Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:14 am BST

PDB ID	:	4U7D
Title	:	Structure of human RECQ-like helicase in complex with an oligonucleotide
Authors	:	Pike, A.C.W.; Zhang, Y.; Schnecke, C.; Cooper, C.D.O.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on	:	2014-07-30
Resolution	:	3.40 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

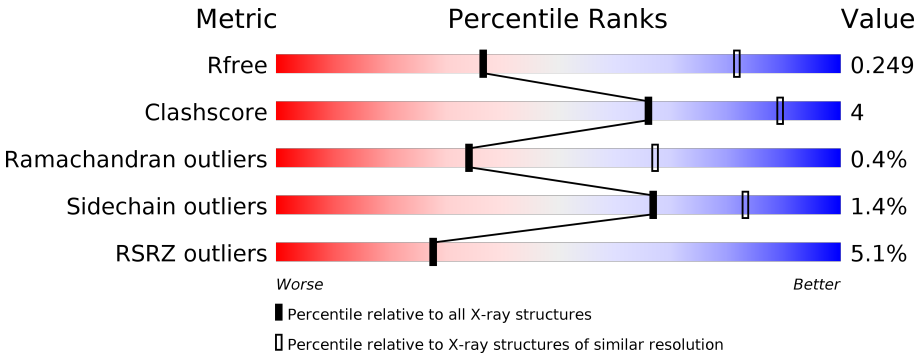
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	A	591	3% 80% 9% 11%
1	B	591	% 79% 10% 11%
1	C	591	6% 81% 9% 10%
1	D	591	9% 81% 8% 10%
2	P	20	5% 30% 55% 15%
2	Q	20	35% 45% 20%

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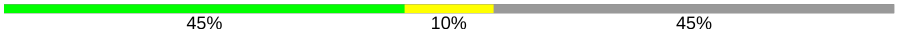
Mol	Chain	Length	Quality of chain
2	R	20	
2	S	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17224 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	527	Total	C	N	O	S	0	0	0
			4056	2594	678	751	33			
1	B	527	Total	C	N	O	S	0	0	0
			4052	2594	675	749	34			
1	C	530	Total	C	N	O	S	0	0	0
			4062	2601	677	751	33			
1	D	530	Total	C	N	O	S	0	0	0
			4070	2604	678	755	33			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	-	initiating methionine	UNP P46063
A	611	SER	GLY	conflict	UNP P46063
A	617	ALA	-	expression tag	UNP P46063
A	618	GLU	-	expression tag	UNP P46063
A	619	ASN	-	expression tag	UNP P46063
A	620	LEU	-	expression tag	UNP P46063
A	621	TYR	-	expression tag	UNP P46063
A	622	PHE	-	expression tag	UNP P46063
A	623	GLN	-	expression tag	UNP P46063
A	624	SER	-	expression tag	UNP P46063
A	625	HIS	-	expression tag	UNP P46063
A	626	HIS	-	expression tag	UNP P46063
A	627	HIS	-	expression tag	UNP P46063
A	628	HIS	-	expression tag	UNP P46063
A	629	HIS	-	expression tag	UNP P46063
A	630	HIS	-	expression tag	UNP P46063
A	631	ASP	-	expression tag	UNP P46063
A	632	TYR	-	expression tag	UNP P46063
A	633	LYS	-	expression tag	UNP P46063
A	634	ASP	-	expression tag	UNP P46063
A	635	ASP	-	expression tag	UNP P46063

