



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2016 – 10:59 AM EDT

PDB ID : 5LBA
Title : Crystal structure of human RECQL5 helicase in complex with DSPL fragment(1-cyclohexyl-3-(oxolan-2-ylmethyl)urea, SGC - Diamond XChem I04-1 fragment screening.
Authors : Newman, J.A.; Aitkenhead, H.; Talon, R.; Savitsky, P.; Krojer, T.; Von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2016-06-15
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

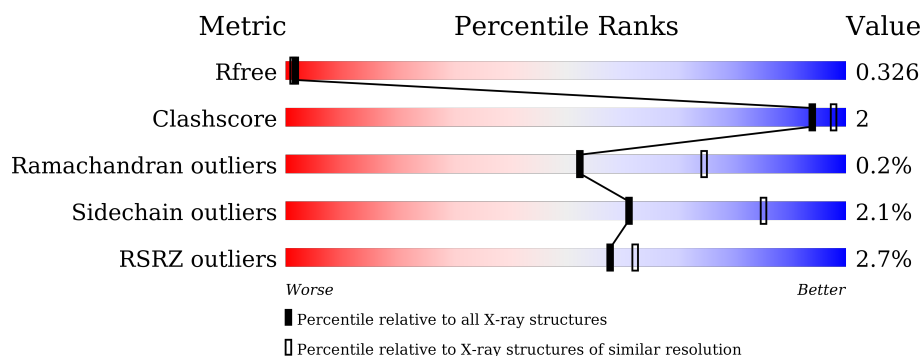
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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-20027790

i

X-RAY DIFFRACTION

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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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>5%</div> <div>90%</div> <div>7%</div> <div>•</div> </div>
1	B	445	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
1	C	445	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>••</div> </div>
1	D	445	<div> <div>1%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13954 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	B	434	Total	C	N	O	S	0	3	0
			3383	2137	604	618	24			
1	A	430	Total	C	N	O	S	0	1	0
			3352	2120	599	611	22			
1	C	432	Total	C	N	O	S	0	0	0
			3343	2113	595	613	22			
1	D	437	Total	C	N	O	S	0	1	0
			3394	2147	604	620	23			

There are 8 discrepancies between the modelled and reference sequences:

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

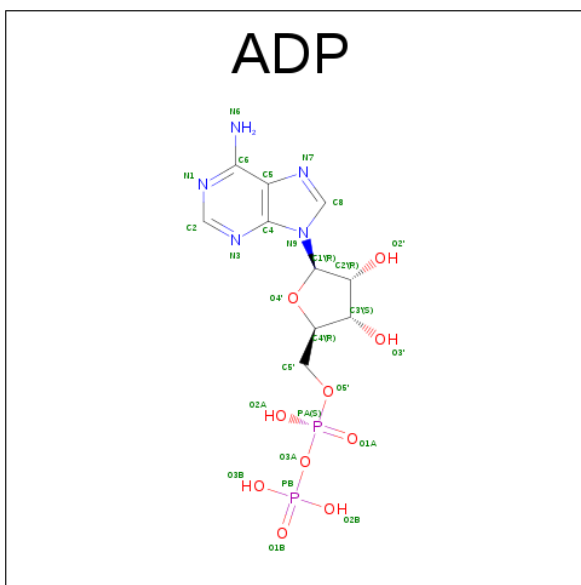
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



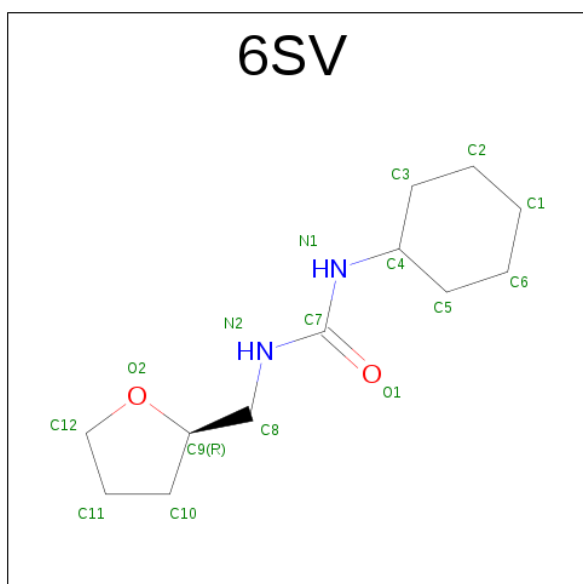
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is 1-cyclohexyl-3-[[[(2 {R})-oxolan-2-yl]methyl]urea (three-letter code: 6SV) (formula: C₁₂H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			16	12	2	2		

