



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2016 – 05:07 PM EST

PDB ID : 5K78
Title : Dbr1 in complex with 16-mer branched RNA
Authors : Clark, N.E.; Taylor, A.B.; Hart, P.J.
Deposited on : 2016-05-25
Resolution : 2.64 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

<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-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

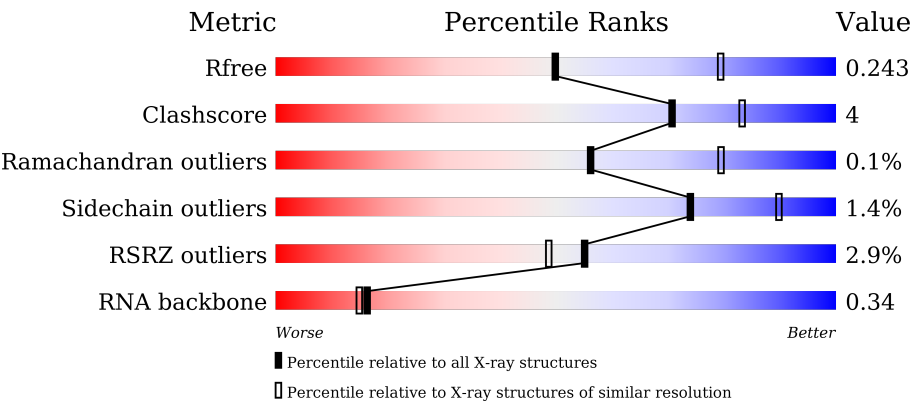
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)
RNA backbone	2183	1002 (3.06-2.22)

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	360	<div><div>%</div><div>83%12% . .</div></div>
1	B	360	<div><div>5%</div><div>85%13% .</div></div>
1	C	360	<div><div>%</div><div>85%12% .</div></div>
1	D	360	<div><div>2%</div><div>83%13% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	E	360	<div><div></div><div>3%</div><div>86%</div><div>10%</div><div></div></div>
2	X	11	<div><div></div><div>9%</div><div>36%</div><div>9%</div><div>55%</div><div></div></div>
2	Y	11	<div><div></div><div>18%</div><div>36%</div><div>64%</div><div></div></div>
3	x	6	<div><div></div><div>17%</div><div>83%</div><div>17%</div><div></div></div>
3	y	6	<div><div></div><div>67%</div><div>83%</div><div>17%</div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14682 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 RNA lariat debranching enzyme, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	1	0
			2840	1848	460	517	15			
1	B	351	Total	C	N	O	S	0	0	0
			2870	1864	468	523	15			
1	C	349	Total	C	N	O	S	0	0	0
			2852	1854	463	520	15			
1	D	349	Total	C	N	O	S	0	0	0
			2852	1854	463	520	15			
1	E	349	Total	C	N	O	S	0	0	0
			2852	1854	463	520	15			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ALA	HIS	engineered mutation	UNP C4M1P9
A	355	HIS	-	expression tag	UNP C4M1P9
A	356	HIS	-	expression tag	UNP C4M1P9
A	357	HIS	-	expression tag	UNP C4M1P9
A	358	HIS	-	expression tag	UNP C4M1P9
A	359	HIS	-	expression tag	UNP C4M1P9
A	360	HIS	-	expression tag	UNP C4M1P9
B	91	ALA	HIS	engineered mutation	UNP C4M1P9
B	355	HIS	-	expression tag	UNP C4M1P9
B	356	HIS	-	expression tag	UNP C4M1P9
B	357	HIS	-	expression tag	UNP C4M1P9
B	358	HIS	-	expression tag	UNP C4M1P9
B	359	HIS	-	expression tag	UNP C4M1P9
B	360	HIS	-	expression tag	UNP C4M1P9
C	91	ALA	HIS	engineered mutation	UNP C4M1P9
C	355	HIS	-	expression tag	UNP C4M1P9
C	356	HIS	-	expression tag	UNP C4M1P9
C	357	HIS	-	expression tag	UNP C4M1P9
C	358	HIS	-	expression tag	UNP C4M1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	359	HIS	-	expression tag	UNP C4M1P9
C	360	HIS	-	expression tag	UNP C4M1P9
D	91	ALA	HIS	engineered mutation	UNP C4M1P9
D	355	HIS	-	expression tag	UNP C4M1P9
D	356	HIS	-	expression tag	UNP C4M1P9
D	357	HIS	-	expression tag	UNP C4M1P9
D	358	HIS	-	expression tag	UNP C4M1P9
D	359	HIS	-	expression tag	UNP C4M1P9
D	360	HIS	-	expression tag	UNP C4M1P9
E	91	ALA	HIS	engineered mutation	UNP C4M1P9
E	355	HIS	-	expression tag	UNP C4M1P9
E	356	HIS	-	expression tag	UNP C4M1P9
E	357	HIS	-	expression tag	UNP C4M1P9
E	358	HIS	-	expression tag	UNP C4M1P9
E	359	HIS	-	expression tag	UNP C4M1P9
E	360	HIS	-	expression tag	UNP C4M1P9