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Chain	Residue	Modelled	Actual	Comment	Reference
A	636	ASP	-	expression tag	UNP P46063
A	637	ASP	-	expression tag	UNP P46063
A	638	LYS	-	expression tag	UNP P46063
B	48	MET	-	initiating methionine	UNP P46063
B	611	SER	GLY	conflict	UNP P46063
B	617	ALA	-	expression tag	UNP P46063
B	618	GLU	-	expression tag	UNP P46063
B	619	ASN	-	expression tag	UNP P46063
B	620	LEU	-	expression tag	UNP P46063
B	621	TYR	-	expression tag	UNP P46063
B	622	PHE	-	expression tag	UNP P46063
B	623	GLN	-	expression tag	UNP P46063
B	624	SER	-	expression tag	UNP P46063
B	625	HIS	-	expression tag	UNP P46063
B	626	HIS	-	expression tag	UNP P46063
B	627	HIS	-	expression tag	UNP P46063
B	628	HIS	-	expression tag	UNP P46063
B	629	HIS	-	expression tag	UNP P46063
B	630	HIS	-	expression tag	UNP P46063
B	631	ASP	-	expression tag	UNP P46063
B	632	TYR	-	expression tag	UNP P46063
B	633	LYS	-	expression tag	UNP P46063
B	634	ASP	-	expression tag	UNP P46063
B	635	ASP	-	expression tag	UNP P46063
B	636	ASP	-	expression tag	UNP P46063
B	637	ASP	-	expression tag	UNP P46063
B	638	LYS	-	expression tag	UNP P46063
C	48	MET	-	initiating methionine	UNP P46063
C	611	SER	GLY	conflict	UNP P46063
C	617	ALA	-	expression tag	UNP P46063
C	618	GLU	-	expression tag	UNP P46063
C	619	ASN	-	expression tag	UNP P46063
C	620	LEU	-	expression tag	UNP P46063
C	621	TYR	-	expression tag	UNP P46063
C	622	PHE	-	expression tag	UNP P46063
C	623	GLN	-	expression tag	UNP P46063
C	624	SER	-	expression tag	UNP P46063
C	625	HIS	-	expression tag	UNP P46063
C	626	HIS	-	expression tag	UNP P46063
C	627	HIS	-	expression tag	UNP P46063
C	628	HIS	-	expression tag	UNP P46063
C	629	HIS	-	expression tag	UNP P46063

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Chain	Residue	Modelled	Actual	Comment	Reference
C	630	HIS	-	expression tag	UNP P46063
C	631	ASP	-	expression tag	UNP P46063
C	632	TYR	-	expression tag	UNP P46063
C	633	LYS	-	expression tag	UNP P46063
C	634	ASP	-	expression tag	UNP P46063
C	635	ASP	-	expression tag	UNP P46063
C	636	ASP	-	expression tag	UNP P46063
C	637	ASP	-	expression tag	UNP P46063
C	638	LYS	-	expression tag	UNP P46063
D	48	MET	-	initiating methionine	UNP P46063
D	611	SER	GLY	conflict	UNP P46063
D	617	ALA	-	expression tag	UNP P46063
D	618	GLU	-	expression tag	UNP P46063
D	619	ASN	-	expression tag	UNP P46063
D	620	LEU	-	expression tag	UNP P46063
D	621	TYR	-	expression tag	UNP P46063
D	622	PHE	-	expression tag	UNP P46063
D	623	GLN	-	expression tag	UNP P46063
D	624	SER	-	expression tag	UNP P46063
D	625	HIS	-	expression tag	UNP P46063
D	626	HIS	-	expression tag	UNP P46063
D	627	HIS	-	expression tag	UNP P46063
D	628	HIS	-	expression tag	UNP P46063
D	629	HIS	-	expression tag	UNP P46063
D	630	HIS	-	expression tag	UNP P46063
D	631	ASP	-	expression tag	UNP P46063
D	632	TYR	-	expression tag	UNP P46063
D	633	LYS	-	expression tag	UNP P46063
D	634	ASP	-	expression tag	UNP P46063
D	635	ASP	-	expression tag	UNP P46063
D	636	ASP	-	expression tag	UNP P46063
D	637	ASP	-	expression tag	UNP P46063
D	638	LYS	-	expression tag	UNP P46063

- Molecule 2 is a DNA chain called DNA oligonucleotide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	17	Total	C	N	O	P	0	0	0
			323	154	54	99	16			
2	Q	16	Total	C	N	O	P	0	0	0
			311	149	54	93	15			
2	R	9	Total	C	N	O	P	0	0	0
			156	74	24	50	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	11	Total	C	N	O	P	0	0	0
			190	89	27	63	11			