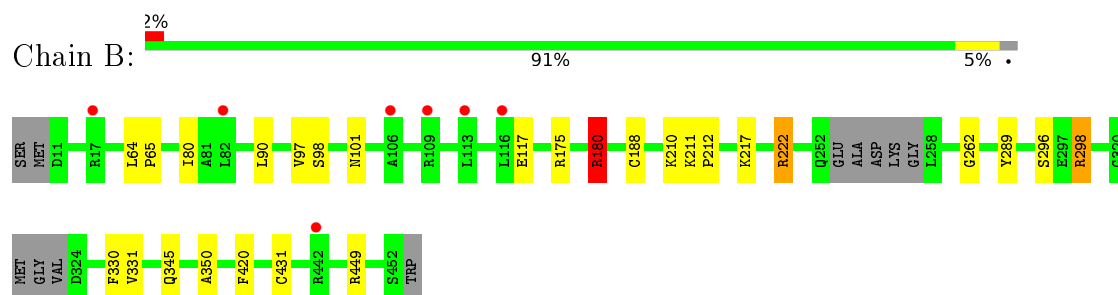
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	101	Total	O	0	0
			101	101		
7	A	88	Total	O	0	0
			88	88		
7	C	68	Total	O	0	0
			68	68		
7	D	81	Total	O	0	0
			81	81		

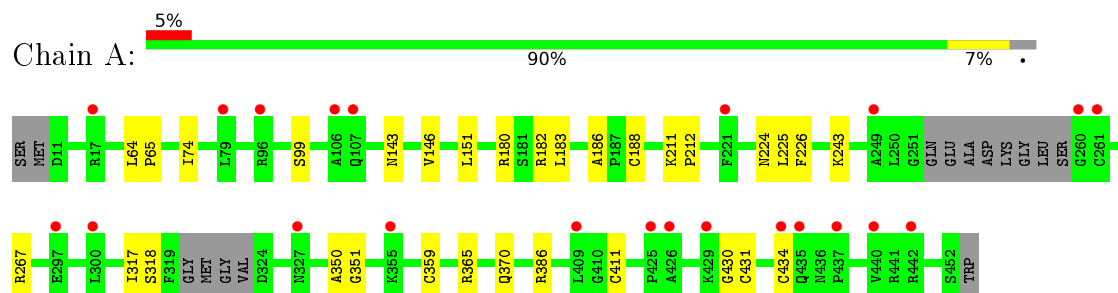
3 Residue-property plots [i](#)

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.

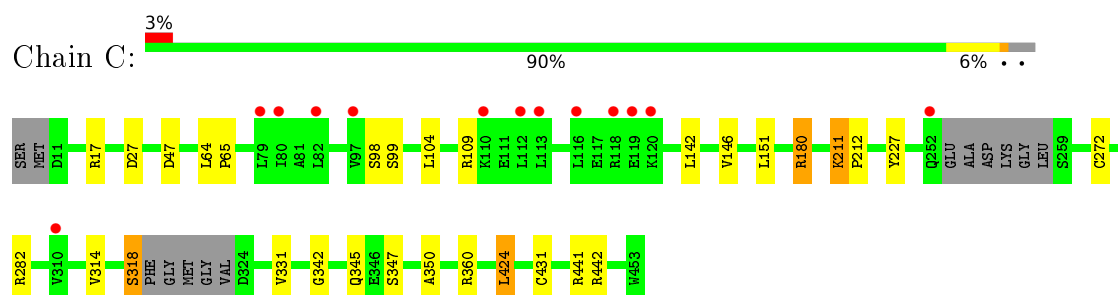
- Molecule 1: ATP-dependent DNA helicase Q5