- Molecule 2 is a RNA chain called branch 1 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	5	Total 68	C 29	N 13	O 22	P 4	0	0	1
2	Y	4	Total 46	C 19	N 8	O 16	P 3	0	0	1

- Molecule 3 is a RNA chain called branch 2 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	x	6	Total 112	C 48	N 19	O 39	P 6	0	0	0
3	y	5	Total 90	C 38	N 14	O 33	P 5	0	0	0

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

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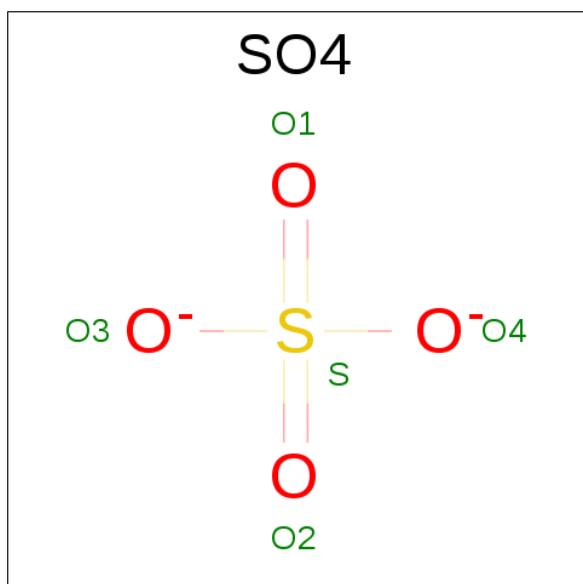
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

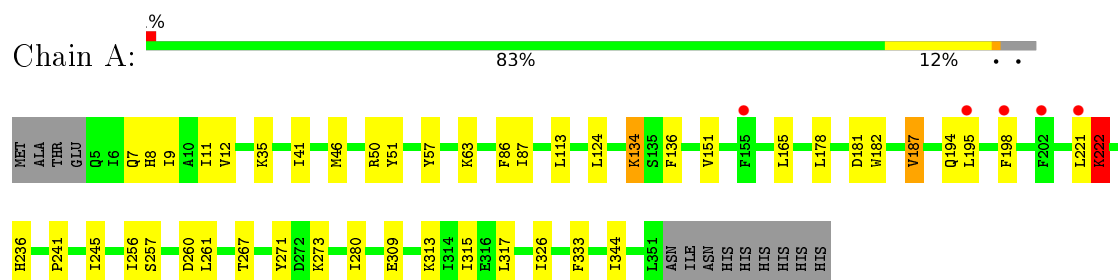
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	B	1	Total	O	0	0
			1	1		
7	C	12	Total	O	0	0
			12	12		
7	D	1	Total	O	0	0
			1	1		
7	E	8	Total	O	0	0
			8	8		

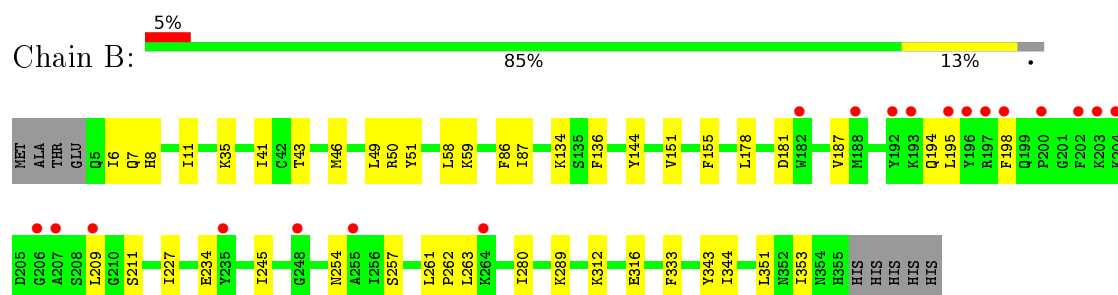
3 Residue-property plots [i](#)

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.