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

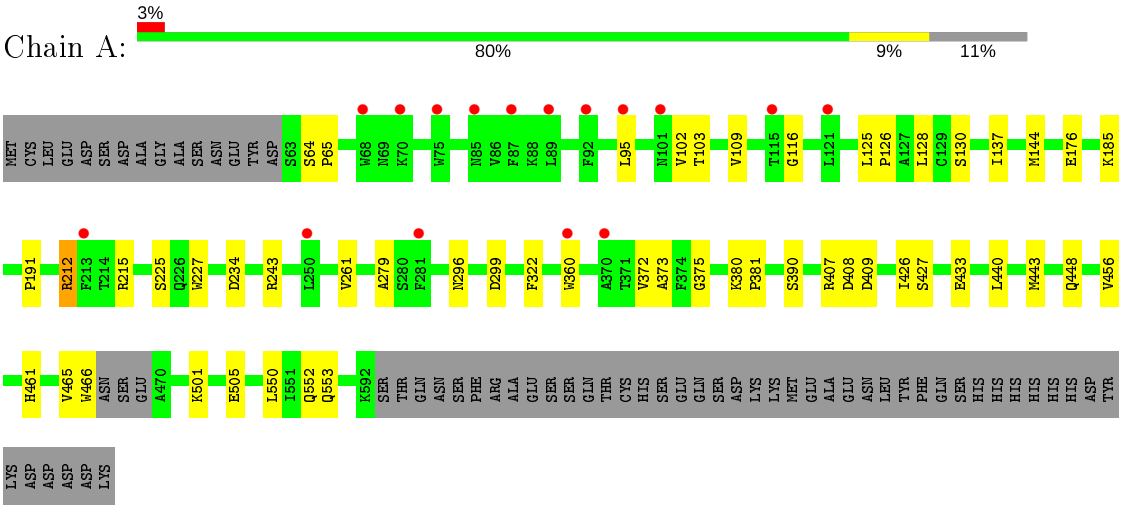
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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 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.

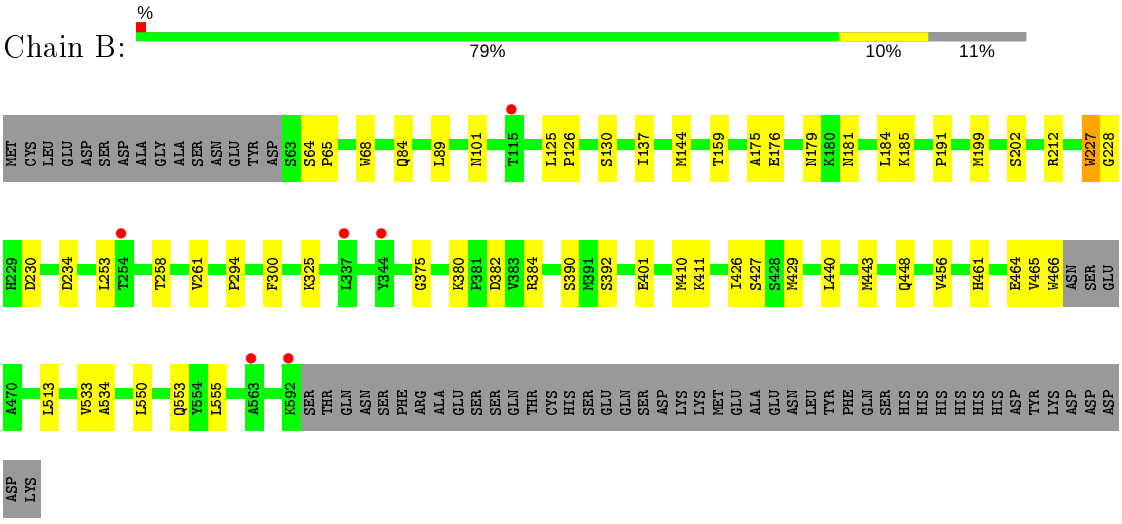
- Molecule 1: ATP-dependent DNA helicase Q1

Chain A:



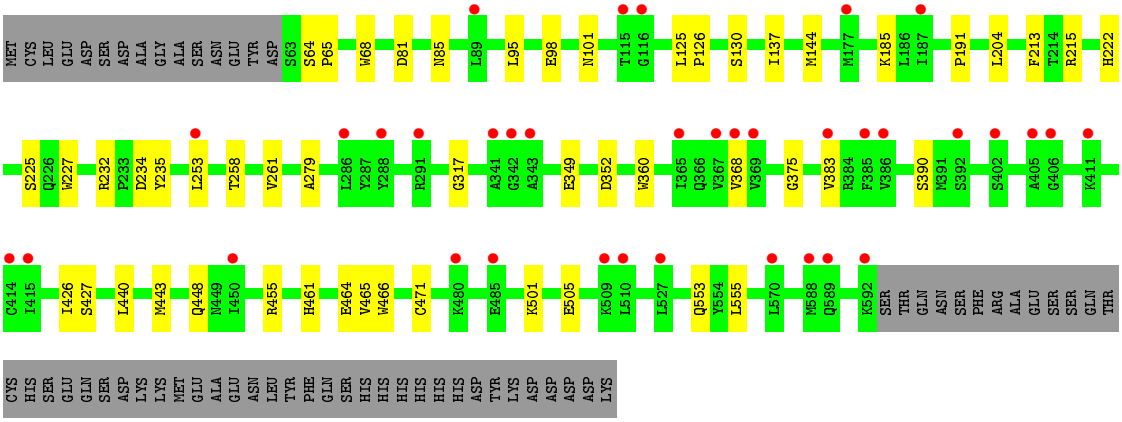
- Molecule 1: ATP-dependent DNA helicase Q1

