.64	0/5694
2	O	0.81	0/64	1.73	1/99 (1.0%)
2	Q	0.97	0/447	1.76	10/686 (1.5%)
2	R	0.87	0/53	1.49	1/81 (1.2%)
2	T	0.78	0/400	1.53	4/613 (0.7%)
3	P	0.88	0/296	1.70	7/455 (1.5%)
3	S	0.77	0/275	1.64	7/423 (1.7%)
All	All	0.64	0/9946	0.91	30/13741 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	12	DC	O4'-C1'-N1	9.26	114.48	108.00
2	Q	24	DC	O4'-C4'-C3'	-8.36	100.98	106.00
2	T	12	DC	O4'-C1'-N1	8.21	113.74	108.00
3	P	13	DC	O4'-C4'-C3'	-7.47	101.51	104.50
2	Q	25	DC	P-O3'-C3'	7.45	128.64	119.70
3	S	9	DG	O4'-C1'-N9	7.34	113.14	108.00
2	R	2	DG	O4'-C1'-N9	6.92	112.84	108.00
2	Q	13	DT	O4'-C1'-N1	-6.77	103.26	108.00
3	S	3	DC	O4'-C1'-N1	-6.54	103.42	108.00
2	T	11	DT	O4'-C1'-N1	6.39	112.47	108.00
3	S	7	DG	O4'-C1'-N9	6.35	112.44	108.00
3	S	11	DT	O4'-C1'-N1	6.25	112.37	108.00
2	Q	13	DT	N3-C4-O4	6.16	123.60	119.90
3	S	2	DG	C8-N9-C4	-6.09	103.97	106.40
2	T	25	DC	P-O3'-C3'	6.07	126.98	119.70
3	P	11	DT	O4'-C1'-N1	5.90	112.13	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	DG	P-O3'-C3'	5.86	126.73	119.70
2	Q	22	DT	N3-C4-O4	5.79	123.37	119.90
2	Q	26	DT	O4'-C1'-N1	5.71	111.99	108.00
2	Q	7	DT	C3'-C2'-C1'	-5.67	95.70	102.50
2	O	4	DT	C4'-C3'-C2'	-5.45	98.20	103.10
2	Q	22	DT	O4'-C1'-N1	5.43	111.80	108.00
2	Q	21	DC	P-O3'-C3'	5.39	126.17	119.70
3	P	5	DT	N3-C4-O4	5.30	123.08	119.90
3	P	3	DC	P-O3'-C3'	5.21	125.95	119.70
3	S	1	DA	O4'-C1'-N9	5.15	111.61	108.00
2	Q	13	DT	C5-C4-O4	-5.14	121.30	124.90
2	T	10	DA	O4'-C1'-N9	5.13	111.59	108.00
3	P	3	DC	O4'-C1'-C2'	-5.10	101.82	105.90
3	S	4	DG	P-O3'-C3'	5.05	125.75	119.70

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	4122	0	4037	39	0
1	B	4119	0	4016	46	0
2	O	59	0	30	4	0
2	Q	402	0	227	11	0
2	R	48	0	22	1	0
2	T	360	0	204	6	0
3	P	264	0	147	4	0
3	S	245	0	136	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	4	0	6	1	0
6	B	4	0	6	0	0
7	A	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	23	0	0	0	0
7	P	3	0	0	0	0
7	Q	4	0	0	0	0
All	All	9733	0	8831	110	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 6.

