



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 06:26 PM EST

PDB ID : 5LB5  
Title : Crystal structure of human RECQL5 helicase in complex with ADP/Mg (triclinic 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 : 2.00 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

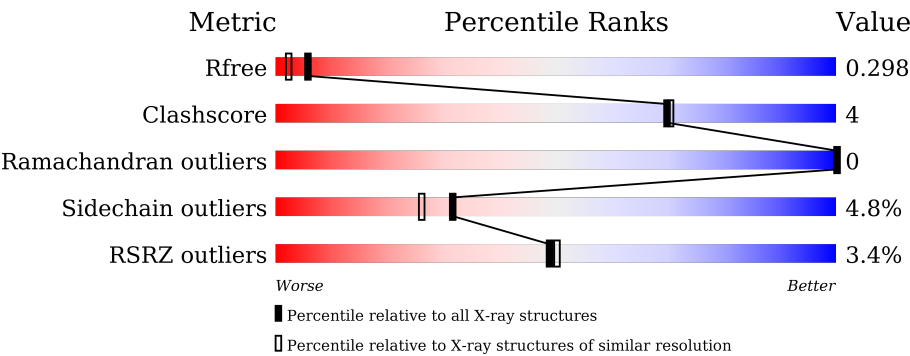
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	A	445	<div><div>2%</div><div><div></div><div>88%</div><div>8%</div><div></div></div><div></div></div>
1	B	445	<div><div>3%</div><div><div></div><div>88%</div><div>8%</div><div></div></div><div></div></div>
1	C	445	<div><div>5%</div><div><div></div><div>85%</div><div>9%</div><div></div></div><div></div></div>
1	D	445	<div><div>4%</div><div><div></div><div>87%</div><div>9%</div><div></div></div><div></div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	501	-	-	-	X
2	ZN	B	501	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13859 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	430	Total	C	N	O	S	0	3	0
			3354	2117	600	615	22			
1	B	433	Total	C	N	O	S	0	3	0
			3352	2119	595	613	25			
1	C	426	Total	C	N	O	S	0	1	0
			3273	2070	576	605	22			
1	D	434	Total	C	N	O	S	0	2	0
			3353	2120	593	618	22			

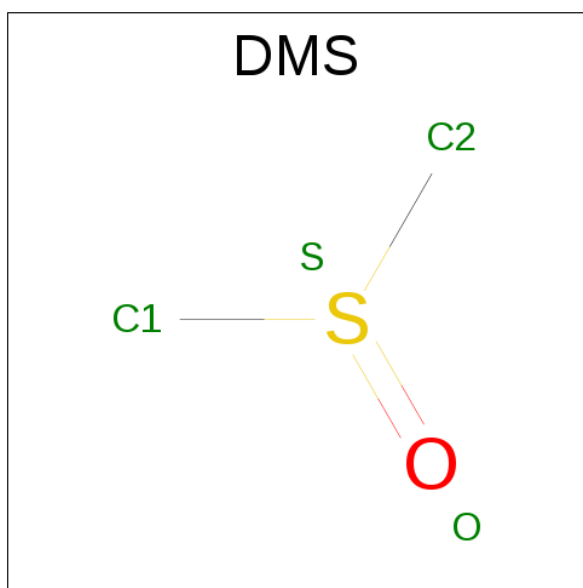
There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).

