



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 02:26 PM EDT

PDB ID : 6DGD  
Title : PriA helicase bound to dsDNA of a DNA replication fork  
Authors : Satyshur, K.A.; Windgassen, T.A.; Keck, J.L.  
Deposited on : 2018-05-17  
Resolution : 2.82 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

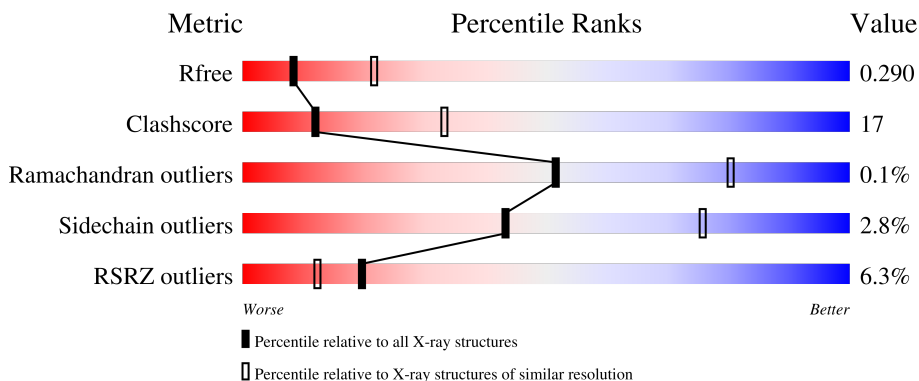
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	 2% 65% 28% • 6%
1	B	751	 7% 64% 28% • 7%
2	W	12	 50% 75% 25%
3	X	12	 50% 50% 50%
3	Z	12	 58% 42% 58%

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Mol	Chain	Length	Quality of chain
4	Y	13	<p>54% 69% 31%</p>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	809	-	-	-	X
6	SO4	B	805	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11648 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 Primosomal protein N'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	704	5391	3436	966	972	17	0	0	0
1	B	701	5186	3319	910	940	17	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A0A1W2ITH4
A	-18	GLY	-	expression tag	UNP A0A1W2ITH4
A	-17	SER	-	expression tag	UNP A0A1W2ITH4
A	-16	SER	-	expression tag	UNP A0A1W2ITH4
A	-15	HIS	-	expression tag	UNP A0A1W2ITH4
A	-14	HIS	-	expression tag	UNP A0A1W2ITH4
A	-13	HIS	-	expression tag	UNP A0A1W2ITH4
A	-12	HIS	-	expression tag	UNP A0A1W2ITH4
A	-11	HIS	-	expression tag	UNP A0A1W2ITH4
A	-10	HIS	-	expression tag	UNP A0A1W2ITH4
A	-9	SER	-	expression tag	UNP A0A1W2ITH4
A	-8	SER	-	expression tag	UNP A0A1W2ITH4
A	-7	GLY	-	expression tag	UNP A0A1W2ITH4
A	-6	LEU	-	expression tag	UNP A0A1W2ITH4
A	-5	VAL	-	expression tag	UNP A0A1W2ITH4
A	-4	PRO	-	expression tag	UNP A0A1W2ITH4
A	-3	ARG	-	expression tag	UNP A0A1W2ITH4
A	-2	GLY	-	expression tag	UNP A0A1W2ITH4
A	-1	SER	-	expression tag	UNP A0A1W2ITH4
A	0	HIS	-	expression tag	UNP A0A1W2ITH4
B	-19	MET	-	expression tag	UNP A0A1W2ITH4
B	-18	GLY	-	expression tag	UNP A0A1W2ITH4
B	-17	SER	-	expression tag	UNP A0A1W2ITH4
B	-16	SER	-	expression tag	UNP A0A1W2ITH4
B	-15	HIS	-	expression tag	UNP A0A1W2ITH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A0A1W2ITH4
B	-13	HIS	-	expression tag	UNP A0A1W2ITH4
B	-12	HIS	-	expression tag	UNP A0A1W2ITH4
B	-11	HIS	-	expression tag	UNP A0A1W2ITH4
B	-10	HIS	-	expression tag	UNP A0A1W2ITH4
B	-9	SER	-	expression tag	UNP A0A1W2ITH4
B	-8	SER	-	expression tag	UNP A0A1W2ITH4
B	-7	GLY	-	expression tag	UNP A0A1W2ITH4
B	-6	LEU	-	expression tag	UNP A0A1W2ITH4
B	-5	VAL	-	expression tag	UNP A0A1W2ITH4
B	-4	PRO	-	expression tag	UNP A0A1W2ITH4
B	-3	ARG	-	expression tag	UNP A0A1W2ITH4
B	-2	GLY	-	expression tag	UNP A0A1W2ITH4
B	-1	SER	-	expression tag	UNP A0A1W2ITH4
B	0	HIS	-	expression tag	UNP A0A1W2ITH4

- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*GP\*CP\*AP\*CP\*GP\*CP\*CP\*GP\*AP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	W	12	244	115	47	70	12	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(P\*GP\*TP\*CP\*GP\*GP\*CP\*GP\*TP\*GP\*CP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	X	12	246	116	43	75	12	0	0	0
3	Z	12	243	116	43	73	11	0	0	0