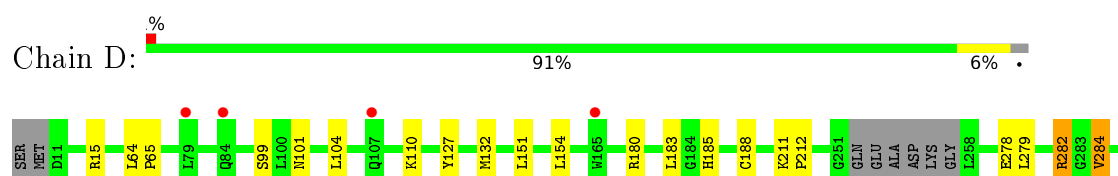
- Molecule 1: ATP-dependent DNA helicase Q5



- 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, α , β , γ	63.93 Å 85.26 Å 105.92 Å 109.90° 90.02° 97.01°	Depositor
Resolution (Å)	79.49 – 2.50 76.13 – 2.47	Depositor EDS
% Data completeness (in resolution range)	92.3 (79.49-2.50) 80.8 (76.13-2.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.237 , 0.303 0.269 , 0.326	Depositor DCC
R_{free} test set	2994 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13954	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.24 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.9809e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, DMS, 6SV, 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	0.61	0/3416	0.74	1/4617 (0.0%)
1	B	0.64	0/3447	0.78	4/4660 (0.1%)
1	C	0.59	0/3408	0.74	4/4613 (0.1%)
1	D	0.60	0/3461	0.74	2/4683 (0.0%)
All	All	0.61	0/13732	0.75	11/18573 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	LEU	CA-CB-CG	6.58	130.43	115.30
1	D	360	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	386	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	222	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	298	ARG	NE-CZ-NH1	5.67	123.14	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	LYS	Peptide
1	B	211	LYS	Peptide
1	C	211	LYS	Peptide
1	D	211	LYS	Peptide

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	3352	0	3371	13	0
1	B	3383	0	3386	11	0
1	C	3343	0	3331	13	0
1	D	3394	0	3393	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	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
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	B	16	0	0	0	0
7	A	88	0	0	1	0
7	B	101	0	0	2	0
7	C	68	0	0	3	0
7	D	81	0	0	1	0
All	All	13954	0	13547	49	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 2.

The worst 5 of 49 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:C:342:GLY:O	7:C:601:HOH:O	1.89	0.91
1:B:180:ARG:HD3	1:B:188:CYS:HB2	1.80	0.62
1:A:365:ARG:NH2	7:A:603:HOH:O	2.37	0.58
1:A:180:ARG:HD3	1:A:188:CYS:HB2	1.87	0.57
1:C:47:ASP:OD2	1:C:180:ARG:NH1	2.38	0.56

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	425/445 (96%)	410 (96%)	14 (3%)	1 (0%)	52	75
1	B	431/445 (97%)	420 (97%)	10 (2%)	1 (0%)	52	75
1	C	426/445 (96%)	408 (96%)	17 (4%)	1 (0%)	52	75
1	D	434/445 (98%)	419 (96%)	14 (3%)	1 (0%)	52	75
All	All	1716/1780 (96%)	1657 (97%)	55 (3%)	4 (0%)	52	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	212	PRO
1	B	212	PRO
1	C	212	PRO
1	A	212	PRO

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	358/373 (96%)	353 (99%)	5 (1%)	74	91
1	B	361/373 (97%)	354 (98%)	7 (2%)	65	87
1	C	355/373 (95%)	346 (98%)	9 (2%)	55	82
1	D	361/373 (97%)	352 (98%)	9 (2%)	55	82
All	All	1435/1492 (96%)	1405 (98%)	30 (2%)	61	85