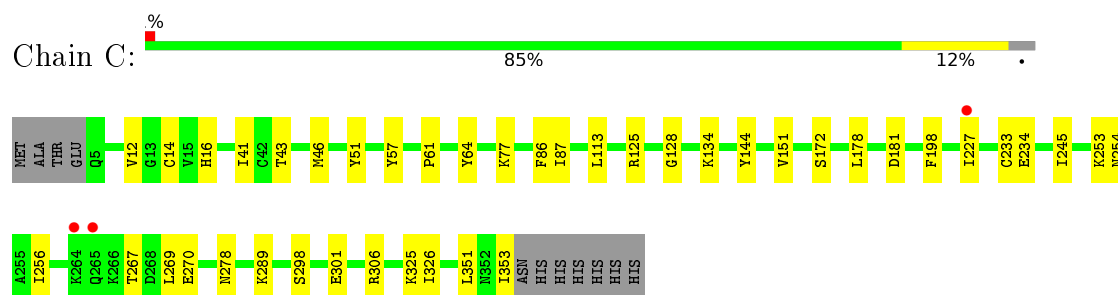
- Molecule 1: RNA lariat debranching enzyme, putative



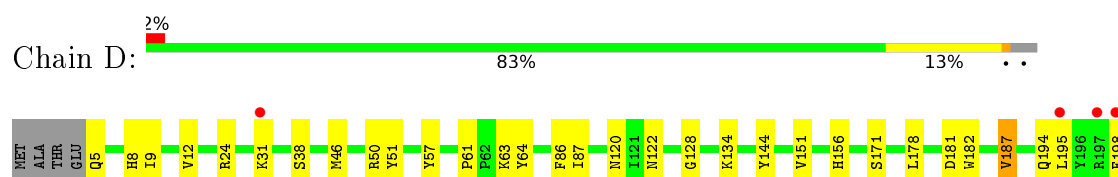
- Molecule 1: RNA lariat debranching enzyme, putative



- Molecule 1: RNA lariat debranching enzyme, putative

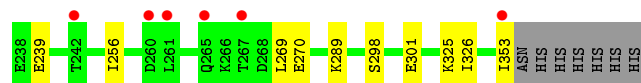
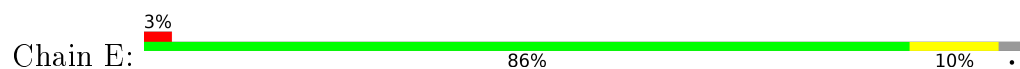


- Molecule 1: RNA lariat debranching enzyme, putative

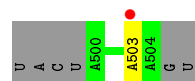
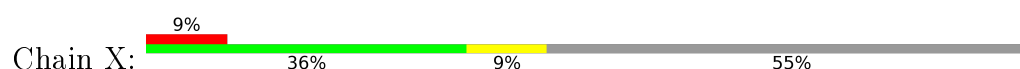




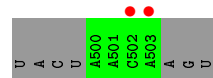
- Molecule 1: RNA lariat debranching enzyme, putative



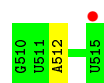
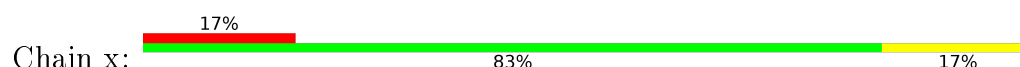
- Molecule 2: branch 1 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'



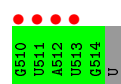
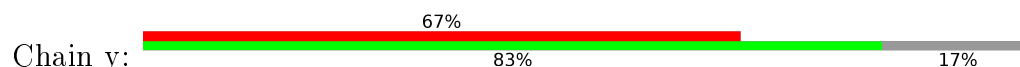
- Molecule 2: branch 1 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'