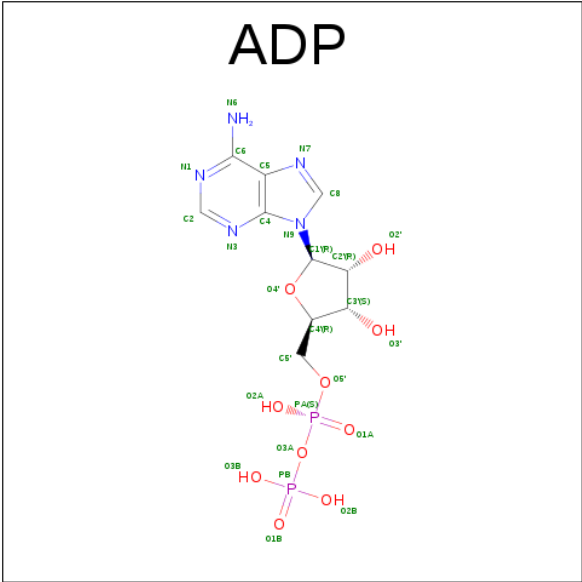


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

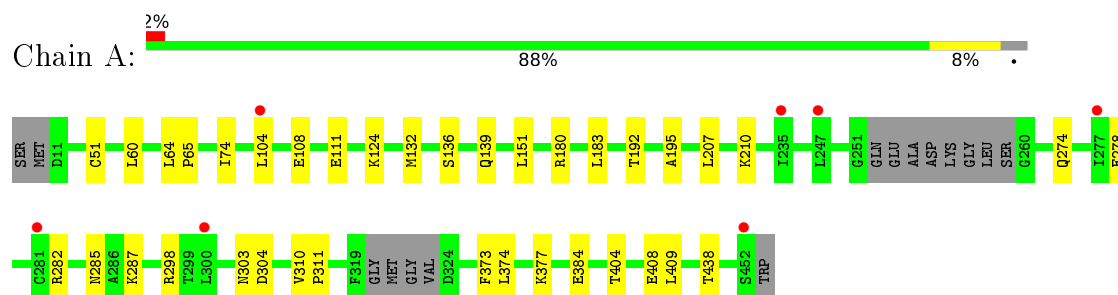
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	115	Total	O	0	0
			115	115		
6	B	113	Total	O	0	0
			113	113		
6	C	93	Total	O	0	0
			93	93		
6	D	78	Total	O	0	0
			78	78		

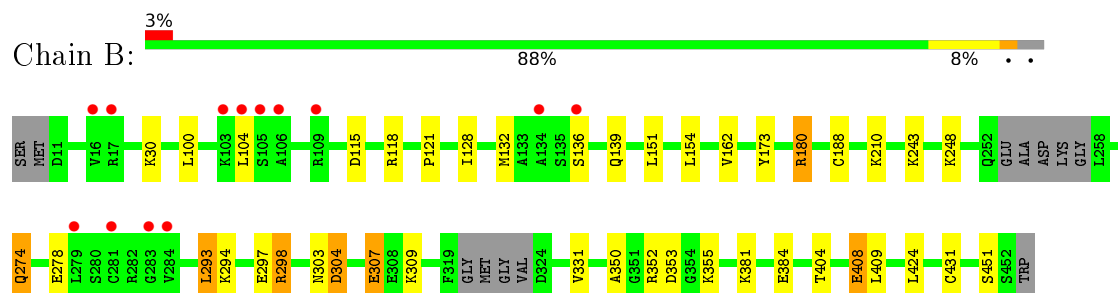
### 3 Residue-property plots [i](#)

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.

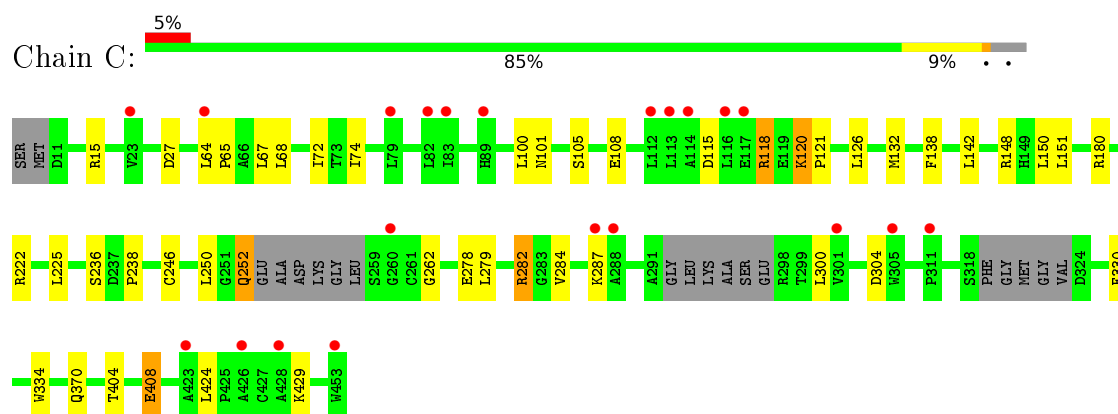
- Molecule 1: ATP-dependent DNA helicase Q5