All (110) 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:P:12:DC:H2''	3:P:13:DC:H5''	1.48	0.93
1:B:206:LYS:HE2	2:O:4:DT:OP1	1.86	0.76
1:B:552:GLN:O	1:B:575:LYS:HE2	1.86	0.74
1:A:227:TRP:N	1:A:227:TRP:CD1	2.52	0.73
1:B:258:THR:HG22	1:B:260:HIS:H	1.52	0.73
1:B:392:SER:HB2	1:B:443:MET:HE2	1.69	0.72
1:A:392:SER:HB2	1:A:443:MET:HE2	1.73	0.70
1:A:70:LYS:O	1:A:71:GLU:HG3	1.97	0.65
2:T:11:DT:H2''	2:T:12:DC:H5''	1.77	0.65
1:A:227:TRP:HD1	1:A:227:TRP:N	1.94	0.65
2:O:2:DG:H1'	2:O:3:DG:OP2	1.98	0.64
2:Q:15:DG:H2''	2:Q:16:DA:C8	2.34	0.63
3:S:9:DG:H2''	3:S:10:DA:OP2	1.98	0.63
2:Q:8:DG:H2''	2:Q:9:DG:H5'	1.81	0.61
2:T:9:DG:H2''	2:T:10:DA:OP2	2.00	0.60
1:A:69:ASN:OD1	1:A:97:LEU:HD23	2.02	0.60
2:Q:9:DG:H2''	2:Q:10:DA:OP2	2.01	0.60
1:B:223:CYS:SG	1:B:232:ARG:NH1	2.76	0.59
1:B:408:ASP:O	1:B:409:ASP:HB2	2.03	0.59
1:B:70:LYS:O	1:B:71:GLU:HG3	2.04	0.57
3:P:12:DC:C2'	3:P:13:DC:H5''	2.29	0.57
1:A:258:THR:HG22	1:A:260:HIS:H	1.69	0.57
1:A:567:ILE:HD11	1:A:569:TYR:CZ	2.40	0.57
2:Q:12:DC:H5'	2:Q:12:DC:H6	1.68	0.57
2:T:11:DT:H2''	2:T:12:DC:C5'	2.35	0.56
3:S:1:DA:H2'	3:S:2:DG:C8	2.40	0.56
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.71	0.56
1:B:567:ILE:HD11	1:B:569:TYR:CZ	2.41	0.56
1:A:408:ASP:O	1:A:409:ASP:HB2	2.06	0.55
2:Q:15:DG:H2''	2:Q:16:DA:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD12	1:B:173:VAL:HG11	1.92	0.52
2:Q:25:DC:H4'	2:Q:26:DT:OP1	2.10	0.52
1:A:78:LYS:O	1:A:82:ILE:HG13	2.10	0.52
1:B:346:ALA:HB2	2:T:24:DC:H5'	1.92	0.52
1:A:519:TRP:O	1:A:534:ALA:HB2	2.10	0.51
1:B:78:LYS:O	1:B:82:ILE:HG13	2.10	0.50
2:T:25:DC:H4'	2:T:26:DT:OP1	2.12	0.50
1:B:519:TRP:O	1:B:534:ALA:HB2	2.10	0.50
1:B:231:PHE:CE2	1:B:233:PRO:HA	2.47	0.49
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.95	0.49
1:B:272:GLU:HA	1:B:272:GLU:OE1	2.12	0.48
1:B:140:LEU:HB2	1:B:143:LEU:HD12	1.96	0.48
1:A:140:LEU:HB2	1:A:143:LEU:HD12	1.96	0.48
1:B:574:PRO:O	1:B:576:ALA:N	2.47	0.48
2:Q:12:DC:H2''	2:Q:13:DT:O5'	2.14	0.48
1:B:488:ASN:HA	1:B:587:THR:HG22	1.95	0.47
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.97	0.47
1:A:231:PHE:CE2	1:A:233:PRO:HA	2.49	0.47
1:A:488:ASN:HA	1:A:587:THR:HG22	1.97	0.47
1:A:162:ASN:OD1	1:A:163:ALA:N	2.47	0.47
1:A:398:TYR:CE2	1:A:416:LEU:HD12	2.50	0.47
1:B:398:TYR:CE2	1:B:416:LEU:HD12	2.49	0.47
1:A:227:TRP:HB2	1:A:261:VAL:HG22	1.97	0.46
1:B:303:ASP:OD1	1:B:303:ASP:N	2.46	0.46
1:A:184:LEU:HA	1:A:184:LEU:HD12	1.61	0.45
2:O:4:DT:H4'	2:O:5:DA:OP1	2.17	0.45
1:A:226:GLN:HB2	1:A:227:TRP:CD1	2.51	0.45
1:A:492:TYR:CE1	1:A:535:PRO:HG3	2.51	0.45