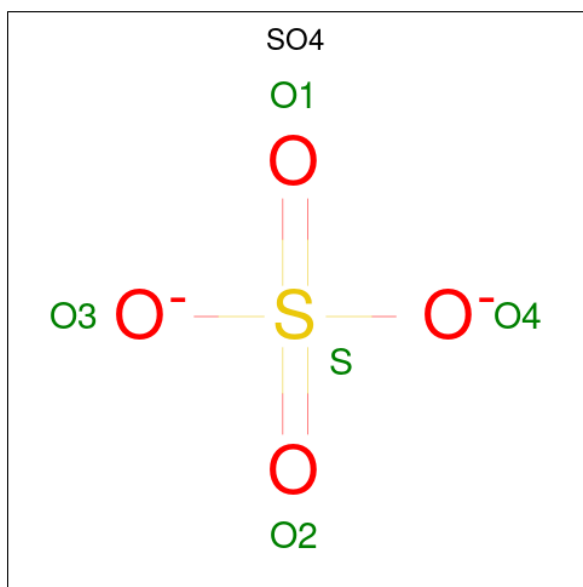
- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*AP\*GP\*CP\*AP\*CP\*GP\*CP\*CP\*GP\*AP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	Y	13	267	125	52	77	13	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

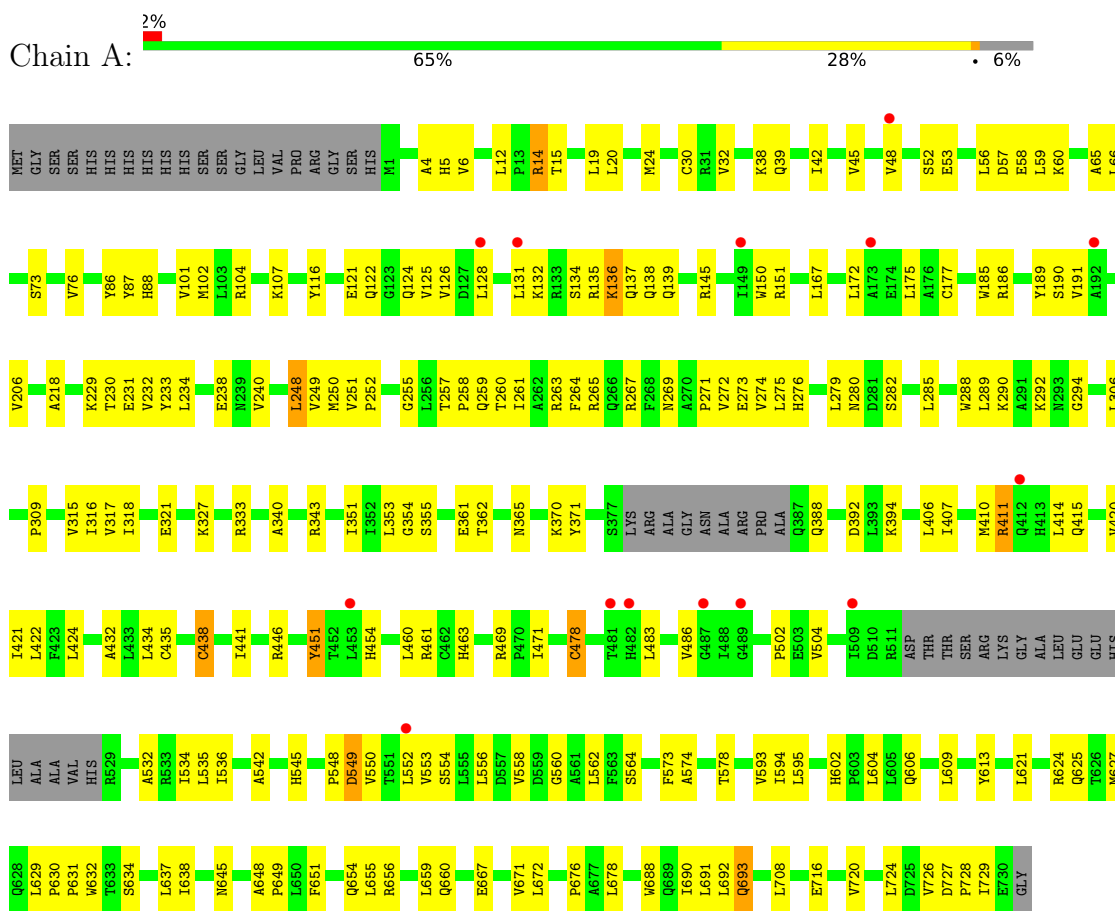
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		

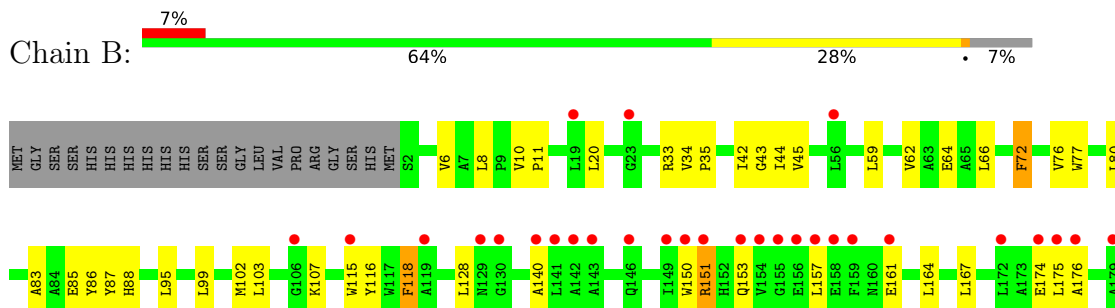
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