Chain B:



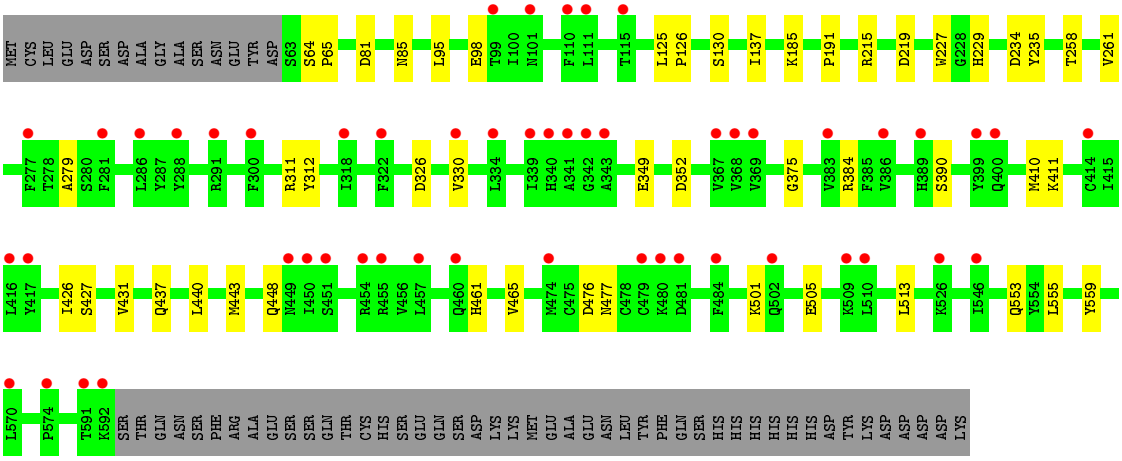
- Molecule 1: ATP-dependent DNA helicase Q1

Chain C:



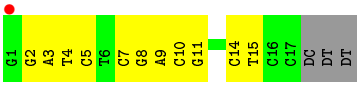
• Molecule 1: ATP-dependent DNA helicase Q1

Chain D:



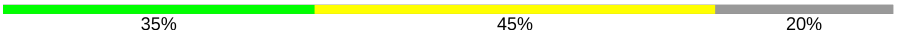
• Molecule 2: DNA oligonucleotide

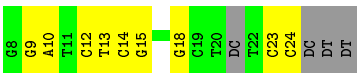
Chain P:



• Molecule 2: DNA oligonucleotide

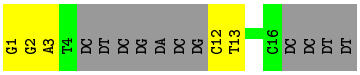
Chain Q:





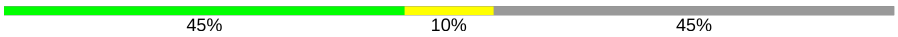
• Molecule 2: DNA oligonucleotide

Chain R:



- Molecule 2: DNA oligonucleotide

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.38Å 138.22Å 207.58Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.90 – 3.40 83.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.90-3.40) 94.9 (83.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1682)	Depositor
R, R_{free}	0.205 , 0.249 0.210 , 0.249	Depositor DCC
R_{free} test set	1888 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.337 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17224	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.67% 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

5.1 Standard geometry

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

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	0.40	0/4137	0.58	0/5606
1	B	0.39	0/4133	0.61	0/5601
1	C	0.37	0/4144	0.57	0/5619
1	D	0.35	0/4152	0.56	0/5629
2	P	0.86	0/360	0.95	0/552
2	Q	0.85	0/346	0.91	0/529
2	R	0.71	0/172	0.96	0/262
2	S	0.62	0/211	0.91	0/322
All	All	0.42	0/17655	0.61	0/24120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4056	0	3918	31	0
1	B	4052	0	3919	31	0
1	C	4062	0	3917	27	0
1	D	4070	0	3928	25	0
2	P	323	0	182	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	311	0	174	9	0
2	R	156	0	88	4	0
2	S	190	0	104	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17224	0	16230	130	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 4.