- Molecule 3: branch 2 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'



- Molecule 3: branch 2 of branched RNA 5'-UACUAA(2'-GUAUGU)CAAGU-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.89Å 142.67Å 215.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.34 – 2.64 71.34 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (71.34-2.64) 95.7 (71.34-2.64)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.195 , 0.246 0.188 , 0.243	Depositor DCC
R_{free} test set	3231 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14682	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, FE2, SO4

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	0.26	0/2920	0.45	0/3947
1	B	0.26	0/2948	0.44	0/3985
1	C	0.26	0/2929	0.42	0/3959
1	D	0.24	0/2929	0.43	0/3959
1	E	0.27	1/2929 (0.0%)	0.43	0/3959
2	X	0.28	0/75	0.79	0/116
2	Y	0.33	0/50	0.70	0/77
3	x	0.12	0/124	0.63	0/189
3	y	0.14	0/99	0.68	0/151
All	All	0.26	1/15003 (0.0%)	0.44	0/20342

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	TYR	C-N	5.08	1.45	1.34

There are no bond angle outliers.

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	2840	0	2821	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2870	0	2842	27	0
1	C	2852	0	2829	23	0
1	D	2852	0	2829	31	0
1	E	2852	0	2829	21	0
2	X	68	0	33	0	0
2	Y	46	0	22	0	0
3	x	112	0	53	0	0
3	y	90	0	42	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
4	E	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	10	0	0	0	0
6	B	15	0	0	0	0
6	C	20	0	0	0	0
6	D	15	0	0	1	0
6	E	5	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	12	0	0	0	0
7	D	1	0	0	0	0
7	E	8	0	0	0	0
All	All	14682	0	14300	126	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 (126) 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:234:GLU:HG3	1:D:254:ASN:HB3	1.70	0.73
1:E:270:GLU:HG2	1:E:325:LYS:HA	1.81	0.61
1:C:61:PRO:HG2	1:C:64:TYR:HD2	1.66	0.61
1:D:254:ASN:N	1:D:254:ASN:OD1	2.34	0.60
1:A:195:LEU:HA	1:A:198:PHE:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HA	1:B:198:PHE:HD2	1.67	0.59
1:D:195:LEU:HA	1:D:198:PHE:HD2	1.67	0.59
1:E:195:LEU:HA	1:E:198:PHE:HD2	1.67	0.59
1:B:134:LYS:HE3	1:B:136:PHE:CE2	2.39	0.57
1:D:24:ARG:NH2	6:D:405:SO4:O2	2.38	0.56
1:D:171:SER:OG	1:D:274:ASP:OD2	2.20	0.55
1:E:41:ILE:HG23	1:E:178:LEU:HD21	1.88	0.54
1:B:41:ILE:HG23	1:B:178:LEU:HD21	1.90	0.53
1:E:12:VAL:HG22	1:E:256:ILE:HG12	1.88	0.53
1:B:8:HIS:NE2	1:B:35:LYS:HD3	2.24	0.53
1:B:7:GLN:HB3	1:B:263:LEU:HD13	1.91	0.52
1:D:5:GLN:HG3	1:D:263:LEU:HB3	1.92	0.52
1:C:278:ASN:OD1	1:C:306:ARG:NH1	2.41	0.52
1:D:57:TYR:HA	1:D:151:VAL:HG22	1.91	0.51
1:B:312:LYS:O	1:B:316:GLU:HG2	2.10	0.51
1:B:59:LYS:HB2	1:B:151:VAL:HG22	1.92	0.51
1:D:128:GLY:HA2	1:D:178:LEU:HB2	1.92	0.51
1:D:237:ALA:HB3	1:D:244:PHE:HB3	1.92	0.51
1:E:87:ILE:HD13	1:E:178:LEU:HB3	1.93	0.51
1:A:46:MET:HG3	1:A:86:PHE:CD1	2.46	0.50
1:C:12:VAL:HG22	1:C:256:ILE:HG12	1.93	0.50
1:B:187:VAL:HG21	1:B:209:LEU:HD23	1.94	0.50
1:A:41:ILE:HG23	1:A:178:LEU:HD21	1.94	0.49
1:E:144:TYR:HB3	1:E:289:LYS:O	2.12	0.49
1:C:128:GLY:HA2	1:C:178:LEU:HB2	1.94	0.49
1:A:11:ILE:HD11	1:A:257:SER:HB3	1.94	0.49
1:D:144:TYR:HB3	1:D:289:LYS:O	2.12	0.49
1:D:182:TRP:HZ3	1:D:187:VAL:HG23	1.76	0.49
1:C:46:MET:HG3	1:C:86:PHE:CD2	2.47	0.49
1:E:21:GLU:HG3	1:E:24:ARG:HH12	1.78	0.49
1:D:46:MET:HG3	1:D:86:PHE:CD2	2.48	0.49
1:D:87:ILE:HD13	1:D:178:LEU:HB3	1.95	0.49
1:A:222:LYS:HG2	1:A:222:LYS:O	2.13	0.49
1:B:87:ILE:HD13	1:B:178:LEU:HB3	1.95	0.48
1:B:234:GLU:HG3	1:B:254:ASN:HB2	1.95	0.48
1:B:351:LEU:O	1:B:353:ILE:N	2.45	0.48
1:C:125:ARG:NH1	1:C:172:SER:O	2.46	0.48
1:E:57:TYR:HA	1:E:151:VAL:HG22	1.95	0.48
1:D:12:VAL:HG22	1:D:256:ILE:HG12	1.96	0.48
1:A:8:HIS:ND1	1:A:260:ASP:OD1	2.43	0.47
1:B:144:TYR:HB3	1:B:289:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:PRO:HG2	1:D:64:TYR:HD2	1.80	0.47