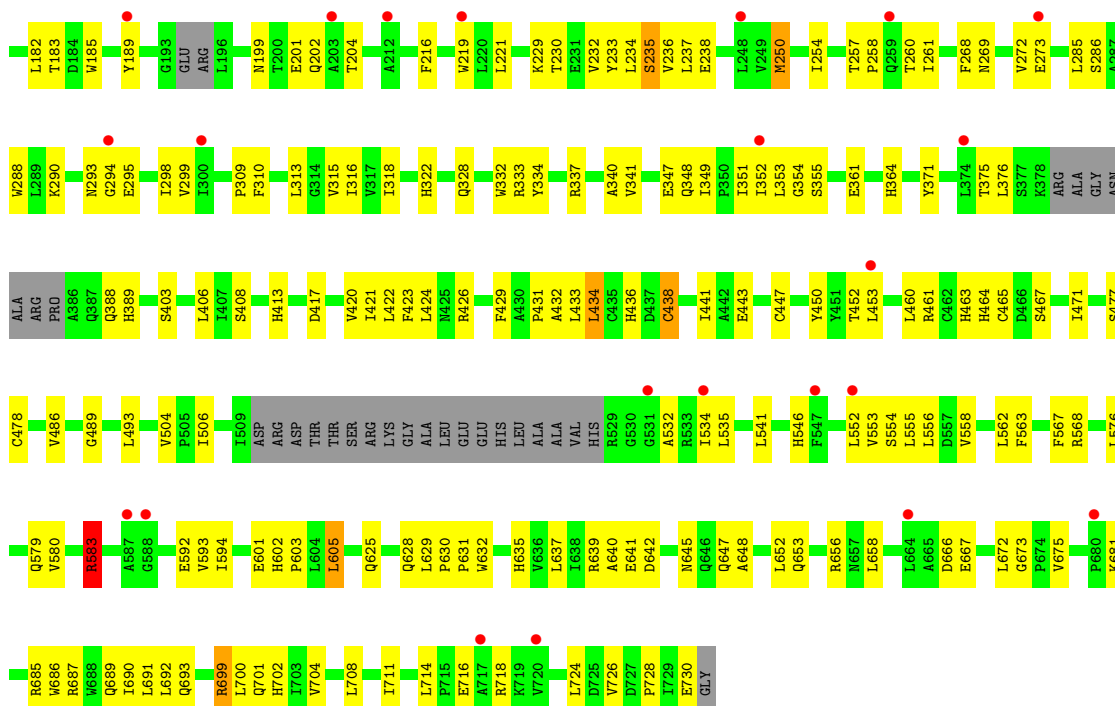
#### • Molecule 1: Primosomal protein N<sup>1</sup>



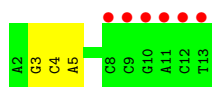
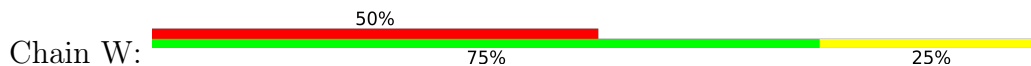
#### • Molecule 1: Primosomal protein N<sup>1</sup>



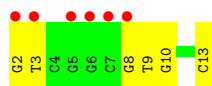




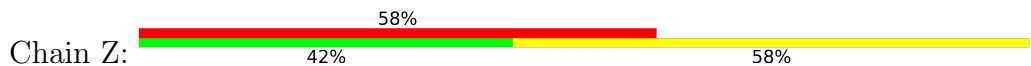
- Molecule 2: DNA (5'-D(P\*AP\*GP\*CP\*AP\*CP\*GP\*CP\*CP\*GP\*AP\*CP\*T)-3')



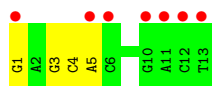
- Molecule 3: DNA (5'-D(P\*GP\*TP\*CP\*GP\*GP\*CP\*GP\*TP\*GP\*CP\*TP\*C)-3')



- Molecule 3: DNA (5'-D(P\*GP\*TP\*CP\*GP\*GP\*CP\*GP\*TP\*GP\*CP\*TP\*C)-3')



- Molecule 4: DNA (5'-D(P\*GP\*AP\*GP\*CP\*AP\*CP\*GP\*CP\*CP\*GP\*AP\*CP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.56Å 106.76Å 256.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.82 49.34 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.34-2.82) 98.8 (49.34-2.82)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.247 , 0.290 0.247 , 0.290	Depositor DCC
$R_{free}$ test set	1999 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.6	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 105.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: SO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.44	0/5526	0.61	0/7545
1	B	0.49	1/5317 (0.0%)	0.64	0/7287
2	W	0.60	0/273	0.85	0/418
3	X	0.58	0/274	0.95	0/421
3	Z	0.58	0/271	0.92	0/417
4	Y	0.82	1/299 (0.3%)	0.86	0/457
All	All	0.49	2/11960 (0.0%)	0.66	0/16545

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	1	DG	OP3-P	-10.79	1.48	1.61
1	B	299	VAL	CB-CG2	-5.26	1.41	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	583	ARG	Sidechain

## 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	5391	0	5269	172	1
1	B	5186	0	4946	205	0
2	W	244	0	134	8	0
3	X	246	0	136	8	0
3	Z	243	0	137	5	0
4	Y	267	0	145	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	40	0	0	2	0
6	B	25	0	0	5	0
7	A	2	0	0	0	0
All	All	11648	0	10767	386	1

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 17.