All (130) 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:B:130:SER:O	1:B:185:LYS:NZ	2.15	0.78
1:D:130:SER:O	1:D:185:LYS:NZ	2.22	0.72
1:A:130:SER:O	1:A:185:LYS:NZ	2.23	0.70
2:P:4:DT:O2	2:Q:18:DG:N2	2.30	0.64
1:A:243:ARG:NH2	1:D:431:VAL:O	2.26	0.64
1:C:130:SER:O	1:C:185:LYS:NZ	2.31	0.63
1:A:227:TRP:HB2	1:A:261:VAL:HG22	1.84	0.60
2:P:2:DG:C6	2:P:3:DA:C6	2.92	0.58
1:B:456:VAL:HG22	1:B:466:TRP:CD1	2.38	0.58
1:B:392:SER:OG	1:B:401:GLU:OE1	2.22	0.57
1:A:433:GLU:OE2	2:Q:23:DC:N4	2.38	0.57
1:A:373:ALA:HA	2:Q:24:DC:H4'	1.86	0.57
1:C:258:THR:HB	1:C:261:VAL:HG23	1.88	0.56
2:P:9:DA:C2	2:P:10:DC:N3	2.75	0.55
2:R:1:DG:N2	2:R:2:DG:N3	2.54	0.55
1:D:125:LEU:HB3	1:D:126:PRO:HD3	1.89	0.54
2:Q:14:DC:H2'	2:Q:15:DG:C8	2.44	0.53
1:B:325:LYS:HZ1	2:P:14:DC:P	2.31	0.53
1:A:130:SER:HB2	1:A:215:ARG:HH21	1.74	0.52
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.92	0.52
1:C:464:GLU:O	1:C:466:TRP:N	2.42	0.52
1:C:125:LEU:HB3	1:C:126:PRO:HD3	1.91	0.52
2:P:4:DT:H2"	2:P:5:DC:H5'	1.91	0.52
1:D:95:LEU:HD12	1:D:279:ALA:HA	1.90	0.52
1:B:513:LEU:HD13	2:Q:10:DA:H5'	1.91	0.52
1:D:426:ILE:HG21	1:D:440:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:13:DT:H1'	2:Q:14:DC:H5'	1.93	0.51
1:A:381:PRO:HA	1:A:407:ARG:HB2	1.91	0.51
1:C:426:ILE:HG21	1:C:440:LEU:HD13	1.92	0.51
1:A:95:LEU:HD12	1:A:279:ALA:HA	1.93	0.50
1:A:176:GLU:O	1:A:212:ARG:NH2	2.43	0.50
1:D:191:PRO:HB2	1:D:234:ASP:HB3	1.94	0.50
2:P:9:DA:C2	2:Q:12:DC:N3	2.80	0.50
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.94	0.49
1:B:137:ILE:N	1:B:137:ILE:HD12	2.27	0.49
1:C:137:ILE:HD12	1:C:137:ILE:N	2.27	0.49
1:A:95:LEU:HD12	1:A:279:ALA:CA	2.42	0.49
1:C:95:LEU:HA	1:C:98:GLU:OE1	2.12	0.49
1:D:81:ASP:OD1	1:D:85:ASN:ND2	2.47	0.48
1:D:513:LEU:HD13	2:R:3:DA:H5'	1.95	0.48
1:C:553:GLN:HA	1:C:555:LEU:O	2.14	0.48
1:D:258:THR:HB	1:D:261:VAL:HG23	1.96	0.48
1:B:191:PRO:HB2	1:B:234:ASP:HB3	1.95	0.48
1:B:325:LYS:NZ	2:P:14:DC:OP1	2.39	0.47
1:B:426:ILE:HG21	1:B:440:LEU:HD13	1.96	0.47
2:P:10:DC:H2"	2:P:11:DG:H5'	1.96	0.47
1:A:137:ILE:N	1:A:137:ILE:HD12	2.30	0.47
1:D:227:TRP:CD1	1:D:227:TRP:N	2.82	0.47
1:B:84:GLN:HA	1:B:89:LEU:O	2.14	0.47