1:B:280:ILE:HD13	1:B:344:ILE:HG23	1.96	0.47
1:A:182:TRP:HZ3	1:A:187:VAL:HG23	1.80	0.47
1:E:46:MET:HG3	1:E:86:PHE:CD1	2.49	0.47
1:A:57:TYR:HA	1:A:151[A]:VAL:HG12	1.98	0.46
1:E:16:HIS:HD1	1:E:47:GLN:HE21	1.63	0.46
1:B:6:ILE:HD13	1:B:262:PRO:HA	1.97	0.46
1:D:332:THR:OG1	1:D:335:ILE:HD13	2.15	0.46
1:C:227:ILE:HA	1:C:245:ILE:O	2.15	0.46
1:C:234:GLU:HB2	1:C:254:ASN:HB2	1.97	0.46
1:E:181:ASP:OD1	1:E:181:ASP:N	2.49	0.46
1:E:269:LEU:HG	1:E:326:ILE:HD12	1.98	0.46
1:C:57:TYR:HA	1:C:151:VAL:HG22	1.98	0.46
1:D:50:ARG:HD3	1:D:333:PHE:CE2	2.51	0.46
1:E:25:GLN:O	1:E:28:GLU:HG2	2.16	0.46
1:D:9:ILE:HD12	1:D:261:LEU:HD22	1.97	0.45
1:C:181:ASP:N	1:C:181:ASP:OD1	2.49	0.45
1:E:8:HIS:NE2	1:E:35:LYS:HD3	2.32	0.45
1:A:87:ILE:HD13	1:A:178:LEU:HB3	1.98	0.45
1:A:313:LYS:HD2	1:A:313:LYS:HA	1.74	0.45
1:C:87:ILE:HD13	1:C:178:LEU:HB3	1.98	0.44
1:D:63:LYS:HE3	1:D:64:TYR:CE2	2.53	0.44
1:D:120:ASN:OD1	1:D:272:ASP:HA	2.18	0.44
1:B:181:ASP:OD2	1:B:211:SER:HB2	2.18	0.44
1:B:181:ASP:N	1:B:181:ASP:OD1	2.49	0.44
1:D:134:LYS:HD2	1:D:156:HIS:CE1	2.51	0.44
1:A:181:ASP:N	1:A:181:ASP:OD1	2.50	0.44
1:C:14:CYS:HB3	1:C:16:HIS:CD2	2.53	0.44
1:C:43:THR:HG21	1:C:227:ILE:HG22	2.00	0.44
1:B:49:LEU:HD11	1:B:58:LEU:HD22	2.00	0.43
1:D:181:ASP:OD1	1:D:181:ASP:N	2.49	0.43
1:A:280:ILE:HD13	1:A:344:ILE:HG23	2.00	0.43
1:A:50:ARG:HD3	1:A:333:PHE:CE2	2.53	0.43
1:B:227:ILE:HA	1:B:245:ILE:O	2.17	0.43
1:A:7:GLN:HE22	1:A:124:LEU:HD11	1.82	0.43
1:B:59:LYS:HD2	1:B:155:PHE:CZ	2.53	0.43
1:E:194:GLN:HG2	1:E:198:PHE:CE2	2.53	0.43
1:A:236:HIS:HD2	1:A:245:ILE:HA	1.83	0.43
1:B:194:GLN:HG2	1:B:198:PHE:CE2	2.54	0.43
1:A:57:TYR:HA	1:A:151[B]:VAL:HG22	2.02	0.42
1:A:12:VAL:HG22	1:A:256:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ILE:HA	1:D:245:ILE:O	2.19	0.42
1:D:8:HIS:ND1	1:D:260:ASP:OD1	2.40	0.42
1:D:308:LYS:HB3	1:D:308:LYS:HE3	1.66	0.42
1:B:43:THR:HG21	1:B:227:ILE:HG22	2.01	0.42
1:B:46:MET:HG3	1:B:86:PHE:CD1	2.55	0.42
1:E:165:LEU:O	1:E:221:LEU:HD21	2.20	0.42
1:A:9:ILE:HD12	1:A:261:LEU:HD12	2.01	0.42
1:C:198:PHE:CE2	1:C:233:CYS:HB3	2.55	0.42
1:C:253:LYS:HE2	1:C:253:LYS:HB3	1.80	0.42
1:A:194:GLN:HG2	1:A:198:PHE:CE2	2.54	0.42
1:C:41:ILE:HG23	1:C:178:LEU:HD11	2.00	0.42
1:A:165:LEU:O	1:A:221:LEU:HD21	2.19	0.42
1:A:134:LYS:HG2	1:A:136:PHE:CZ	2.55	0.41
1:D:194:GLN:HG2	1:D:198:PHE:CE2	2.54	0.41
1:D:31:LYS:HD3	1:D:31:LYS:HA	1.69	0.41
1:E:194:GLN:HG2	1:E:198:PHE:HE2	1.85	0.41
1:A:7:GLN:NE2	1:A:124:LEU:HD11	2.36	0.41
1:C:270:GLU:HG2	1:C:325:LYS:HD3	2.02	0.41
1:C:134:LYS:HA	1:C:134:LYS:HD3	1.92	0.41
1:D:248:GLY:N	1:D:254:ASN:O	2.30	0.41
1:D:38:SER:OG	1:D:122:ASN:ND2	2.54	0.41
1:E:81:PRO:HG2	1:E:82:TYR:CD2	2.55	0.41
1:B:312:LYS:HD3	1:B:312:LYS:HA	1.87	0.41
1:B:50:ARG:HD3	1:B:333:PHE:CE2	2.55	0.41
1:B:343:TYR:OH	1:E:51:TYR:HA	2.20	0.41
1:D:313:LYS:HE3	1:D:317:LEU:HD11	2.03	0.41
1:A:271:TYR:CZ	1:A:326:ILE:HG12	2.56	0.41
1:B:11:ILE:HD11	1:B:257:SER:HB3	2.02	0.41
1:A:8:HIS:CD2	1:A:35:LYS:HB3	2.55	0.41
1:C:351:LEU:O	1:C:353:ILE:HG23	2.21	0.41
1:D:194:GLN:HG2	1:D:198:PHE:HE2	1.86	0.41
1:E:14:CYS:HB3	1:E:16:HIS:CD2	2.55	0.41
1:B:194:GLN:HG2	1:B:198:PHE:HE2	1.86	0.41
1:C:144:TYR:HB3	1:C:289:LYS:O	2.20	0.41
1:C:77:LYS:HD3	1:C:77:LYS:HA	1.88	0.41
1:A:273:LYS:HG3	1:A:315:ILE:HD11	2.03	0.40
1:E:298:SER:HB3	1:E:301:GLU:HB3	2.02	0.40
1:C:269:LEU:HG	1:C:326:ILE:HD12	2.04	0.40
1:C:298:SER:HB3	1:C:301:GLU:HB3	2.04	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	346/360 (96%)	332 (96%)	13 (4%)	1 (0%)	46	70
1	B	349/360 (97%)	339 (97%)	10 (3%)	0	100	100
1	C	347/360 (96%)	336 (97%)	11 (3%)	0	100	100
1	D	347/360 (96%)	335 (96%)	12 (4%)	0	100	100
1	E	347/360 (96%)	333 (96%)	14 (4%)	0	100	100
All	All	1736/1800 (96%)	1675 (96%)	60 (4%)	1 (0%)	56	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LYS