All (386) 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:B:422:LEU:HD23	1:B:554:SER:OG	1.47	1.11
1:A:59:LEU:HD23	3:X:13:DC:H2''	1.26	1.09
1:A:59:LEU:CD2	3:X:13:DC:H2''	1.95	0.95
1:B:185:TRP:CD1	1:B:295:GLU:O	2.20	0.94
1:B:293:ASN:HD22	1:B:295:GLU:CD	1.71	0.93
1:A:637:LEU:HD13	1:A:728:PRO:HG3	1.54	0.90
1:A:59:LEU:HD23	3:X:13:DC:C2'	2.02	0.89
1:B:422:LEU:HD23	1:B:554:SER:HG	1.37	0.89
1:B:293:ASN:ND2	1:B:295:GLU:CD	2.27	0.88
1:A:248:LEU:HB3	1:A:316:ILE:HG22	1.57	0.86
1:B:293:ASN:ND2	1:B:295:GLU:CG	2.39	0.85
1:B:424:LEU:HD23	1:B:489:GLY:HA2	1.60	0.84
1:B:605:LEU:O	1:B:605:LEU:HD12	1.79	0.81
1:B:420:VAL:HG13	1:B:552:LEU:O	1.80	0.80
1:A:638:ILE:HG12	1:A:724:LEU:CD1	2.12	0.79
1:B:422:LEU:CD2	1:B:554:SER:OG	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ILE:HG12	1:B:534:ILE:HB	1.64	0.78
1:B:640:ALA:HB3	1:B:652:LEU:HD11	1.66	0.77
1:B:594:ILE:HD12	1:B:594:ILE:O	1.84	0.77
3:Z:9:DT:H2''	3:Z:10:DG:H5''	1.67	0.76
1:B:558:VAL:O	1:B:562:LEU:HD12	1.86	0.75
1:B:310:PHE:CG	1:B:313:LEU:HD21	2.23	0.73
1:B:506:ILE:CG1	1:B:534:ILE:HB	2.18	0.73
1:B:628:GLN:O	1:B:693:GLN:NE2	2.21	0.72
1:B:33:ARG:HD3	1:B:42:ILE:HD11	1.70	0.71
1:B:322:HIS:ND1	1:B:355:SER:OG	2.22	0.71
1:B:421:ILE:HG12	1:B:535:LEU:HB2	1.74	0.70
1:B:6:VAL:HG22	1:B:45:VAL:HA	1.75	0.69
1:A:638:ILE:HG12	1:A:724:LEU:HD13	1.72	0.69
1:B:238:GLU:HG2	1:B:268:PHE:CZ	2.28	0.68
1:B:59:LEU:HD23	3:Z:13:DC:H2''	1.75	0.68
1:A:249:VAL:HG23	1:A:317:VAL:HG13	1.75	0.68
1:B:562:LEU:HD22	1:B:602:HIS:ND1	2.09	0.68
1:B:20:LEU:HD12	1:B:62:VAL:HG11	1.74	0.68
1:A:275:LEU:HA	1:A:279:LEU:HD11	1.77	0.67
1:B:72:PHE:CE1	1:B:99:LEU:HD21	2.30	0.67
1:B:185:TRP:HD1	1:B:295:GLU:O	1.75	0.67
1:A:56:LEU:HA	1:A:59:LEU:HD12	1.77	0.67
1:B:72:PHE:HE1	1:B:99:LEU:HD21	1.59	0.66
1:A:578:THR:HG21	1:A:613:TYR:HB2	1.77	0.66
1:B:656:ARG:NH1	1:B:673:GLY:O	2.29	0.66
1:A:252:PRO:HD2	1:A:255:GLY:HA3	1.76	0.66
1:B:293:ASN:ND2	1:B:295:GLU:HG3	2.11	0.65
1:B:182:LEU:HD23	1:B:182:LEU:H	1.61	0.65
1:B:293:ASN:OD1	1:B:294:GLY:N	2.30	0.65
1:B:406:LEU:O	1:B:406:LEU:HD12	1.97	0.65
1:B:76:VAL:O	1:B:80:LEU:HD12	1.97	0.65
1:A:122:GLN:O	1:A:126:VAL:HG22	1.97	0.65
1:B:637:LEU:HG	1:B:728:PRO:HG3	1.78	0.65
1:B:568:ARG:NH1	1:B:730:GLU:O	2.31	0.64
1:A:60:LYS:NZ	3:X:13:DC:OP2	2.27	0.64
1:B:164:LEU:HD12	1:B:167:LEU:HD12	1.80	0.64
1:A:407:ILE:O	1:A:411:ARG:HG2	1.97	0.64
1:B:424:LEU:HD21	1:B:493:LEU:HD13	1.79	0.64
1:A:536:ILE:HD12	1:A:536:ILE:O	1.98	0.64
1:B:553:VAL:HB	1:B:593:VAL:HG23	1.80	0.63
1:B:293:ASN:ND2	1:B:295:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:HD11	1:B:471:ILE:HA	1.80	0.63
1:A:136:LYS:HB3	1:A:139:GLN:HE21	1.63	0.62
1:B:272:VAL:HG12	1:B:298:ILE:HG12	1.80	0.62
1:A:122:GLN:HA	1:A:125:VAL:HG22	1.80	0.62
1:A:250:MET:HB2	1:A:318:ILE:HG22	1.82	0.62
1:B:576:LEU:O	1:B:580:VAL:HG22	2.00	0.61