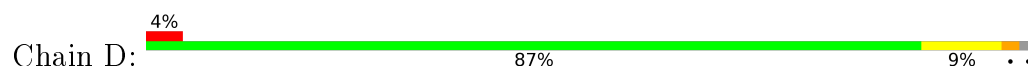
- Molecule 1: ATP-dependent DNA helicase Q5

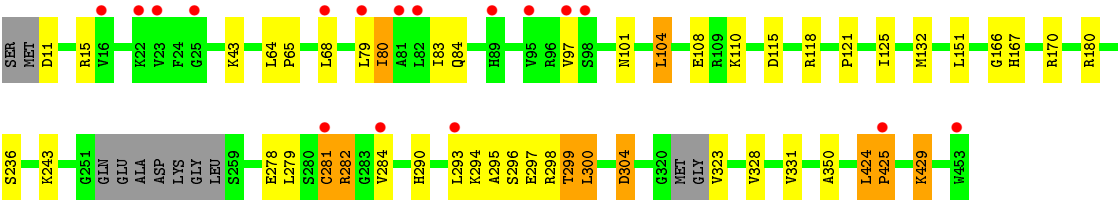


- Molecule 1: ATP-dependent DNA helicase Q5



- Molecule 1: ATP-dependent DNA helicase Q5







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.59 Å   84.75 Å   106.69 Å 108.82°   90.06°   96.86°	Depositor
Resolution (Å)	100.90 – 2.00 100.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (100.90-2.00) 87.5 (100.90-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.00 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.244   ,   0.282 0.258   ,   0.298	Depositor DCC
$R_{free}$ test set	6950 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.70% 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, DMS, MG, ADP

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	0.52	0/3418	0.64	0/4624
1	B	0.54	0/3416	0.68	0/4624
1	C	0.50	0/3337	0.65	1/4526 (0.0%)
1	D	0.55	0/3418	0.68	1/4631 (0.0%)
All	All	0.53	0/13589	0.66	2/18405 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	424	LEU	C-N-CD	5.25	139.43	128.40
1	C	120	LYS	C-N-CD	5.25	139.41	128.40

