



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:02 AM UTC

PDB ID : 5LB8 / pdb_00005lb8
Title : Crystal structure of human RECQL5 helicase APO form.
Authors : Newman, J.A.; Aitkenhead, H.; Savitsky, P.; Krojer, T.; von Delft, F.; Arrow-smith, C.H.; Edwards, A.M.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2016-06-15
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

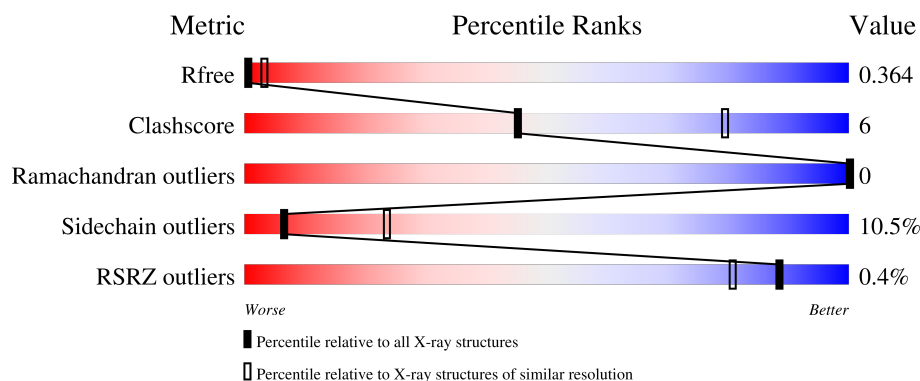
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	518	63% 18% • 18%
1	D	518	64% 18% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6566 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 Q5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3266	2070	572	602	22			
1	D	426	Total	C	N	O	S	0	0	0
			3298	2087	584	605	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 1: ATP-dependent DNA helicase Q5



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.74Å 68.74Å 396.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.40 48.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-3.40) 99.7 (48.61-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.301 , 0.322 0.317 , 0.364	Depositor DCC
R_{free} test set	684 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	139.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 126.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6566	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.333 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

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	0.80	0/3330	1.38	5/4513 (0.1%)
1	D	0.74	0/3362	1.36	8/4550 (0.2%)
All	All	0.77	0/6692	1.37	13/9063 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ALA	N-CA-C	8.88	121.92	111.71
1	A	164	GLN	N-CA-C	-6.67	104.45	112.59
1	A	309	LYS	N-CA-C	-5.98	105.81	113.23
1	A	231	PHE	CA-C-N	5.53	127.95	120.38
1	A	231	PHE	C-N-CA	5.53	127.95	120.38
1	D	184	GLY	CA-C-N	5.36	131.79	121.18
1	D	184	GLY	C-N-CA	5.36	131.79	121.18
1	D	231	PHE	CA-C-N	5.08	127.33	120.38
1	D	231	PHE	C-N-CA	5.08	127.33	120.38
1	D	110	LYS	CA-C-N	5.07	127.58	120.28
1	D	110	LYS	C-N-CA	5.07	127.58	120.28
1	D	141	THR	CA-C-N	5.03	127.02	120.28
1	D	141	THR	C-N-CA	5.03	127.02	120.28