1:A:595:LEU:HD21	1:A:609:LEU:HD21	1.82	0.61
1:B:648:ALA:O	1:B:652:LEU:HD12	2.00	0.61
1:B:675:VAL:O	1:B:689:GLN:HG2	2.01	0.60
1:A:88:HIS:HB2	1:A:724:LEU:HD23	1.82	0.60
1:B:421:ILE:HA	1:B:535:LEU:O	2.01	0.60
1:B:182:LEU:HB2	1:B:295:GLU:OE2	2.01	0.59
1:B:183:THR:O	1:B:295:GLU:HG2	2.03	0.59
1:B:238:GLU:HG2	1:B:268:PHE:CE1	2.37	0.59
1:A:438:CYS:HB3	1:A:478:CYS:SG	2.42	0.59
1:A:562:LEU:HD21	1:A:602:HIS:CG	2.37	0.59
1:B:34:VAL:HG12	1:B:62:VAL:HG23	1.84	0.59
1:A:553:VAL:O	1:A:593:VAL:HA	2.03	0.59
1:A:56:LEU:HD23	1:A:59:LEU:HD12	1.84	0.59
1:B:328:GLN:NE2	1:B:332:TRP:O	2.36	0.59
1:A:265:ARG:NH2	1:B:438:CYS:HB2	2.18	0.59
1:A:87:TYR:HA	1:A:726:VAL:HG21	1.85	0.58
1:A:306:LEU:O	1:A:343:ARG:NH1	2.36	0.58
1:B:318:ILE:HD12	1:B:351:ILE:HD11	1.85	0.58
1:B:72:PHE:CD2	1:B:77:TRP:HE3	2.21	0.58
1:B:583:ARG:NH2	6:B:805:SO4:S	2.72	0.58
1:B:681:LYS:HA	1:B:685:ARG:O	2.04	0.58
1:B:504:VAL:O	1:B:506:ILE:HD12	2.04	0.58
1:A:257:THR:O	1:A:260:THR:N	2.35	0.57
1:B:420:VAL:HG12	1:B:421:ILE:N	2.17	0.57
1:A:638:ILE:HB	1:A:690:ILE:CG2	2.33	0.57
1:B:558:VAL:HG12	1:B:562:LEU:HD11	1.86	0.57
1:B:443:GLU:HG2	1:B:450:TYR:HD1	1.70	0.57
1:B:257:THR:HG1	1:B:260:THR:HG1	1.47	0.57
1:B:221:LEU:HD23	1:B:229:LYS:HB3	1.87	0.57
1:B:422:LEU:HD22	1:B:556:LEU:HD21	1.86	0.57
1:B:72:PHE:HD2	1:B:77:TRP:HE3	1.53	0.57
1:B:594:ILE:HD12	1:B:594:ILE:C	2.25	0.56
1:A:57:ASP:OD1	1:A:58:GLU:N	2.39	0.56
1:A:257:THR:O	1:A:259:GLN:N	2.38	0.56
1:B:700:LEU:O	1:B:704:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLU:O	1:A:365:ASN:ND2	2.38	0.56
1:A:406:LEU:HD12	1:A:594:ILE:HG21	1.87	0.56
1:A:602:HIS:CE1	1:A:604:LEU:HB2	2.41	0.56
1:B:310:PHE:CD1	1:B:313:LEU:HD21	2.41	0.56
1:A:435:CYS:HA	1:A:483:LEU:HD22	1.87	0.56
1:B:8:LEU:HD23	1:B:43:GLY:HA3	1.89	0.55
1:B:353:LEU:HD11	1:B:371:TYR:HE2	1.71	0.55
1:A:637:LEU:HD11	1:A:691:LEU:HD13	1.89	0.55
1:A:280:ASN:OD1	1:A:282:SER:N	2.40	0.55
1:A:318:ILE:HD11	1:A:353:LEU:HD12	1.89	0.55
1:B:347:GLU:HB2	1:B:349:ILE:HG22	1.89	0.55
1:B:221:LEU:HD23	1:B:229:LYS:CB	2.36	0.55
1:B:315:VAL:HG22	1:B:316:ILE:N	2.22	0.55
1:B:452:THR:HG22	1:B:461:ARG:O	2.07	0.55
1:A:671:VAL:HG12	1:A:692:LEU:HG	1.89	0.55
1:B:219:TRP:HB2	1:B:352:ILE:HG12	1.89	0.55
1:A:14:ARG:HG3	1:A:15:THR:O	2.07	0.54
1:A:422:LEU:CD2	1:A:554:SER:HB2	2.37	0.54
1:B:293:ASN:HD21	1:B:295:GLU:HB2	1.71	0.54
1:B:691:LEU:HD12	1:B:692:LEU:N	2.21	0.54
1:B:433:LEU:HD13	1:B:453:LEU:HD13	1.89	0.54
1:A:38:LYS:NZ	2:W:5:DA:P	2.80	0.54
1:B:232:VAL:O	1:B:236:VAL:HG22	2.08	0.54
1:A:420:VAL:HG21	1:A:552:LEU:HD23	1.89	0.54
1:A:432:ALA:H	1:A:486:VAL:HG22	1.72	0.54
1:B:34:VAL:CG1	1:B:62:VAL:HG23	2.37	0.54
1:B:151:ARG:NH2	1:B:161:GLU:OE2	2.41	0.53
1:B:216:PHE:HB2	1:B:348:GLN:HA	1.90	0.53
1:B:199:ASN:HB3	1:B:202:GLN:OE1	2.09	0.53
1:A:128:LEU:HD11	1:A:138:GLN:HG3	1.91	0.53