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	3354	0	3334	14	0
1	B	3352	0	3330	32	0
1	C	3273	0	3211	37	0
1	D	3353	0	3312	36	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
3	D	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	0	0
6	A	115	0	0	0	0
6	B	113	0	0	2	0
6	C	93	0	0	0	0
6	D	78	0	0	0	0
All	All	13859	0	13253	119	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 (119) 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:D:278:GLU:O	1:D:282:ARG:CD	1.96	1.13
1:D:278:GLU:O	1:D:282:ARG:CG	1.98	1.11
1:C:118:ARG:HD3	1:C:121:PRO:HA	1.38	1.04
1:D:278:GLU:O	1:D:282:ARG:HG2	1.59	1.02
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.23	0.98
1:D:293:LEU:O	1:D:298:ARG:NH2	1.98	0.96
1:C:279:LEU:HB3	1:C:284:VAL:HG13	1.48	0.95
1:B:293:LEU:HB2	1:B:297:GLU:OE2	1.77	0.85
1:C:278:GLU:O	1:C:282:ARG:CD	2.24	0.85
1:B:180:ARG:HD3	1:B:188:CYS:HB2	1.61	0.81
1:D:278:GLU:O	1:D:282:ARG:HD2	1.81	0.81
1:C:118:ARG:NH1	1:C:118:ARG:HG3	1.93	0.79
1:C:278:GLU:O	1:C:282:ARG:HD3	1.86	0.74
1:D:429:LYS:HD3	1:D:429:LYS:C	2.07	0.74
1:D:290:HIS:H	1:D:293:LEU:HD12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ALA:O	1:D:299:THR:OG1	2.07	0.73
1:C:279:LEU:HB3	1:C:284:VAL:CG1	2.19	0.72
1:C:72:ILE:HD11	1:C:121:PRO:HG2	1.70	0.72
1:B:298:ARG:HG2	1:B:298:ARG:NH1	2.06	0.70
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.57	0.69
1:D:279:LEU:HA	1:D:282:ARG:HG3	1.74	0.69
1:B:180:ARG:HH22	1:B:210:LYS:HG3	1.58	0.69
1:C:279:LEU:O	1:C:284:VAL:HG12	1.93	0.68
1:C:279:LEU:O	1:C:284:VAL:CG1	2.44	0.66
1:D:278:GLU:O	1:D:282:ARG:HD3	1.94	0.66
1:B:293:LEU:HG	1:B:297:GLU:HB3	1.78	0.65
1:A:180:ARG:HG2	1:A:207:LEU:O	1.96	0.65
1:C:278:GLU:O	1:C:282:ARG:HG2	1.98	0.63
1:D:80:ILE:HA	1:D:83:ILE:HD12	1.80	0.63
1:C:278:GLU:O	1:C:282:ARG:CG	2.46	0.63
1:C:105:SER:HB3	1:C:108:GLU:HG3	1.81	0.63
1:C:246:CYS:O	1:C:250:LEU:HD12	1.99	0.62
1:C:279:LEU:CB	1:C:284:VAL:HG13	2.28	0.61
1:C:262:GLY:HA3	1:C:330:PHE:CE2	2.37	0.60
1:B:128:ILE:HD11	1:B:132[A]:MET:HG3	1.82	0.60
1:B:298:ARG:HH11	1:B:298:ARG:CG	2.14	0.59
1:B:180:ARG:NH2	1:B:210:LYS:HG3	2.18	0.59
1:C:118:ARG:CG	1:C:118:ARG:HH11	2.09	0.58
1:D:115:ASP:O	1:D:118:ARG:HB2	2.03	0.57
1:B:294:LYS:O	1:B:297:GLU:HB2	2.05	0.56
1:C:279:LEU:HD22	1:C:284:VAL:HG11	1.88	0.56
1:D:278:GLU:OE1	1:D:282:ARG:NH1	2.37	0.56
1:B:293:LEU:HD23	1:B:293:LEU:O	2.06	0.55
1:D:79:LEU:O	1:D:83:ILE:HG13	2.07	0.55
1:B:303:ASN:O	1:B:307:GLU:HG2	2.07	0.54
1:B:304:ASP:HA	1:B:309:LYS:HD2	1.90	0.54
1:B:293:LEU:CD2	1:B:298:ARG:CD	2.85	0.54
1:C:279:LEU:CD2	1:C:284:VAL:HG11	2.38	0.53
1:D:328:VAL:HB	1:D:350:ALA:HA	1.90	0.53
1:D:290:HIS:H	1:D:293:LEU:CD1	2.20	0.53
1:B:293:LEU:HB2	1:B:297:GLU:CD	2.30	0.52
1:C:279:LEU:C	1:C:284:VAL:HG13	2.30	0.52
1:D:331:VAL:HG23	1:D:350:ALA:HB2	1.92	0.51
1:D:300:LEU:HD12	1:D:304:ASP:OD2	2.10	0.51
1:B:293:LEU:HD23	1:B:293:LEU:C	2.31	0.51
1:C:15:ARG:HG2	1:C:68:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:HH21	1:A:210:LYS:HG3	1.76	0.51
1:D:101:ASN:H	1:D:104:LEU:HD12	1.76	0.50
1:B:293:LEU:CD2	1:B:298:ARG:HD3	2.42	0.50
1:B:293:LEU:HD23	1:B:298:ARG:HD3	1.94	0.49