1:B:227:TRP:N	1:B:227:TRP:CD1	2.83	0.47
1:D:137:ILE:HD12	1:D:137:ILE:N	2.30	0.47
1:C:349:GLU:O	1:C:352:ASP:N	2.47	0.47
1:A:103:THR:O	1:A:215:ARG:NH1	2.47	0.47
1:D:384:ARG:NH1	1:D:410:MET:O	2.48	0.47
1:A:372:VAL:HG23	2:Q:24:DC:C5'	2.45	0.46
1:C:95:LEU:HD12	1:C:279:ALA:HA	1.98	0.46
1:C:68:TRP:O	1:C:101:ASN:ND2	2.44	0.46
1:B:294:PRO:HG2	1:B:300:PHE:HA	1.98	0.46
1:B:550:LEU:O	1:B:553:GLN:N	2.44	0.46
1:B:380:LYS:NZ	1:B:382:ASP:OD1	2.41	0.46
1:B:68:TRP:O	1:B:101:ASN:ND2	2.48	0.46
1:C:227:TRP:CD1	1:C:227:TRP:N	2.84	0.46
1:C:191:PRO:HB2	1:C:234:ASP:HB3	1.98	0.46
2:Q:9:DG:C6	2:Q:10:DA:N6	2.83	0.45
1:A:322:PHE:CE1	1:A:426:ILE:HG12	2.52	0.45
1:A:116:GLY:HA3	1:A:407:ARG:NH1	2.31	0.45
1:C:227:TRP:HB2	1:C:261:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LYS:O	1:A:505:GLU:HG3	2.16	0.45
1:C:204:LEU:HD22	1:C:213:PHE:CE2	2.52	0.45
1:C:225:SER:HB3	1:C:261:VAL:HG13	1.98	0.45
1:C:95:LEU:HD12	1:C:279:ALA:CA	2.47	0.45
1:D:384:ARG:NE	1:D:411:LYS:O	2.44	0.45
1:A:191:PRO:HB2	1:A:234:ASP:HB3	1.99	0.44
1:C:455:ARG:HD2	1:C:471:CYS:SG	2.58	0.44
1:C:501:LYS:O	1:C:505:GLU:HG3	2.16	0.44
1:A:426:ILE:HG21	1:A:440:LEU:HD13	2.00	0.44
1:B:464:GLU:O	1:B:466:TRP:N	2.50	0.44
1:A:102:VAL:HG11	1:A:109:VAL:HB	1.98	0.44
1:C:81:ASP:OD1	1:C:85:ASN:ND2	2.51	0.43
1:D:476:ASP:OD2	1:D:477:ASN:N	2.52	0.43
1:B:64:SER:HB2	1:B:65:PRO:HD2	1.99	0.43
1:D:95:LEU:HD12	1:D:279:ALA:CA	2.49	0.43
1:A:64:SER:HB2	1:A:65:PRO:HD2	2.00	0.43
1:B:175:ALA:O	1:B:179:ASN:HB2	2.17	0.43
1:C:317:GLY:HA2	1:C:383:VAL:HG13	2.00	0.43
1:C:360:TRP:CG	1:C:368:VAL:CG2	3.01	0.43
1:D:95:LEU:HA	1:D:98:GLU:OE1	2.19	0.43
1:A:550:LEU:O	1:A:553:GLN:N	2.49	0.43
1:D:326:ASP:O	1:D:330:VAL:HG23	2.18	0.43
1:D:553:GLN:HA	1:D:555:LEU:O	2.19	0.43
2:S:3:DA:H2"	2:S:4:DT:H5'	2.00	0.43
1:D:130:SER:HB2	1:D:215:ARG:HH21	1.82	0.43
1:B:179:ASN:OD1	1:B:181:ASN:N	2.51	0.42
1:A:227:TRP:N	1:A:227:TRP:CD1	2.87	0.42
1:B:258:THR:HB	1:B:261:VAL:HG23	2.01	0.42
2:P:7:DC:H2'	2:P:8:DG:C8	2.54	0.42
1:A:225:SER:HB3	1:A:261:VAL:HG13	2.01	0.42
1:C:144:MET:HB2	1:C:144:MET:HE3	1.89	0.42
1:B:384:ARG:NH1	1:B:410:MET:O	2.52	0.42
1:D:437:GLN:NE2	1:D:559:TYR:OH	2.49	0.42