1:A:463:HIS:CD2	1:A:678:LEU:HD11	2.44	0.53
1:B:286:SER:OG	1:B:290:LYS:HE3	2.09	0.53
1:A:186:ARG:NH2	1:A:294:GLY:O	2.38	0.53
1:B:434:LEU:HB3	1:B:441:ILE:HG22	1.90	0.53
3:Z:7:DC:H2''	3:Z:8:DG:O4'	2.09	0.53
1:B:102:MET:CE	1:B:285:LEU:HD12	2.39	0.53
1:A:654:GLN:NE2	1:A:716:GLU:OE2	2.41	0.53
1:B:140:ALA:HB1	1:B:164:LEU:HD13	1.89	0.53
1:A:333:ARG:NH1	6:A:805:SO4:O1	2.42	0.52
1:B:254:ILE:O	1:B:254:ILE:HG22	2.08	0.52
1:B:447:CYS:SG	1:B:464:HIS:HB3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ARG:HA	1:B:467:SER:O	2.09	0.52
1:A:121:GLU:O	1:A:124:GLN:HG2	2.08	0.52
1:A:230:THR:O	1:A:234:LEU:HD12	2.10	0.52
1:A:258:PRO:HB2	1:B:601:GLU:HG3	1.90	0.52
1:B:602:HIS:CD2	1:B:603:PRO:HD2	2.44	0.52
1:B:72:PHE:HB3	1:B:76:VAL:HG13	1.90	0.52
1:A:38:LYS:HZ2	2:W:5:DA:C4'	2.22	0.52
1:A:536:ILE:HD12	1:A:536:ILE:C	2.28	0.52
1:B:258:PRO:HA	1:B:261:ILE:CG1	2.40	0.52
1:B:258:PRO:HA	1:B:261:ILE:HG12	1.92	0.52
1:A:553:VAL:CG2	1:A:593:VAL:HG12	2.39	0.52
1:B:221:LEU:CD2	1:B:229:LYS:CB	2.88	0.52
1:B:233:TYR:OH	1:B:354:GLY:HA3	2.10	0.52
1:A:116:TYR:O	1:A:175:LEU:HD12	2.10	0.52
1:B:423:PHE:C	1:B:424:LEU:HD12	2.30	0.52
1:A:150:TRP:CD1	1:A:151:ARG:N	2.78	0.51
1:B:423:PHE:HB2	1:B:555:LEU:HD23	1.91	0.51
3:X:9:DT:H2''	3:X:10:DG:H5'	1.93	0.51
1:B:443:GLU:HG2	1:B:450:TYR:CD1	2.46	0.51
1:A:392:ASP:OD2	1:A:394:LYS:HE3	2.11	0.51
1:A:649:PRO:HG3	1:A:688:TRP:CE2	2.46	0.51
1:B:219:TRP:O	1:B:352:ILE:HA	2.11	0.51
1:A:285:LEU:O	1:A:289:LEU:HD12	2.11	0.51
1:B:232:VAL:HA	1:B:235:SER:HB3	1.92	0.51
1:A:38:LYS:HZ3	2:W:5:DA:P	2.33	0.50
1:B:42:ILE:HD12	1:B:66:LEU:HD11	1.93	0.50
1:B:221:LEU:CD2	1:B:229:LYS:HB3	2.41	0.50
1:B:87:TYR:CE1	1:B:334:TYR:HA	2.46	0.50
1:B:153:GLN:O	1:B:157:LEU:HD13	2.11	0.50
1:B:417:ASP:OD1	1:B:532:ALA:HB2	2.11	0.50
1:A:602:HIS:HE1	1:A:604:LEU:HB2	1.76	0.50
1:B:234:LEU:O	1:B:238:GLU:HG3	2.12	0.50
1:B:375:THR:O	1:B:376:LEU:HD23	2.11	0.50
1:A:6:VAL:N	1:A:15:THR:HG22	2.27	0.50
1:A:38:LYS:NZ	2:W:4:DC:O3'	2.42	0.50
1:A:261:ILE:HD13	1:A:274:VAL:HG21	1.94	0.50
1:A:434:LEU:HD22	1:A:435:CYS:H	1.75	0.50
1:A:39:GLN:NE2	2:W:3:DG:O3'	2.45	0.50
1:A:150:TRP:CZ2	1:A:282:SER:OG	2.64	0.50
1:A:131:LEU:HD13	1:A:134:SER:OG	2.12	0.49
1:A:206:VAL:HG22	1:A:232:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:2:DG:H2'	3:Z:3:DT:H5'	1.93	0.49
1:A:257:THR:HG22	1:A:259:GLN:CB	2.43	0.49
1:B:388:GLN:HB3	1:B:593:VAL:HG12	1.94	0.49
1:B:506:ILE:HG13	1:B:534:ILE:HB	1.94	0.49
1:B:552:LEU:HA	1:B:592:GLU:O	2.12	0.49
1:A:124:GLN:HA	1:A:145:ARG:HE	1.77	0.49
1:B:234:LEU:HD12	1:B:234:LEU:H	1.77	0.49
1:B:116:TYR:HB3	1:B:150:TRP:HA	1.94	0.49
2:W:5:DA:N6	3:X:8:DG:O6	2.46	0.49
1:A:548:PRO:HG2	1:A:549:ASP:OD1	2.13	0.49
1:B:33:ARG:CD	1:B:42:ILE:HD11	2.40	0.49
1:B:102:MET:HE3	1:B:285:LEU:HD12	1.95	0.49
1:A:218:ALA:HA	1:A:351:ILE:HG23	1.93	0.49