1:A:373:PHE:CZ	1:A:377:LYS:HE2	2.47	0.49
1:D:15:ARG:HE	1:D:68:LEU:HD22	1.78	0.48
1:B:293:LEU:CD2	1:B:298:ARG:HD2	2.44	0.48
1:D:101:ASN:HA	1:D:132:MET:HG3	1.95	0.48
1:D:294:LYS:O	1:D:297:GLU:N	2.46	0.48
1:D:424:LEU:HG	1:D:425:PRO:HD2	1.96	0.48
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.96	0.47
1:C:404:THR:O	1:C:408:GLU:HB2	2.13	0.47
1:C:118:ARG:O	1:C:148:ARG:NH1	2.46	0.47
1:A:136:SER:HA	1:A:139:GLN:HG2	1.97	0.47
1:A:74:ILE:HG13	1:A:151:LEU:HD21	1.97	0.47
1:A:278:GLU:O	1:A:282:ARG:HG2	2.14	0.47
1:B:154:LEU:HD23	1:B:180:ARG:HG2	1.97	0.47
1:D:429:LYS:HD3	1:D:429:LYS:O	2.15	0.47
1:B:162:VAL:HG12	1:B:173:TYR:HB3	1.97	0.46
1:D:323:VAL:HG12	1:D:323:VAL:O	2.14	0.46
1:C:284:VAL:HG13	1:C:284:VAL:O	2.16	0.46
1:C:148:ARG:HB3	1:C:150:LEU:HD13	1.98	0.46
1:C:279:LEU:O	1:C:284:VAL:HG13	2.15	0.46
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.98	0.46
1:C:115:ASP:O	1:C:121:PRO:HB3	2.16	0.45
1:D:282:ARG:HG2	1:D:282:ARG:H	1.46	0.45
1:D:80:ILE:H	1:D:80:ILE:HG13	1.46	0.45
1:A:195:ALA:H	3:A:502:DMS:H23	1.80	0.45
1:C:101:ASN:HA	1:C:132:MET:HG3	1.98	0.45
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.99	0.45
1:B:115:ASP:O	1:B:121:PRO:HB3	2.16	0.45
1:A:104:LEU:HD22	1:A:108:GLU:HB3	1.99	0.44
1:D:424:LEU:HG	1:D:425:PRO:N	2.32	0.44
1:A:274:GLN:O	1:A:278:GLU:HB2	2.17	0.44
1:B:118:ARG:HD3	6:B:683:HOH:O	2.16	0.44
1:C:222:ARG:HB3	1:C:225:LEU:HD13	1.99	0.43
1:C:74:ILE:HD12	1:C:126:LEU:HD23	2.01	0.43
1:C:118:ARG:HD3	1:C:120:LYS:O	2.18	0.43
1:D:294:LYS:O	1:D:297:GLU:HB2	2.19	0.43
1:C:252:GLN:HA	1:C:252:GLN:OE1	2.19	0.42
1:D:281:CYS:SG	1:D:282:ARG:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASP:O	1:C:118:ARG:HD2	2.19	0.42
1:D:424:LEU:HG	1:D:425:PRO:CD	2.50	0.42
1:B:248:LYS:HE3	6:B:690:HOH:O	2.19	0.42
1:C:279:LEU:CB	1:C:284:VAL:CG1	2.94	0.42
1:A:404:THR:O	1:A:408:GLU:HB2	2.20	0.41
1:B:293:LEU:HD21	1:B:298:ARG:HD2	2.02	0.41
1:B:331:VAL:HG23	1:B:350:ALA:HB2	2.02	0.41
1:B:353:ASP:OD1	1:B:355:LYS:HB2	2.19	0.41
1:A:287:LYS:HB2	1:A:310:VAL:HG11	2.02	0.41
1:B:274:GLN:O	1:B:278:GLU:HG2	2.19	0.41
1:B:293:LEU:HD21	1:B:298:ARG:CD	2.51	0.41
1:B:408:GLU:HG2	1:B:409:LEU:N	2.35	0.41
1:D:115:ASP:O	1:D:121:PRO:HB3	2.19	0.41
1:B:404:THR:O	1:B:408:GLU:HB3	2.21	0.41
1:A:285:ASN:HB3	1:A:311:PRO:HD2	2.03	0.41
1:B:136:SER:HA	1:B:139:GLN:HG2	2.03	0.41
1:C:138:PHE:CE2	1:C:142:LEU:HD13	2.56	0.40
1:D:424:LEU:HG	1:D:425:PRO:O	2.22	0.40
1:D:97:VAL:HG23	1:D:125:ILE:HB	2.02	0.40
1:D:166:GLY:O	1:D:167:HIS:CB	2.69	0.40
1:A:51:CYS:HA	1:A:192:THR:O	2.22	0.40
1:C:238:PRO:HB2	1:C:334:TRP:HH2	1.86	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	427/445 (96%)	418 (98%)	9 (2%)	0	100	100
1	B	430/445 (97%)	422 (98%)	8 (2%)	0	100	100
1	C	419/445 (94%)	411 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	430/445 (97%)	424 (99%)	6 (1%)	0	100	100
All	All	1706/1780 (96%)	1675 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	355/373 (95%)	343 (97%)	12 (3%)	44	41
1	B	355/373 (95%)	337 (95%)	18 (5%)	29	23
1	C	344/373 (92%)	328 (95%)	16 (5%)	32	27
1	D	353/373 (95%)	332 (94%)	21 (6%)	24	18
All	All	1407/1492 (94%)	1340 (95%)	67 (5%)	31	26