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	314/325 (97%)	304 (97%)	10 (3%)	46	73
1	B	317/325 (98%)	315 (99%)	2 (1%)	90	97
1	C	315/325 (97%)	312 (99%)	3 (1%)	82	93
1	D	315/325 (97%)	311 (99%)	4 (1%)	76	91
1	E	315/325 (97%)	312 (99%)	3 (1%)	82	93
All	All	1576/1625 (97%)	1554 (99%)	22 (1%)	74	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	63	LYS
1	A	113	LEU
1	A	134	LYS
1	A	187	VAL
1	A	222	LYS
1	A	241	PRO
1	A	267	THR
1	A	309	GLU
1	A	317	LEU
1	B	51	TYR
1	B	261	LEU
1	C	51	TYR
1	C	113	LEU
1	C	267	THR
1	D	51	TYR
1	D	187	VAL
1	D	254	ASN
1	D	261	LEU
1	E	51	TYR
1	E	239	GLU
1	E	353	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	B	16	HIS
1	B	47	GLN
1	B	352	ASN
1	C	66	GLN
1	C	120	ASN
1	C	170	GLN
1	D	122	ASN
1	E	47	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	1/11 (9%)	1 (100%)	0
2	Y	0/11	-	-
3	x	4/6 (66%)	1 (25%)	0
3	y	3/6 (50%)	0	0
All	All	8/34 (23%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	503	A
3	x	512	A

