



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 07:28 AM EST

PDB ID : 1S06  
Title : Crystal Structure of the R253K Mutant of 7,8-Diaminopelargonic Acid Synthase  
Authors : Sandmark, J.; Eliot, A.C.; Famm, K.; Schneider, G.; Kirsch, J.F.  
Deposited on : 2003-12-30  
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

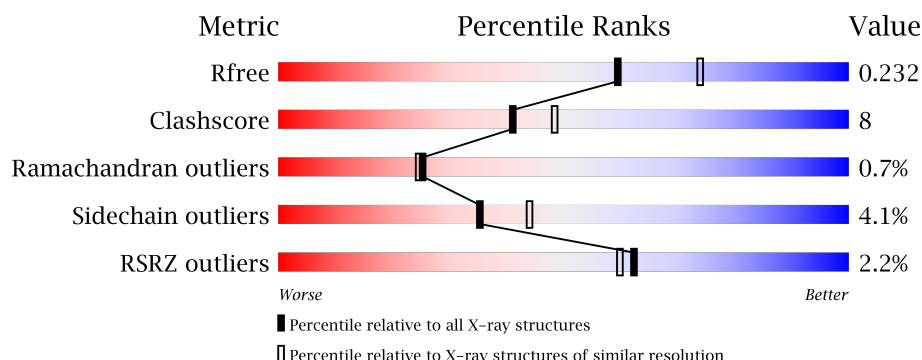
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	429	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	429	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7004 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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	P	S	18	2	0
			3329	2114	575	606	1	33			
1	B	428	Total	C	N	O	P	S	14	4	0
			3337	2122	577	604	1	33			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
A	253	LYS	ARG	ENGINEERED	UNP P12995
A	274	LLP	LYS	MODIFIED RESIDUE	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	253	LYS	ARG	ENGINEERED	UNP P12995
B	274	LLP	LYS	MODIFIED RESIDUE	UNP P12995

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

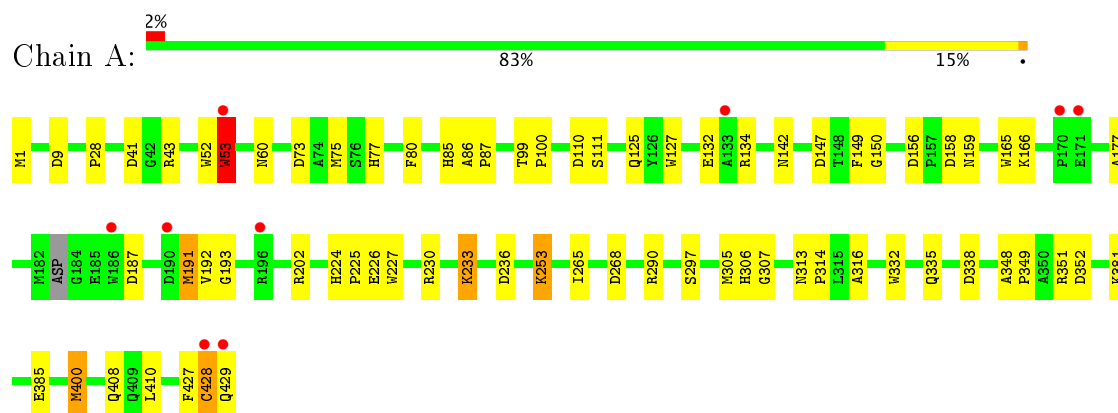
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		
3	B	145	Total	O	0	0
			145	145		