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	111	GLU
1	A	124	LYS
1	A	132	MET
1	A	183	LEU
1	A	298	ARG
1	A	303	ASN
1	A	304	ASP
1	A	374	LEU
1	A	384	GLU
1	A	409	LEU
1	A	438	THR
1	B	30	LYS
1	B	100	LEU
1	B	104	LEU
1	B	151	LEU

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Mol	Chain	Res	Type
1	B	180	ARG
1	B	243	LYS
1	B	274	GLN
1	B	293	LEU
1	B	298	ARG
1	B	304	ASP
1	B	307	GLU
1	B	352	ARG
1	B	381	LYS
1	B	384	GLU
1	B	408	GLU
1	B	424	LEU
1	B	431	CYS
1	B	451	SER
1	C	27	ASP
1	C	67	LEU
1	C	100	LEU
1	C	118	ARG
1	C	151	LEU
1	C	180	ARG
1	C	236	SER
1	C	252	GLN
1	C	282	ARG
1	C	287	LYS
1	C	300	LEU
1	C	304	ASP
1	C	370	GLN
1	C	408	GLU
1	C	424	LEU
1	C	429	LYS
1	D	11	ASP
1	D	43	LYS
1	D	80	ILE
1	D	84	GLN
1	D	104	LEU
1	D	108	GLU
1	D	110	LYS
1	D	151	LEU
1	D	170	ARG
1	D	180	ARG
1	D	236	SER
1	D	243	LYS

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Mol	Chain	Res	Type
1	D	281	CYS
1	D	282	ARG
1	D	284	VAL
1	D	296	SER
1	D	299	THR
1	D	300	LEU
1	D	304	ASP
1	D	425	PRO
1	D	429	LYS

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	303	ASN
1	A	345	GLN
1	B	122	GLN
1	C	122	GLN
1	C	274	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DMS	A	502	-	3,3,3	0.28	0	3,3,3	0.70	0
5	ADP	A	504	4	24,29,29	0.64	0	23,45,45	0.68	0
3	DMS	B	502	-	3,3,3	0.34	0	3,3,3	0.29	0
5	ADP	B	504	4	24,29,29	0.69	0	23,45,45	0.68	0
5	ADP	C	503	4	24,29,29	0.63	0	23,45,45	0.59	0
3	DMS	D	502	-	3,3,3	0.23	0	3,3,3	0.37	0
5	ADP	D	504	4	24,29,29	0.60	0	23,45,45	0.60	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
3	DMS	A	502	-	-	0/0/0/0	0/0/0/0
5	ADP	A	504	4	-	0/12/32/32	0/3/3/3
3	DMS	B	502	-	-	0/0/0/0	0/0/0/0
5	ADP	B	504	4	-	0/12/32/32	0/3/3/3
5	ADP	C	503	4	-	0/12/32/32	0/3/3/3
3	DMS	D	502	-	-	0/0/0/0	0/0/0/0
5	ADP	D	504	4	-	0/12/32/32	0/3/3/3