2:Q:17:DC:H2''	2:Q:18:DG:C8	2.52	0.45
1:A:281:PHE:HD2	1:A:464:GLU:OE1	1.99	0.45
1:B:169:HIS:O	1:B:173:VAL:HG23	2.16	0.45
1:B:206:LYS:CE	2:O:4:DT:OP1	2.61	0.45
1:A:227:TRP:CZ3	1:A:260:HIS:HB3	2.52	0.45
1:B:266:GLN:HG2	1:B:266:GLN:O	2.16	0.45
1:A:373:ALA:HB2	2:Q:24:DC:H5''	1.99	0.45
3:S:7:DG:C2	3:S:8:DA:C2	3.05	0.44
1:A:226:GLN:HB2	1:A:227:TRP:HD1	1.82	0.44
1:B:272:GLU:HA	1:B:273:LYS:HA	1.79	0.44
2:T:25:DC:O2	2:T:25:DC:H2'	2.18	0.44
1:A:111:LEU:HD12	1:A:112:VAL:N	2.33	0.44
1:B:536:THR:C	1:B:537:LEU:HG	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:O	1:A:193:LYS:HB2	2.17	0.44
1:A:502:GLN:OE1	1:A:529:VAL:HG22	2.18	0.44
1:B:375:GLY:O	1:B:378:ILE:HG12	2.17	0.44
3:P:11:DT:H2''	3:P:12:DC:O5'	2.18	0.44
1:A:148:LEU:HD11	1:A:160:MET:HG2	1.99	0.44
1:A:141:ILE:O	1:A:145:GLU:HG3	2.18	0.43
1:B:141:ILE:O	1:B:145:GLU:HG3	2.17	0.43
1:A:227:TRP:CZ3	1:A:260:HIS:CG	3.06	0.43
1:B:574:PRO:C	1:B:576:ALA:H	2.20	0.43
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.18	0.43
1:B:84:GLN:HG2	1:B:89:LEU:O	2.19	0.43
1:B:111:LEU:HD12	1:B:112:VAL:N	2.34	0.43
1:A:221:VAL:HG22	1:A:221:VAL:O	2.19	0.43
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.90	0.42
1:B:497:ILE:HG23	1:B:572:ILE:CD1	2.49	0.42
1:B:296:ASN:OD1	1:B:296:ASN:C	2.58	0.42
1:B:296:ASN:OD1	1:B:298:GLU:N	2.51	0.42
1:B:536:THR:O	1:B:537:LEU:HG	2.19	0.42
1:A:84:GLN:HG2	1:A:89:LEU:O	2.19	0.42
2:R:3:DG:H2''	3:S:1:DA:O5'	2.20	0.42
1:B:534:ALA:HA	1:B:535:PRO:HD3	1.90	0.42
1:B:502:GLN:OE1	1:B:529:VAL:HG22	2.19	0.42
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.35	0.41
1:B:272:GLU:CD	1:B:273:LYS:HA	2.41	0.41
1:B:462:PHE:CD1	1:B:462:PHE:N	2.88	0.41
1:A:418:TYR:CE2	6:A:2001:EDO:H12	2.54	0.41
1:B:266:GLN:NE2	1:B:272:GLU:OE1	2.53	0.41
3:S:12:DC:H2'	3:S:12:DC:O2	2.20	0.41
1:A:471:CYS:O	1:A:472:ASN:HB2	2.20	0.41
1:A:271:ILE:CG2	1:A:272:GLU:N	2.84	0.41
1:A:64:SER:HA	1:A:65:PRO:HD2	1.80	0.41
1:B:65:PRO:O	1:B:66:ALA:C	2.59	0.41
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.91	0.41
1:B:78:LYS:O	1:B:81:ASP:HB3	2.21	0.41
3:P:12:DC:H42	2:Q:9:DG:H1	1.68	0.41
1:A:73:PHE:CD2	1:A:75:TRP:CZ2	3.09	0.41
1:B:324:GLN:O	1:B:327:SER:HB3	2.21	0.41
1:B:69:ASN:OD1	1:B:97:LEU:HD23	2.20	0.40
2:Q:12:DC:C6	2:Q:12:DC:H5'	2.54	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	528/591 (89%)	493 (93%)	32 (6%)	3 (1%)	25	58
1	B	529/591 (90%)	492 (93%)	35 (7%)	2 (0%)	34	66
All	All	1057/1182 (89%)	985 (93%)	67 (6%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASP
1	A	375	GLY
1	B	375	GLY
1	A	230	ASP
1	A	228	GLY