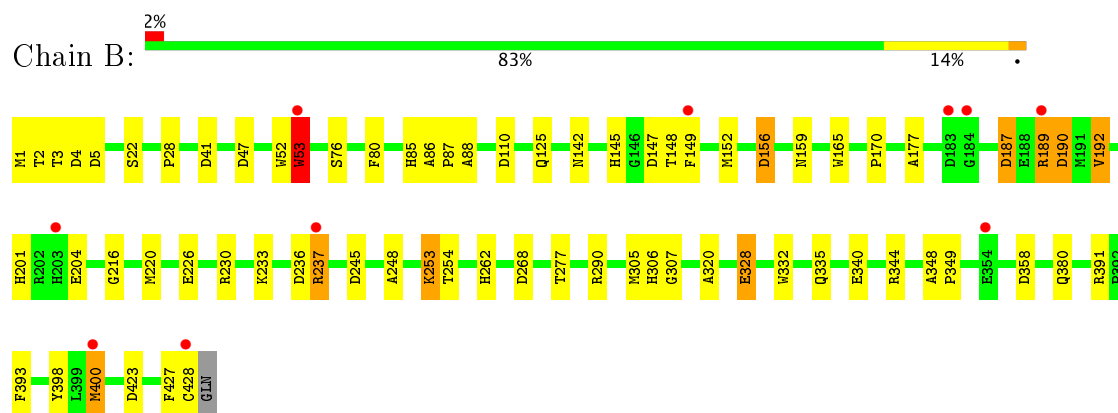
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.08 Å 56.53 Å 120.99 Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.20) 98.2 (20.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.19 Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.191 , 0.226 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	2010 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.61% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.58	1/3391 (0.0%)	0.86	17/4601 (0.4%)
1	B	0.64	3/3409 (0.1%)	0.94	18/4628 (0.4%)
All	All	0.61	4/6800 (0.1%)	0.90	35/9229 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLU	CB-CG	-8.74	1.35	1.52
1	A	191	MET	C-N	-6.19	1.19	1.34
1	B	53[A]	TRP	CB-CG	5.98	1.61	1.50
1	B	53[B]	TRP	CB-CG	5.98	1.61	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400[A]	MET	CG-SD-CE	-17.65	71.96	100.20
1	B	400[B]	MET	CG-SD-CE	-17.65	71.96	100.20
1	B	328	GLU	CA-CB-CG	9.94	135.26	113.40
1	B	53[A]	TRP	CA-CB-CG	9.82	132.36	113.70
1	B	53[B]	TRP	CA-CB-CG	9.82	132.36	113.70
1	A	191	MET	O-C-N	-8.82	108.59	122.70
1	A	53[A]	TRP	CA-CB-CG	7.77	128.47	113.70
1	A	53[B]	TRP	CA-CB-CG	7.77	128.47	113.70
1	B	400[A]	MET	CA-CB-CG	-7.39	100.73	113.30
1	B	400[B]	MET	CA-CB-CG	-7.39	100.73	113.30
1	A	338	ASP	CB-CG-OD2	6.91	124.52	118.30
1	B	4	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	53[A]	TRP	N-CA-CB	6.30	121.94	110.60
1	A	53[B]	TRP	N-CA-CB	6.30	121.94	110.60
1	A	9	ASP	CB-CG-OD2	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	MET	CA-C-N	6.14	130.71	117.20
1	B	187	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	328	GLU	CB-CG-CD	6.03	130.47	114.20
1	A	192	VAL	O-C-N	-5.80	113.34	123.20
1	A	73	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	268	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	236	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	358	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	41	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	328	GLU	CB-CA-C	-5.33	99.74	110.40
1	A	352	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	156	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	423	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	236	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	53[A]	TRP	CB-CA-C	-5.18	100.05	110.40
1	A	53[B]	TRP	CB-CA-C	-5.18	100.05	110.40
1	A	158	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	187	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	268	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	47	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3329	0	3275	46	1
1	B	3337	0	3283	66	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	191	0	0	2	0
3	B	145	0	0	1	1
All	All	7004	0	6558	106	2

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 8.