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	3266	0	3229	44	0
1	D	3298	0	3290	34	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
All	All	6566	0	6519	77	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 (77) 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:162:VAL:CG1	1:A:173:TYR:HB3	2.09	0.81
1:A:162:VAL:HG13	1:A:173:TYR:HB3	1.62	0.81
1:A:75:VAL:HA	1:A:155:VAL:HB	1.78	0.66
1:A:54:THR:HA	1:A:58:LYS:HD3	1.80	0.63
1:A:163:SER:O	1:A:169:PHE:HD1	1.80	0.63
1:D:287:LYS:HD2	1:D:301:VAL:HG11	1.82	0.62
1:A:174:LEU:HD22	1:D:175:ARG:HE	1.65	0.62
1:D:48:VAL:HG12	1:D:214:ALA:HB3	1.84	0.59
1:A:48:VAL:HG12	1:A:214:ALA:HB3	1.84	0.59
1:D:149:HIS:HA	1:D:185:HIS:NE2	2.18	0.59
1:D:142:LEU:HD21	1:D:183:LEU:HD11	1.85	0.58
1:A:162:VAL:HG12	1:A:173:TYR:HB3	1.85	0.58
1:A:438:THR:HG22	1:A:441:ARG:HH21	1.71	0.56
1:D:326:ALA:HA	1:D:352:ARG:HB2	1.88	0.56
1:A:326:ALA:HA	1:A:352:ARG:HB2	1.88	0.55
1:A:84:GLN:HA	1:A:87:VAL:HG22	1.89	0.54
1:D:438:THR:HG22	1:D:441:ARG:HH21	1.72	0.54
1:A:116:LEU:HB3	1:A:145:LEU:HD11	1.89	0.53
1:D:75:VAL:HA	1:D:155:VAL:HB	1.90	0.53
1:A:160:HIS:ND1	1:A:192:THR:OG1	2.34	0.53
1:A:180:ARG:HH12	1:A:184:GLY:HA2	1.72	0.53
1:D:364:SER:HB3	1:D:367:ASP:HB2	1.89	0.53
1:A:96:ARG:HB2	1:A:123:THR:HA	1.90	0.53
1:A:163:SER:O	1:A:169:PHE:CD1	2.61	0.52
1:A:48:VAL:HG23	1:A:189:VAL:HG13	1.91	0.51
1:A:400:ASP:HA	1:A:403:VAL:HG22	1.93	0.51
1:D:48:VAL:HG23	1:D:189:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:HG2	1:A:391:SER:HB3	1.93	0.51
1:D:400:ASP:HA	1:D:403:VAL:HG22	1.93	0.51
1:D:264:VAL:HG12	1:D:332:ALA:HB3	1.94	0.50
1:D:226:PHE:HD2	1:D:358:TRP:HD1	1.59	0.50
1:A:431:CYS:HB3	1:A:434:CYS:SG	2.53	0.49
1:D:431:CYS:HB3	1:D:434:CYS:SG	2.53	0.48
1:A:413:HIS:HA	1:A:416:ILE:HD12	1.96	0.48
1:A:204:PHE:HA	1:A:209:LEU:HD12	1.97	0.47
1:D:159:ALA:O	1:D:162:VAL:HG22	2.15	0.47
1:D:413:HIS:HA	1:D:416:ILE:HD12	1.97	0.47
1:D:204:PHE:HA	1:D:209:LEU:HD12	1.96	0.46
1:A:167:HIS:HB3	1:A:341:ALA:HB3	1.98	0.46
1:D:73:THR:HG23	1:D:153:TYR:HB2	1.97	0.46
1:D:267:ARG:HE	1:D:371:VAL:HG22	1.80	0.46
1:D:178:ALA:O	1:D:182:ARG:HB2	2.16	0.46
1:D:88:ASP:HA	1:D:91:LEU:HD12	1.97	0.46
1:A:87:VAL:HG11	1:A:99:SER:HB3	1.99	0.45
1:D:115:ASP:O	1:D:121:PRO:HB3	2.17	0.45
1:A:177:GLY:HA2	1:A:207:LEU:HA	1.98	0.45
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.99	0.45
1:D:167:HIS:HB3	1:D:341:ALA:HB3	1.99	0.44
1:A:96:ARG:H	1:A:96:ARG:HG2	1.59	0.44
1:D:113:LEU:HA	1:D:116:LEU:HD12	2.00	0.44
1:A:161:CYS:HB3	1:A:170:ARG:HG3	1.99	0.43
1:A:331:VAL:HG23	1:A:350:ALA:HB2	1.99	0.43
1:A:338:LYS:HG3	1:A:375:ILE:HD11	1.99	0.43
1:A:41:VAL:HG22	1:A:48:VAL:HG21	1.99	0.43
1:A:173:TYR:HA	1:A:176:LEU:HD12	2.00	0.43
1:D:338:LYS:HG3	1:D:375:ILE:HD12	2.00	0.43
1:A:98:SER:HB3	1:A:123:THR:HG21	2.00	0.43
1:A:312:VAL:HG22	1:A:330:PHE:HZ	1.82	0.43
1:A:162:VAL:HG12	1:A:173:TYR:C	2.43	0.43
1:A:37:ALA:O	1:A:41:VAL:HG23	2.19	0.43
1:D:41:VAL:HG22	1:D:48:VAL:HG21	2.01	0.43
1:A:264:VAL:HG12	1:A:332:ALA:HB3	2.00	0.42
1:A:67:LEU:HD23	1:A:124:LYS:HG2	2.01	0.42
1:A:72:ILE:HG22	1:A:124:LYS:HA	2.01	0.42
1:A:242:LEU:HD23	1:A:279:LEU:HD21	2.00	0.42
1:D:266:CYS:SG	1:D:272:CYS:HB3	2.60	0.42
1:D:379:VAL:HG11	1:D:396:ILE:HD11	2.02	0.42
1:D:162:VAL:HG13	1:D:173:TYR:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HG23	1:A:313:ILE:HG23	2.03	0.41
1:A:266:CYS:SG	1:A:272:CYS:HB3	2.61	0.41
1:D:37:ALA:O	1:D:41:VAL:HG23	2.20	0.41
1:D:287:LYS:HB2	1:D:310:VAL:HG11	2.03	0.41
1:A:379:VAL:HG11	1:A:396:ILE:HD11	2.03	0.41
1:A:83:ILE:HG12	1:A:127:TYR:HD1	1.85	0.40
1:D:140:PRO:HA	1:D:143:ASN:HD22	1.86	0.40
1:A:203:VAL:HG13	1:A:207:LEU:HD12	2.03	0.40
1:D:232:LYS:HB2	1:D:364:SER:HB2	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	421/518 (81%)	394 (94%)	27 (6%)	0	100	100
1	D	420/518 (81%)	390 (93%)	30 (7%)	0	100	100
All	All	841/1036 (81%)	784 (93%)	57 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/432 (80%)	305 (89%)	39 (11%)	5	21
1	D	351/432 (81%)	317 (90%)	34 (10%)	8	28
All	All	695/864 (80%)	622 (90%)	73 (10%)	6	23