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	SER
1	C	180	ARG
1	D	284	VAL
1	C	151	LEU
1	C	282	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	GLN
1	A	345	GLN
1	C	86	GLN
1	C	345	GLN
1	D	164	GLN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADP	A	502	2	24,29,29	1.03	1 (4%)	23,45,45	2.02	3 (13%)
5	DMS	A	504	-	3,3,3	0.51	0	3,3,3	0.71	0
4	ADP	B	503	2	24,29,29	1.16	2 (8%)	23,45,45	2.04	3 (13%)
5	DMS	B	504	-	3,3,3	0.42	0	3,3,3	0.75	0
6	6SV	B	505	-	17,17,17	0.32	0	20,21,21	1.02	2 (10%)
4	ADP	C	503	2	24,29,29	0.97	1 (4%)	23,45,45	2.18	3 (13%)
4	ADP	D	503	2	24,29,29	1.17	3 (12%)	23,45,45	2.21	2 (8%)
5	DMS	D	504	-	3,3,3	0.45	0	3,3,3	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	502	2	-	0/12/32/32	0/3/3/3
5	DMS	A	504	-	-	0/0/0/0	0/0/0/0
4	ADP	B	503	2	-	0/12/32/32	0/3/3/3
5	DMS	B	504	-	-	0/0/0/0	0/0/0/0
6	6SV	B	505	-	-	0/9/24/24	0/2/2/2
4	ADP	C	503	2	-	0/12/32/32	0/3/3/3
4	ADP	D	503	2	-	0/12/32/32	0/3/3/3
5	DMS	D	504	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	ADP	C2'-C1'	-2.28	1.50	1.53
4	D	503	ADP	C2-N3	2.08	1.35	1.32
4	B	503	ADP	O4'-C1'	2.40	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	ADP	C5-C4	3.05	1.47	1.40
4	C	503	ADP	C5-C4	3.05	1.47	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	ADP	N3-C2-N1	-8.59	122.12	128.87
4	D	503	ADP	N3-C2-N1	-8.19	122.43	128.87
4	B	503	ADP	N3-C2-N1	-7.66	122.85	128.87
4	A	502	ADP	N3-C2-N1	-7.48	122.99	128.87
6	B	505	6SV	C6-C5-C4	-2.34	107.57	111.15

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 [i](#)

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	430/445 (96%)	0.32	22 (5%) 32 36	21, 50, 86, 116	0
1	B	434/445 (97%)	0.08	7 (1%) 74 78	21, 43, 78, 101	0
1	C	432/445 (97%)	0.13	13 (3%) 54 59	22, 45, 83, 118	0
1	D	437/445 (98%)	-0.04	5 (1%) 82 84	20, 42, 77, 92	0
All	All	1733/1780 (97%)	0.12	47 (2%) 58 62	20, 45, 82, 118	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	LEU	7.9
1	A	107	GLN	5.1
1	A	442	ARG	4.7
1	A	426	ALA	4.5
1	C	252	GLN	4.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
6	6SV	B	505	16/16	0.83	0.23	1.99	46,65,84,85	0
5	DMS	D	504	4/4	0.95	0.16	0.57	51,55,57,61	0
5	DMS	A	504	4/4	0.95	0.17	0.38	41,43,43,48	0
4	ADP	A	502	27/27	0.95	0.15	-0.19	35,62,79,81	0
4	ADP	B	503	27/27	0.94	0.13	-0.65	30,43,48,48	0
4	ADP	D	503	27/27	0.96	0.11	-1.00	35,50,57,60	0
4	ADP	C	503	27/27	0.95	0.11	-1.34	39,46,51,52	0
5	DMS	B	504	4/4	0.95	0.14	-1.58	43,45,48,49	0
3	ZN	A	503	1/1	0.98	0.12	-2.19	53,53,53,53	0
3	ZN	D	502	1/1	0.99	0.07	-3.28	26,26,26,26	0
3	ZN	B	502	1/1	0.98	0.07	-4.04	35,35,35,35	0
3	ZN	C	502	1/1	0.98	0.09	-5.05	34,34,34,34	0
2	MG	C	501	1/1	0.95	0.08	-	49,49,49,49	0
2	MG	B	501	1/1	0.97	0.07	-	35,35,35,35	0
2	MG	A	501	1/1	0.93	0.06	-	43,43,43,43	0
2	MG	D	501	1/1	0.98	0.08	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.