There are no RNA pucker outliers to report.

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 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	$\# Z > 2$
6	SO4	A	403	-	4,4,4	0.21	0	6,6,6	0.06	0
6	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	B	404	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	B	405	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	C	403	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	C	404	-	4,4,4	0.22	0	6,6,6	0.05	0
6	SO4	C	405	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	C	406	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	D	404	-	4,4,4	0.26	0	6,6,6	0.06	0
6	SO4	D	405	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	E	403	-	4,4,4	0.21	0	6,6,6	0.07	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	SO4	A	403	-	-	0/0/0/0	0/0/0/0
6	SO4	A	404	-	-	0/0/0/0	0/0/0/0
6	SO4	B	403	-	-	0/0/0/0	0/0/0/0
6	SO4	B	404	-	-	0/0/0/0	0/0/0/0
6	SO4	B	405	-	-	0/0/0/0	0/0/0/0
6	SO4	C	403	-	-	0/0/0/0	0/0/0/0
6	SO4	C	404	-	-	0/0/0/0	0/0/0/0
6	SO4	C	405	-	-	0/0/0/0	0/0/0/0
6	SO4	C	406	-	-	0/0/0/0	0/0/0/0
6	SO4	D	403	-	-	0/0/0/0	0/0/0/0
6	SO4	D	404	-	-	0/0/0/0	0/0/0/0
6	SO4	D	405	-	-	0/0/0/0	0/0/0/0
6	SO4	E	403	-	-	0/0/0/0	0/0/0/0