### 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	433/520 (83%)	409 (94%)	24 (6%)	21	53
1	B	429/520 (82%)	411 (96%)	18 (4%)	30	63
All	All	862/1040 (83%)	820 (95%)	42 (5%)	25	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU

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Mol	Chain	Res	Type
1	A	160	MET
1	A	184	LEU
1	A	213	PHE
1	A	227	TRP
1	A	230	ASP
1	A	280	SER
1	A	303	ASP
1	A	352	ASP
1	A	357	HIS
1	A	367	VAL
1	A	411	LYS
1	A	427	SER
1	A	431	VAL
1	A	434	ASN
1	A	445	SER
1	A	458	MET
1	A	461	HIS
1	A	486	ARG
1	A	536	THR
1	A	540	GLU
1	A	567	ILE
1	A	568	SER
1	A	582	GLU
1	B	108	GLU
1	B	161	LEU
1	B	203	ARG
1	B	213	PHE
1	B	230	ASP
1	B	280	SER
1	B	295	SER
1	B	297	THR
1	B	355	THR
1	B	367	VAL
1	B	427	SER
1	B	434	ASN
1	B	439	LYS
1	B	445	SER
1	B	448	GLN
1	B	461	HIS
1	B	567	ILE
1	B	568	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no



such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	SO4	A	2000	-	4,4,4	0.16	0	6,6,6	0.20	0
5	SO4	B	2000	-	4,4,4	0.15	0	6,6,6	0.80	0
5	SO4	B	1597	-	4,4,4	0.15	0	6,6,6	0.14	0
5	SO4	A	1596	-	4,4,4	0.17	0	6,6,6	0.28	0
6	EDO	A	2001	-	3,3,3	0.56	0	2,2,2	0.14	0
6	EDO	B	2001	-	3,3,3	0.46	0	2,2,2	0.30	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
6	EDO	A	2001	-	-	0/1/1/1	-
6	EDO	B	2001	-	-	0/1/1/1	-

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
6	A	2001	EDO	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	A	530/591 (89%)	-0.21	5 (0%) 84 84	30, 70, 145, 191	0
1	B	530/591 (89%)	-0.11	7 (1%) 77 77	42, 76, 130, 177	0
2	O	5/27 (18%)	0.04	0 100 100	91, 106, 180, 221	0
2	Q	20/27 (74%)	0.08	0 100 100	51, 97, 154, 179	0
2	R	3/27 (11%)	1.66	1 (33%) 0 0	147, 147, 168, 191	0
2	T	18/27 (66%)	0.55	3 (16%) 1 1	78, 162, 235, 272	0
3	P	13/13 (100%)	-0.05	0 100 100	59, 95, 134, 150	0
3	S	12/13 (92%)	1.26	3 (25%) 0 0	105, 158, 265, 265	0
All	All	1131/1316 (85%)	-0.12	19 (1%) 70 69	30, 75, 147, 272	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	GLU	4.1
3	S	12	DC	4.0
1	B	466	TRP	3.9
1	B	465	VAL	3.8
1	B	468	SER	3.5
2	T	10	DA	3.3
2	T	9	DG	3.1
1	A	184	LEU	3.0
2	R	2	DG	2.7
1	A	87	PHE	2.6
2	T	11	DT	2.3
1	B	64	SER	2.3
1	A	131	ASP	2.3
1	B	362	ALA	2.2
1	A	468	SER	2.2
3	S	7	DG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	467	ASN	2.1
1	B	274	CYS	2.1
3	S	6	DC	2.1

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1596	5/5	0.81	0.19	152,152,152,152	0
6	EDO	A	2001	4/4	0.96	0.20	64,64,64,64	0
5	SO4	B	1597	5/5	0.97	0.22	113,113,113,113	0
5	SO4	B	2000	5/5	0.98	0.19	72,72,72,72	0
5	SO4	A	2000	5/5	0.98	0.17	82,82,82,82	0
6	EDO	B	2001	4/4	0.98	0.20	82,82,82,82	0
4	ZN	A	1595	1/1	0.99	0.14	59,59,59,59	0
4	ZN	B	1595	1/1	0.99	0.16	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.