1:A:574:ALA:O	1:A:578:THR:HG23	2.12	0.49
1:A:121:GLU:O	1:A:125:VAL:HG13	2.13	0.49
1:B:6:VAL:HG13	1:B:44:ILE:O	2.13	0.49
1:A:20:LEU:HD13	1:A:24:MET:O	2.12	0.48
1:A:136:LYS:O	1:A:137:GLN:C	2.51	0.48
1:A:671:VAL:CG1	1:A:692:LEU:HG	2.42	0.48
1:A:233:TYR:OH	1:A:354:GLY:HA3	2.13	0.48
1:B:708:LEU:HA	1:B:711:ILE:HD12	1.96	0.48
1:B:8:LEU:O	1:B:10:VAL:N	2.46	0.48
1:A:406:LEU:HD11	1:A:554:SER:OG	2.14	0.48
1:A:645:ASN:OD1	1:A:645:ASN:O	2.32	0.48
1:A:651:PHE:CD2	1:A:720:VAL:HG21	2.49	0.48
1:B:420:VAL:CG1	1:B:421:ILE:N	2.76	0.48
1:B:140:ALA:HB1	1:B:164:LEU:CD1	2.44	0.48
1:B:656:ARG:HG2	1:B:656:ARG:HH11	1.79	0.48
1:A:230:THR:HA	1:A:233:TYR:CD2	2.48	0.47
1:A:420:VAL:HG23	1:A:552:LEU:HB3	1.95	0.47
1:A:460:LEU:HD11	1:A:471:ILE:HA	1.94	0.47
1:A:60:LYS:H	3:X:13:DC:H3'	1.79	0.47
1:B:639:ARG:HH22	1:B:730:GLU:HB3	1.78	0.47
1:B:389:HIS:HB2	1:B:594:ILE:HG22	1.96	0.47
1:B:429:PHE:O	1:B:431:PRO:HD3	2.14	0.47
1:A:73:SER:OG	1:A:76:VAL:HG12	2.14	0.47
1:A:191:VAL:HG11	1:A:238:GLU:OE2	2.13	0.47
1:A:421:ILE:HG12	1:A:550:VAL:HG11	1.97	0.47
1:A:624:ARG:NH1	1:A:630:PRO:O	2.47	0.47
1:A:240:VAL:HG21	1:A:315:VAL:HB	1.95	0.47
1:B:645:ASN:ND2	1:B:686:TRP:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:HD11	1:B:340:ALA:CB	2.44	0.47
1:B:460:LEU:HD11	1:B:471:ILE:HG13	1.97	0.47
1:B:605:LEU:HD12	1:B:605:LEU:C	2.27	0.47
2:W:4:DC:H2''	2:W:5:DA:O5'	2.14	0.47
3:X:2:DG:H2'	3:X:3:DT:C6	2.50	0.47
1:B:128:LEU:HD13	1:B:128:LEU:O	2.15	0.47
1:B:426:ARG:HG2	6:B:807:SO4:O3	2.15	0.47
1:B:724:LEU:HD21	1:B:726:VAL:HG23	1.96	0.47
1:B:33:ARG:NH2	1:B:64:GLU:OE1	2.48	0.47
1:B:450:TYR:CE2	1:B:563:PHE:HD1	2.32	0.47
1:B:406:LEU:HD13	1:B:594:ILE:HD11	1.95	0.47
1:B:465:CYS:SG	1:B:467:SER:OG	2.72	0.47
1:B:628:GLN:O	1:B:629:LEU:HD23	2.16	0.46
3:Z:8:DG:H2'	3:Z:9:DT:C5	2.50	0.46
1:A:190:SER:N	1:A:269:ASN:OD1	2.44	0.46
1:A:257:THR:O	1:A:258:PRO:C	2.54	0.46
1:A:273:GLU:OE2	1:A:290:LYS:HD2	2.14	0.46
1:A:558:VAL:HG12	1:A:573:PHE:CE1	2.50	0.46
1:B:103:LEU:CD1	1:B:285:LEU:HG	2.45	0.46
1:B:151:ARG:HH21	1:B:161:GLU:CD	2.19	0.46
1:B:85:GLU:HG3	1:B:701:GLN:NE2	2.30	0.46
1:A:627:MET:HB2	1:A:629:LEU:HD12	1.97	0.46
1:B:118:PHE:HE1	1:B:174:GLU:HB3	1.81	0.46
1:A:560:GLY:O	1:A:564:SER:HB2	2.16	0.46
1:A:627:MET:HB2	1:A:629:LEU:CD1	2.46	0.46
1:A:422:LEU:HD13	1:A:556:LEU:HD11	1.98	0.46
1:B:182:LEU:H	1:B:182:LEU:CD2	2.29	0.46
1:A:32:VAL:HG12	1:A:65:ALA:HA	1.97	0.46
1:A:56:LEU:HD23	1:A:59:LEU:CD1	2.46	0.46
1:A:292:LYS:HB2	1:A:309:PRO:HB2	1.98	0.46
1:B:583:ARG:NH2	6:B:805:SO4:O4	2.49	0.46
1:A:276:HIS:O	1:A:279:LEU:HD12	2.16	0.45
1:A:388:GLN:HA	1:A:593:VAL:O	2.16	0.45
1:B:691:LEU:HD12	1:B:692:LEU:H	1.81	0.45
1:B:116:TYR:CB	1:B:150:TRP:HA	2.46	0.45
1:B:673:GLY:HA3	1:B:690:ILE:HG22	1.98	0.45
1:B:714:LEU:C	1:B:716:GLU:H	2.19	0.45
1:A:12:LEU:O	1:A:14:ARG:N	2.45	0.45