All (106) 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:53[B]:TRP:CD1	1:A:400[B]:MET:SD	2.34	1.20
1:A:53[A]:TRP:CZ3	1:A:400[A]:MET:HB2	1.87	1.09
1:B:253:LYS:HG3	1:B:400[A]:MET:HE1	1.49	0.93
1:B:125:GLN:HE22	1:B:305:MET:H	1.24	0.81
1:A:428:CYS:O	1:A:429:GLN:HB2	1.78	0.81
1:A:226:GLU:OE1	1:A:230:ARG:NH1	2.16	0.79
1:A:53[A]:TRP:CZ3	1:A:400[A]:MET:CB	2.66	0.79
1:A:125:GLN:HE22	1:A:305:MET:H	1.31	0.78
1:B:226:GLU:OE1	1:B:230:ARG:NH1	2.16	0.78
1:B:253:LYS:CG	1:B:400[A]:MET:HE1	2.15	0.76
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:CB	2.70	0.74
1:A:53[B]:TRP:CG	1:A:400[B]:MET:SD	2.80	0.73
1:B:201:HIS:HD2	1:B:204:GLU:OE2	1.72	0.72
1:A:150:GLY:HA3	1:B:149[A]:PHE:CD1	2.28	0.68
1:B:253:LYS:HD2	1:B:400[A]:MET:HE3	1.75	0.67
1:A:142:ASN:HD22	1:A:177:ALA:HB2	1.60	0.66
1:B:52:TRP:C	1:B:53[B]:TRP:CG	2.65	0.65
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.32	0.65
1:A:253:LYS:HD3	1:A:400[A]:MET:CE	2.28	0.63
1:A:313:ASN:ND2	1:A:316:ALA:H	1.97	0.63
1:A:381:LYS:NZ	1:A:385:GLU:OE2	2.32	0.62
1:A:150:GLY:HA3	1:B:149[A]:PHE:HD1	1.64	0.62
1:B:253:LYS:CG	1:B:400[A]:MET:CE	2.79	0.60
1:B:427:PHE:O	1:B:428:CYS:HB2	2.01	0.60
1:B:53[A]:TRP:HH2	1:B:220:MET:HE2	1.67	0.60
1:A:52:TRP:C	1:A:53[B]:TRP:CG	2.75	0.60
1:B:125:GLN:NE2	1:B:305:MET:H	1.98	0.59
1:B:187:ASP:O	1:B:190:ASP:HB2	2.03	0.59
1:B:52:TRP:O	1:B:53[A]:TRP:HB2	2.03	0.58
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.87	0.57
1:A:332:TRP:HA	1:A:335:GLN:HE21	1.69	0.56
1:B:253:LYS:HD2	1:B:400[A]:MET:CE	2.36	0.56
1:B:340:GLU:O	1:B:344:ARG:HG3	2.07	0.54
1:B:53[A]:TRP:CH2	1:B:220:MET:HE2	2.42	0.54
1:B:52:TRP:C	1:B:53[B]:TRP:CD1	2.81	0.54
1:B:22:SER:O	1:B:22:SER:OG	2.17	0.54
1:B:53[A]:TRP:CH2	1:B:220:MET:CE	2.91	0.53
1:A:253:LYS:HD3	1:A:400[A]:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[A]:TRP:CD1	1:A:253:LYS:HD2	2.44	0.53
1:B:142:ASN:HD22	1:B:177:ALA:HB2	1.75	0.52
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:CG	2.93	0.51
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.91	0.51
1:B:53[A]:TRP:CZ2	1:B:220:MET:HE1	2.45	0.51
1:A:156:ASP:HB3	1:A:159:ASN:HB2	1.92	0.51
1:B:145:HIS:HD2	1:B:245:ASP:OD2	1.94	0.51
1:B:52:TRP:HA	1:B:53[B]:TRP:CD1	2.45	0.51
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.47	0.50
1:B:53[B]:TRP:HZ3	1:B:248:ALA:HB2	1.76	0.50
1:A:149:PHE:HB3	1:B:149[B]:PHE:CD2	2.47	0.49
1:A:41:ASP:OD2	1:A:43:ARG:NE	2.43	0.49
1:A:77:HIS:HA	1:A:314:PRO:HD2	1.92	0.49