1:B:199:MET:O	1:B:202:SER:OG	2.34	0.42
1:B:429:MET:CE	2:P:15:DT:H2"	2.49	0.42
1:D:219:ASP:O	1:D:235:TYR:OH	2.29	0.42
1:D:501:LYS:O	1:D:505:GLU:HG3	2.19	0.42
1:A:408:ASP:O	1:A:409:ASP:HB2	2.20	0.42
2:P:4:DT:H2"	2:P:5:DC:C5'	2.50	0.41
1:C:232:ARG:O	1:C:235:TYR:HB2	2.19	0.41
1:A:296:ASN:HB3	1:A:299:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:HB2	1:C:65:PRO:HD2	2.02	0.41
1:D:64:SER:HB2	1:D:65:PRO:HD2	2.02	0.41
2:P:11:DG:N3	2:P:11:DG:H2'	2.34	0.41
1:D:349:GLU:O	1:D:352:ASP:N	2.48	0.41
1:B:159:THR:CG2	1:B:184:LEU:HD21	2.50	0.41
2:S:3:DA:H1'	2:S:4:DT:C5'	2.51	0.41
1:A:128:LEU:HA	1:A:185:LYS:HD2	2.03	0.41
1:A:456:VAL:HG22	1:A:466:TRP:CD1	2.56	0.41
1:B:228:GLY:O	1:B:230:ASP:N	2.53	0.41
1:B:384:ARG:NE	1:B:411:LYS:O	2.43	0.41
1:B:553:GLN:HA	1:B:555:LEU:O	2.21	0.41
2:R:1:DG:C2	2:R:2:DG:C4	3.08	0.41
1:C:222:HIS:HB2	1:C:261:VAL:HG11	2.03	0.41
1:B:144:MET:HB2	1:B:144:MET:HE2	1.94	0.41
1:A:144:MET:HE3	1:A:144:MET:HB2	1.90	0.40
1:A:360:TRP:CH2	1:A:380:LYS:HD3	2.56	0.40
1:A:552:GLN:O	1:A:553:GLN:HB2	2.21	0.40
1:D:311:ARG:HD2	1:D:312:TYR:CZ	2.56	0.40
1:B:176:GLU:O	1:B:212:ARG:NH2	2.54	0.40
1:C:130:SER:HB2	1:C:215:ARG:HH21	1.86	0.40
1:B:533:VAL:HG12	1:B:534:ALA:O	2.22	0.40
2:R:12:DC:H2'	2:R:13:DT:H71	2.03	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	
1	A	523/591 (88%)	499 (95%)	22 (4%)	2 (0%)	34	67
1	B	523/591 (88%)	500 (96%)	21 (4%)	2 (0%)	34	67
1	C	528/591 (89%)	504 (96%)	22 (4%)	2 (0%)	34	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	528/591 (89%)	503 (95%)	22 (4%)	3 (1%)	25 57
All	All	2102/2364 (89%)	2006 (95%)	87 (4%)	9 (0%)	34 67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	VAL
1	A	375	GLY
1	A	465	VAL
1	B	375	GLY
1	B	465	VAL
1	C	375	GLY
1	D	229	HIS
1	D	375	GLY
1	D	465	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	416/521 (80%)	410 (99%)	6 (1%)	67 83
1	B	416/521 (80%)	409 (98%)	7 (2%)	60 80
1	C	414/521 (80%)	408 (99%)	6 (1%)	67 83
1	D	417/521 (80%)	412 (99%)	5 (1%)	71 85
All	All	1663/2084 (80%)	1639 (99%)	24 (1%)	67 83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	390	SER
1	A	427	SER
1	A	443	MET
1	A	448	GLN