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	D	405	SO4	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, 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	347/360 (96%)	0.31	5 (1%) 78 74	46, 76, 120, 173	0
1	B	351/360 (97%)	0.49	19 (5%) 29 23	42, 74, 137, 232	0
1	C	349/360 (96%)	0.18	3 (0%) 85 83	36, 56, 84, 138	0
1	D	349/360 (96%)	0.26	7 (2%) 68 63	43, 70, 119, 177	0
1	E	349/360 (96%)	0.36	10 (2%) 55 49	40, 67, 110, 166	0
2	X	5/11 (45%)	1.34	1 (20%) 1 1	91, 101, 120, 124	3 (60%)
2	Y	4/11 (36%)	1.82	2 (50%) 0 0	95, 112, 126, 135	3 (75%)
3	x	6/6 (100%)	1.38	1 (16%) 2 1	77, 93, 129, 178	2 (33%)
3	y	5/6 (83%)	2.47	4 (80%) 0 0	120, 138, 147, 182	4 (80%)
All	All	1765/1834 (96%)	0.34	52 (2%) 55 49	36, 68, 120, 232	12 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	198	PHE	6.2
3	x	515	U	5.5
1	B	198	PHE	5.4
1	D	198	PHE	5.4
1	A	198	PHE	5.3
3	y	512	A	5.2
1	B	197	ARG	4.7
1	D	195	LEU	4.5
1	E	353	ILE	4.3
1	D	205	ASP	4.1
1	B	195	LEU	4.0
1	B	209	LEU	4.0
1	B	202	PHE	3.8
1	B	204	LYS	3.8
1	B	206	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	Y	502	C	3.6
1	D	202	PHE	3.5
1	A	195	LEU	3.4
1	B	235	TYR	3.2
1	B	203	LYS	3.2
1	E	5	GLN	3.1
1	E	265	GLN	3.0
3	y	510	G	3.0
1	B	248	GLY	2.9
1	E	260	ASP	2.8
1	B	200	PRO	2.8
1	A	221	LEU	2.8
1	E	237	ALA	2.7
2	Y	503	A	2.7
1	D	316	GLU	2.5
1	D	31	LYS	2.5
2	X	503	A	2.5
1	B	207	ALA	2.5
3	y	513	U	2.5
1	B	196	TYR	2.5
3	y	511	U	2.4
1	C	227	ILE	2.3
1	C	265	GLN	2.3
1	A	202	PHE	2.3
1	C	264	LYS	2.3
1	B	193	LYS	2.3
1	B	182	TRP	2.2
1	B	255	ALA	2.2
1	A	155	PHE	2.2
1	E	261	LEU	2.1
1	D	197	ARG	2.1
1	B	264	LYS	2.1
1	B	192	TYR	2.1
1	E	267	THR	2.1
1	E	242	THR	2.0
1	B	188	MET	2.0
1	E	31	LYS	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, 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(Å ²)	Q<0.9
6	SO4	C	403	5/5	0.94	0.21	1.36	52,54,64,74	0
6	SO4	B	405	5/5	0.92	0.20	0.43	130,135,138,138	0
6	SO4	A	404	5/5	0.53	0.28	0.32	128,138,141,144	0
4	FE2	D	401	1/1	0.98	0.20	0.28	74,74,74,74	0
6	SO4	D	403	5/5	0.97	0.20	-0.25	48,58,109,121	0
4	FE2	C	401	1/1	0.99	0.18	-0.65	48,48,48,48	0
5	ZN	E	402	1/1	0.95	0.18	-0.70	75,75,75,75	0
6	SO4	C	406	5/5	0.95	0.17	-0.73	96,98,100,105	0
4	FE2	B	401	1/1	0.99	0.16	-0.74	82,82,82,82	0
5	ZN	D	402	1/1	0.99	0.10	-1.38	79,79,79,79	0
4	FE2	E	401	1/1	0.95	0.15	-1.43	54,54,54,54	0
5	ZN	B	402	1/1	0.96	0.15	-1.43	122,122,122,122	0
6	SO4	B	403	5/5	0.95	0.17	-1.47	51,53,64,67	0
4	FE2	A	401	1/1	0.98	0.16	-1.48	63,63,63,63	0
6	SO4	B	404	5/5	0.88	0.15	-1.77	107,114,114,116	0
6	SO4	A	403	5/5	0.94	0.15	-2.03	55,65,71,75	0
5	ZN	C	402	1/1	0.98	0.14	-2.29	78,78,78,78	0
5	ZN	A	402	1/1	0.99	0.12	-3.46	95,95,95,95	0
6	SO4	E	403	5/5	0.98	0.14	-3.63	55,56,61,61	0
6	SO4	D	404	5/5	0.91	0.13	-	100,103,141,163	0
6	SO4	C	404	5/5	0.94	0.24	-	91,97,100,100	0
6	SO4	C	405	5/5	0.61	0.23	-	134,137,139,143	0
6	SO4	D	405	5/5	0.68	0.83	-	57,66,112,174	5

6.5 Other polymers [i](#)

There are no such residues in this entry.