1:B:253:LYS:CD	1:B:400[A]:MET:HE3	2.41	0.48
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:HG3	2.48	0.48
1:B:332:TRP:HA	1:B:335:GLN:HE21	1.79	0.48
1:B:53[A]:TRP:CZ3	1:B:398:TYR:CE1	3.02	0.48
1:A:1:MET:HE1	1:A:28:PRO:HB2	1.94	0.48
1:B:248:ALA:O	1:B:253:LYS:HE2	2.14	0.48
1:A:52:TRP:C	1:A:53[B]:TRP:CD1	2.87	0.47
1:B:253:LYS:HG3	1:B:400[A]:MET:CE	2.33	0.47
1:B:2:THR:O	1:B:5:ASP:HB2	2.14	0.47
1:A:306:HIS:CE1	1:B:147:ASP:HB3	2.49	0.47
1:A:253:LYS:HE3	1:A:253:LYS:HB2	1.66	0.47
1:B:148:THR:O	1:B:152:MET:HG3	2.15	0.47
1:B:149[B]:PHE:CZ	1:B:170:PRO:HD3	2.49	0.46
1:B:201:HIS:CD2	1:B:204:GLU:OE2	2.60	0.46
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:HB3	2.51	0.46
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.96	0.46
1:A:99:THR:HB	1:A:100:PRO:HD2	1.97	0.46
1:B:1:MET:HE1	1:B:28:PRO:HB2	1.98	0.45
1:B:53[A]:TRP:HH2	1:B:220:MET:CE	2.28	0.45
1:B:53[B]:TRP:CE2	1:B:400[B]:MET:HE1	2.52	0.45
1:B:348:ALA:N	1:B:349:PRO:CD	2.79	0.45
1:A:348:ALA:N	1:A:349:PRO:CD	2.80	0.45
1:B:53[A]:TRP:CZ3	1:B:398:TYR:CD1	3.06	0.44
1:A:165:TRP:CH2	1:B:125:GLN:HG3	2.53	0.44
1:A:52:TRP:HA	1:A:53[B]:TRP:CD1	2.52	0.44
1:B:85:HIS:CE1	1:B:88:ALA:HB2	2.52	0.44
1:A:191:MET:SD	1:A:227:TRP:CZ3	3.11	0.43
1:B:348:ALA:HB3	1:B:349:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53[A]:TRP:CZ3	1:B:400[A]:MET:CB	3.01	0.43
1:A:233:LYS:N	1:A:233:LYS:HD2	2.33	0.43
1:A:85:HIS:HE1	3:A:503:HOH:O	2.01	0.43
1:A:427:PHE:O	1:A:428:CYS:HB2	2.19	0.43
1:B:189:ARG:O	1:B:192:VAL:HG13	2.17	0.43
1:A:111:SER:HA	3:A:566:HOH:O	2.19	0.43
1:B:254:THR:OG1	1:B:262:HIS:HE1	2.02	0.42
1:B:53[A]:TRP:CD1	1:B:248:ALA:HB1	2.54	0.42
1:B:53[A]:TRP:CE3	1:B:400[A]:MET:HB3	2.55	0.42
1:A:224:HIS:HA	1:A:225:PRO:HD3	1.91	0.42
1:A:313:ASN:HD22	1:A:316:ALA:H	1.68	0.42
1:B:145:HIS:HE1	3:B:525:HOH:O	2.02	0.41
1:B:156:ASP:HB3	1:B:159:ASN:HB2	2.01	0.41
1:A:132:GLU:OE2	1:A:134:ARG:NE	2.36	0.41
1:B:253:LYS:CD	1:B:400[A]:MET:CE	2.98	0.41
1:B:53[A]:TRP:CZ3	1:B:400[A]:MET:HB2	2.55	0.41
1:B:380:GLN:OE1	1:B:391:ARG:HD2	2.21	0.41
1:B:400[A]:MET:HB2	1:B:400[A]:MET:HE2	1.93	0.41
1:B:52:TRP:O	1:B:53[A]:TRP:CB	2.67	0.41
1:B:53[B]:TRP:HB3	1:B:253:LYS:HE3	2.02	0.41
1:B:53[A]:TRP:CZ3	1:B:400[A]:MET:HB3	2.56	0.40
1:A:53[B]:TRP:NE1	1:A:400[B]:MET:SD	2.86	0.40
1:B:277:THR:HA	1:B:320:ALA:HA	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237[A]:ARG:NH1	3:B:576:HOH:O[2_646]	1.78	0.42
1:A:351:ARG:O	1:A:408:GLN:NE2[2_645]	1.91	0.29