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
3	A	502	DMS	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	430/445 (96%)	0.03	7 (1%) 74 75	20, 48, 83, 114	0
1	B	433/445 (97%)	0.07	13 (3%) 54 55	22, 49, 90, 117	0
1	C	426/445 (95%)	0.18	21 (4%) 33 35	28, 57, 97, 123	0
1	D	434/445 (97%)	0.09	17 (3%) 43 45	28, 59, 102, 122	0
All	All	1723/1780 (96%)	0.09	58 (3%) 49 50	20, 53, 96, 123	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	6.7
1	C	23	VAL	5.8
1	C	426	ALA	5.0
1	D	95	VAL	4.7
1	A	247	LEU	4.3
1	B	136	SER	4.3
1	C	113	LEU	4.2
1	C	301	VAL	4.1
1	D	23	VAL	4.0
1	C	260	GLY	3.9
1	D	81	ALA	3.8
1	B	105	SER	3.6
1	C	83	ILE	3.6
1	D	425	PRO	3.6
1	C	112	LEU	3.5
1	D	98	SER	3.3
1	C	114	ALA	3.3
1	D	453	TRP	3.2
1	A	281	CYS	3.1
1	B	134	ALA	3.0
1	D	281	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	117	GLU	3.0
1	C	311	PRO	3.0
1	D	82	LEU	2.9
1	A	452	SER	2.8
1	B	283	GLY	2.7
1	B	17	ARG	2.7
1	B	16	VAL	2.7
1	D	16	VAL	2.6
1	B	103	LYS	2.6
1	B	104	LEU	2.6
1	B	284	VAL	2.6
1	A	104	LEU	2.6
1	C	64	LEU	2.6
1	B	279	LEU	2.5
1	D	97	VAL	2.5
1	D	25	GLY	2.5
1	C	82	LEU	2.4
1	C	305	TRP	2.4
1	D	293	LEU	2.4
1	A	300	LEU	2.4
1	C	89	HIS	2.4
1	D	284	VAL	2.3
1	C	453	TRP	2.3
1	D	89	HIS	2.3
1	D	79	LEU	2.2
1	C	79	LEU	2.2
1	A	235	ILE	2.2
1	C	288	ALA	2.2
1	C	428	ALA	2.2
1	D	22	LYS	2.2
1	C	116	LEU	2.1
1	B	109	ARG	2.1
1	B	281	CYS	2.1
1	C	423	ALA	2.1
1	C	287	LYS	2.0
1	D	68	LEU	2.0
1	B	106	ALA	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	501	1/1	0.98	0.15	2.95	45,45,45,45	0
2	ZN	A	501	1/1	0.98	0.12	2.16	39,39,39,39	0
3	DMS	A	502	4/4	0.94	0.12	1.43	30,37,40,43	0
3	DMS	B	502	4/4	0.93	0.17	1.19	86,87,87,87	0
2	ZN	D	501	1/1	0.97	0.13	0.66	45,45,45,45	0
2	ZN	C	501	1/1	0.98	0.13	0.28	46,46,46,46	0
5	ADP	D	504	27/27	0.95	0.11	-0.19	65,81,87,87	0
5	ADP	C	503	27/27	0.93	0.10	-0.56	60,68,73,73	0
5	ADP	A	504	27/27	0.96	0.10	-0.81	39,46,51,53	0
5	ADP	B	504	27/27	0.98	0.08	-0.91	31,40,44,47	0
3	DMS	D	502	4/4	0.97	0.10	-1.45	71,71,71,71	0
4	MG	B	503	1/1	0.89	0.05	-	50,50,50,50	0
4	MG	C	502	1/1	0.66	0.08	-	71,71,71,71	0
4	MG	D	503	1/1	0.78	0.06	-	68,68,68,68	0
4	MG	A	503	1/1	0.95	0.05	-	53,53,53,53	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.