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Mol	Chain	Res	Type
1	A	461	HIS
1	B	227	TRP
1	B	253	LEU
1	B	390	SER
1	B	427	SER
1	B	443	MET
1	B	448	GLN
1	B	461	HIS
1	C	253	LEU
1	C	390	SER
1	C	427	SER
1	C	443	MET
1	C	448	GLN
1	C	461	HIS
1	D	390	SER
1	D	427	SER
1	D	443	MET
1	D	448	GLN
1	D	461	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	HIS
1	A	389	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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 95^{th} 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	527/591 (89%)	0.33	16 (3%) 50 49	42, 82, 133, 160	0
1	B	527/591 (89%)	0.23	6 (1%) 80 79	52, 78, 110, 131	0
1	C	530/591 (89%)	0.49	36 (6%) 17 19	66, 96, 134, 158	0
1	D	530/591 (89%)	0.65	52 (9%) 7 9	60, 116, 153, 168	0
2	P	17/20 (85%)	0.21	1 (5%) 22 23	78, 99, 108, 111	0
2	Q	16/20 (80%)	0.19	0 100 100	71, 92, 107, 108	0
2	R	9/20 (45%)	-0.55	0 100 100	127, 134, 136, 139	0
2	S	11/20 (55%)	-0.31	0 100 100	109, 131, 137, 140	0
All	All	2167/2444 (88%)	0.41	111 (5%) 28 28	42, 89, 140, 168	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	TYR	5.5
1	C	343	ALA	5.4
1	C	510	LEU	5.0
1	D	510	LEU	5.0
1	D	339	ILE	4.9
1	D	509	LYS	4.7
1	D	480	LYS	4.3
1	D	343	ALA	4.2
1	D	416	LEU	4.2
1	C	367	VAL	3.8
1	D	460	GLN	3.8
1	D	417	TYR	3.7
1	C	405	ALA	3.6
1	D	450	ILE	3.5
1	C	342	GLY	3.4
1	D	286	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	392	SER	3.3
1	D	341	ALA	3.3
1	D	451	SER	3.3
1	D	342	GLY	3.2
1	D	334	LEU	3.1
1	D	399	TYR	3.1
1	A	213	PHE	3.1
1	D	300	PHE	3.1
1	C	592	LYS	3.0
1	D	570	LEU	2.9
1	A	92	PHE	2.8
1	C	288	TYR	2.8
1	D	457	LEU	2.8
1	C	365	ILE	2.7
1	C	341	ALA	2.7
1	C	115	THR	2.7
1	D	281	PHE	2.7
1	D	449	ASN	2.7
1	D	369	VAL	2.7
1	A	95	LEU	2.7
1	C	450	ILE	2.7
1	C	414	CYS	2.7
1	B	344	TYR	2.6
1	D	383	VAL	2.6
1	A	115	THR	2.6
1	D	277	PHE	2.6
1	C	385	PHE	2.6
1	C	415	ILE	2.6
1	D	318	ILE	2.6
1	D	455	ARG	2.6
1	C	589	GLN	2.6
1	A	85	ASN	2.6
1	C	527	LEU	2.5
1	C	177	MET	2.5
1	A	75	TRP	2.5
1	C	386	VAL	2.5
1	D	115	THR	2.5
1	A	89	LEU	2.5
1	B	563	ALA	2.5
1	D	322	PHE	2.5
1	D	110	PHE	2.4
1	A	101	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	368	VAL	2.4
1	D	368	VAL	2.4
1	D	291	ARG	2.4
1	D	546	ILE	2.4
1	C	509	LYS	2.4
1	C	402	SER	2.4
1	D	502	GLN	2.4
1	B	115	THR	2.4
1	D	574	PRO	2.3
1	C	253	LEU	2.3
1	A	360	TRP	2.3
1	A	281	PHE	2.3
1	D	386	VAL	2.3
1	B	337	LEU	2.3
1	D	454	ARG	2.3
1	A	250	LEU	2.3
1	D	484	PHE	2.2
1	D	591	THR	2.2
1	D	592	LYS	2.2
1	D	389	HIS	2.2
1	C	291	ARG	2.2
1	C	485	GLU	2.2
1	A	370	ALA	2.2
1	C	588	MET	2.2
1	D	474	MET	2.2
1	C	570	LEU	2.2
1	C	383	VAL	2.2
1	B	592	LYS	2.2
1	D	526	LYS	2.2
1	B	254	THR	2.2
1	D	400	GLN	2.2
1	D	479	CYS	2.2
1	A	70	LYS	2.2
1	D	99	THR	2.2
1	C	369	VAL	2.1
1	D	414	CYS	2.1
2	P	1	DG	2.1
1	A	68	TRP	2.1
1	A	87	PHE	2.1
1	C	286	LEU	2.1
1	D	111	LEU	2.1
1	D	340	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	116	GLY	2.1
1	D	101	ASN	2.1
1	D	367	VAL	2.1
1	C	89	LEU	2.1
1	D	481	ASP	2.0
1	C	187	ILE	2.0
1	C	480	LYS	2.0
1	C	411	LYS	2.0
1	D	330	VAL	2.0
1	A	121	LEU	2.0
1	C	406	GLY	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. The B-factors column lists the minimum, median, 95^{th} 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
3	ZN	B	701	1/1	0.96	0.14	91,91,91,91	0
3	ZN	D	701	1/1	0.97	0.10	131,131,131,131	0
3	ZN	C	701	1/1	0.98	0.15	94,94,94,94	0
3	ZN	A	701	1/1	0.99	0.17	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.