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	425/429 (99%)	412 (97%)	9 (2%)	4 (1%)	20	18
1	B	429/429 (100%)	416 (97%)	11 (3%)	2 (0%)	32	34
All	All	854/858 (100%)	828 (97%)	20 (2%)	6 (1%)	25	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLY
1	A	75	MET
1	A	428	CYS
1	B	307	GLY
1	A	307	GLY
1	B	216	GLY

### 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	345/344 (100%)	330 (96%)	15 (4%)	33	41
1	B	346/344 (101%)	329 (95%)	17 (5%)	29	35
All	All	691/688 (100%)	659 (95%)	32 (5%)	35	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53[A]	TRP
1	A	53[B]	TRP
1	A	60	ASN
1	A	80	PHE
1	A	110	ASP
1	A	166	LYS
1	A	202	ARG
1	A	233	LYS

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Mol	Chain	Res	Type
1	A	253	LYS
1	A	265	ILE
1	A	290	ARG
1	A	297	SER
1	A	400[A]	MET
1	A	400[B]	MET
1	A	410	LEU
1	B	3	THR
1	B	53[A]	TRP
1	B	53[B]	TRP
1	B	76	SER
1	B	80	PHE
1	B	110	ASP
1	B	165	TRP
1	B	189	ARG
1	B	190	ASP
1	B	192	VAL
1	B	233	LYS
1	B	237[A]	ARG
1	B	237[B]	ARG
1	B	253	LYS
1	B	290	ARG
1	B	328	GLU
1	B	393	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	125	GLN
1	A	135	GLN
1	A	142	ASN
1	A	313	ASN
1	A	335	GLN
1	B	125	GLN
1	B	135	GLN
1	B	142	ASN
1	B	145	HIS
1	B	201	HIS
1	B	262	HIS
1	B	313	ASN
1	B	335	GLN

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Mol	Chain	Res	Type
1	B	342	GLN
1	B	346	GLN
1	B	411	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	LLP	A	274	1	24,24,25	2.04	7 (29%)	28,32,34	1.91	5 (17%)
1	LLP	B	274	1	24,24,25	1.92	5 (20%)	28,32,34	1.90	5 (17%)

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
1	LLP	A	274	1	-	0/15/17/19	0/1/1/1
1	LLP	B	274	1	-	0/15/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	LLP	O3-C3	-5.34	1.24	1.37
1	A	274	LLP	O3-C3	-5.26	1.24	1.37
1	A	274	LLP	C4-C5	-2.25	1.39	1.42
1	B	274	LLP	C3-C2	-2.04	1.39	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	LLP	CD-CE	2.06	1.58	1.51
1	A	274	LLP	C2-N1	2.26	1.38	1.33
1	A	274	LLP	C4-C4'	2.32	1.50	1.46
1	B	274	LLP	C2-N1	2.35	1.38	1.33
1	A	274	LLP	C4'-NZ	2.41	1.34	1.27
1	B	274	LLP	C4-C4'	2.52	1.51	1.46
1	B	274	LLP	CA-C	4.47	1.56	1.50
1	A	274	LLP	CA-C	5.27	1.57	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	LLP	C4-C4'-NZ	-4.47	102.95	124.66
1	A	274	LLP	C4-C4'-NZ	-3.79	106.26	124.66
1	B	274	LLP	C3-C4-C4'	-2.58	115.58	120.52
1	A	274	LLP	C3-C4-C4'	-2.28	116.15	120.52
1	B	274	LLP	C5-C6-N1	-2.09	120.33	123.87
1	B	274	LLP	C5-C4-C4'	2.24	124.71	121.36
1	A	274	LLP	O3-C3-C2	2.52	123.06	117.78
1	A	274	LLP	C3-C4-C5	2.84	120.41	118.24
1	B	274	LLP	OP4-C5'-C5	5.66	120.70	109.32
1	A	274	LLP	OP4-C5'-C5	6.59	122.56	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	191:MET	C	192:VAL	N	1.19

## 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, 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	426/429 (99%)	-0.04	9 (2%) 64 61	16, 25, 38, 48	2 (0%)
1	B	427/429 (99%)	0.01	10 (2%) 61 58	16, 27, 39, 50	3 (0%)
All	All	853/858 (99%)	-0.02	19 (2%) 62 60	16, 26, 39, 50	5 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53[A]	TRP	4.8
1	A	429	GLN	4.0
1	A	53[A]	TRP	3.4
1	B	189	ARG	3.3
1	B	428	CYS	3.3
1	B	149[A]	PHE	3.3
1	B	183	ASP	2.4
1	A	133	ALA	2.4
1	A	170	PRO	2.4
1	A	428	CYS	2.3
1	A	186	TRP	2.3
1	A	171	GLU	2.3
1	B	400[A]	MET	2.3
1	B	354	GLU	2.2
1	B	184	GLY	2.2
1	A	196	ARG	2.1
1	A	190	ASP	2.1
1	B	237[A]	ARG	2.0
1	B	203	HIS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	LLP	A	274	24/25	0.95	0.12	-	15,19,22,25	0
1	LLP	B	274	24/25	0.95	0.10	-	16,20,22,25	0

### 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(Å <sup>2</sup> )	Q<0.9
2	NA	B	502	1/1	0.85	0.23	1.89	15,15,15,15	0
2	NA	A	501	1/1	0.99	0.17	1.08	7,7,7,7	0

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

There are no such residues in this entry.