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	33	LEU
1	A	47	ASP
1	A	54	THR
1	A	64	LEU
1	A	83	ILE
1	A	84	GLN
1	A	90	LEU
1	A	96	ARG
1	A	100	LEU
1	A	104	LEU
1	A	113	LEU
1	A	118	ARG
1	A	126	LEU
1	A	139	GLN
1	A	151	LEU
1	A	163	SER
1	A	164	GLN
1	A	179	LEU
1	A	182	ARG
1	A	196	THR
1	A	202	ASP
1	A	230	GLN
1	A	263	ILE
1	A	264	VAL
1	A	274	GLN
1	A	294	LYS
1	A	297	GLU
1	A	304	ASP
1	A	308	GLU
1	A	309	LYS
1	A	314	VAL
1	A	352	ARG
1	A	381	LYS
1	A	406	CYS

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Mol	Chain	Res	Type
1	A	409	LEU
1	A	433	HIS
1	A	444	LEU
1	A	447	LEU
1	D	33	LEU
1	D	47	ASP
1	D	60	LEU
1	D	72	ILE
1	D	80	ILE
1	D	82	LEU
1	D	83	ILE
1	D	84	GLN
1	D	96	ARG
1	D	100	LEU
1	D	104	LEU
1	D	151	LEU
1	D	164	GLN
1	D	179	LEU
1	D	196	THR
1	D	202	ASP
1	D	230	GLN
1	D	264	VAL
1	D	274	GLN
1	D	294	LYS
1	D	297	GLU
1	D	306	MET
1	D	309	LYS
1	D	313	ILE
1	D	314	VAL
1	D	352	ARG
1	D	367	ASP
1	D	381	LYS
1	D	386	ARG
1	D	406	CYS
1	D	409	LEU
1	D	433	HIS
1	D	444	LEU
1	D	447	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	86	GLN
1	A	89	HIS
1	A	139	GLN
1	A	143	ASN
1	A	164	GLN
1	D	34	GLN
1	D	139	GLN
1	D	143	ASN
1	D	149	HIS
1	D	274	GLN
1	D	370	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/518 (82%)	-0.11	3 (0%) 84 73	83, 141, 176, 189	0
1	D	426/518 (82%)	-0.29	0 100 100	115, 149, 179, 199	0
All	All	853/1036 (82%)	-0.20	3 (0%) 88 81	83, 146, 178, 199	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	CYS	3.0
1	A	133	ALA	2.3
1	A	75	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	D	601	1/1	0.96	0.05	132,132,132,132	0
2	ZN	A	601	1/1	0.97	0.06	166,166,166,166	0

6.5 Other polymers [i](#)

There are no such residues in this entry.