1:A:101:VAL:HA	1:A:104:ARG:HG3	1.99	0.45
1:A:327:LYS:NZ	1:A:333:ARG:O	2.47	0.45
1:B:463:HIS:HA	1:B:675:VAL:HG21	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ALA:HB1	1:B:332:TRP:HZ2	1.81	0.45
1:A:406:LEU:O	1:A:410:MET:N	2.49	0.45
1:A:434:LEU:HD23	1:A:441:ILE:HG13	1.99	0.45
1:B:293:ASN:ND2	1:B:295:GLU:CB	2.79	0.45
1:A:361:GLU:HA	1:A:631:PRO:HG3	1.99	0.45
1:A:621:LEU:HD23	1:A:621:LEU:HA	1.86	0.45
1:A:362:THR:HA	1:A:371:TYR:HE2	1.82	0.45
1:B:86:TYR:CE1	1:B:726:VAL:HG11	2.52	0.45
1:B:272:VAL:CG1	1:B:298:ILE:HG12	2.47	0.45
1:A:420:VAL:HG13	1:A:534:ILE:HG23	1.99	0.44
1:B:436:HIS:O	1:B:436:HIS:ND1	2.50	0.44
1:A:288:TRP:CE2	1:A:309:PRO:HG3	2.52	0.44
1:A:422:LEU:HD22	1:A:554:SER:HB2	1.98	0.44
1:A:434:LEU:HD22	1:A:435:CYS:N	2.32	0.44
1:A:502:PRO:C	1:A:504:VAL:H	2.20	0.44
1:B:273:GLU:OE2	1:B:290:LYS:HD2	2.17	0.44
1:A:461:ARG:NH2	1:A:676:PRO:HG3	2.33	0.44
1:A:132:LYS:HA	1:A:138:GLN:OE1	2.17	0.44
1:A:549:ASP:OD1	1:A:549:ASP:N	2.50	0.44
1:B:293:ASN:ND2	1:B:295:GLU:HB2	2.33	0.44
1:B:647:GLN:NE2	1:B:716:GLU:OE2	2.23	0.44
1:A:729:ILE:HD13	1:A:729:ILE:HA	1.78	0.44
1:B:116:TYR:O	1:B:175:LEU:HD23	2.17	0.44
1:A:558:VAL:HG12	1:A:573:PHE:CZ	2.53	0.44
1:A:321:GLU:HG3	1:A:355:SER:HB2	1.99	0.43
1:A:365:ASN:HB2	1:A:371:TYR:CE2	2.53	0.43
1:B:699:ARG:O	1:B:702:HIS:N	2.51	0.43
1:A:231:GLU:OE2	1:A:263:ARG:NH2	2.51	0.43
1:A:672:LEU:HD13	1:A:691:LEU:HD23	1.99	0.43
1:A:42:ILE:HD12	1:A:66:LEU:HD11	2.00	0.43
1:A:38:LYS:HZ2	2:W:5:DA:H4'	1.81	0.43
1:B:583:ARG:NH2	6:B:805:SO4:O3	2.42	0.43
1:B:656:ARG:NH1	1:B:656:ARG:HG2	2.34	0.43
1:B:687:ARG:NH1	6:B:804:SO4:O4	2.50	0.43
4:Y:4:DC:H2''	4:Y:5:DA:H8	1.84	0.43
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.83	0.43
1:B:433:LEU:HD22	1:B:453:LEU:CD1	2.49	0.43
1:A:4:ALA:HA	1:A:48:VAL:HG23	2.00	0.43
1:B:558:VAL:HG12	1:B:562:LEU:CD1	2.47	0.43
1:B:635:HIS:CG	1:B:691:LEU:HD11	2.54	0.43
1:B:250:MET:HE3	1:B:250:MET:HB3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:OG	1:A:53:GLU:N	2.51	0.42
1:A:672:LEU:HD12	1:A:672:LEU:H	1.84	0.42
1:B:88:HIS:CE1	1:B:704:VAL:HG13	2.54	0.42
1:B:450:TYR:CD2	1:B:563:PHE:HA	2.53	0.42
1:B:463:HIS:CE1	1:B:689:GLN:OE1	2.72	0.42
1:A:638:ILE:HB	1:A:690:ILE:HG23	2.00	0.42
1:B:115:TRP:HB2	1:B:176:ALA:O	2.19	0.42
1:B:432:ALA:O	1:B:486:VAL:HG22	2.20	0.42
1:A:53:GLU:OE2	1:A:53:GLU:HA	2.18	0.42
1:A:370:LYS:NZ	6:A:809:SO4:O2	2.50	0.42
1:A:306:LEU:HD11	1:A:340:ALA:HA	2.01	0.42
1:A:86:TYR:OH	1:A:727:ASP:OD2	2.37	0.42
1:A:185:TRP:HB3	1:A:271:PRO:HD3	2.02	0.42
1:B:625:GLN:HB2	1:B:632:TRP:CE2	2.55	0.42
1:B:233:TYR:O	1:B:237:LEU:HB2	2.19	0.42
1:B:269:ASN:OD1	1:B:269:ASN:N	2.50	0.42
1:B:658:LEU:HD12	1:B:658:LEU:HA	1.78	0.42
1:A:655:LEU:HD23	1:A:659:LEU:HG	2.01	0.42
1:B:229:LYS:H	1:B:229:LYS:HG2	1.68	0.42
1:B:433:LEU:HD22	1:B:453:LEU:HD12	2.01	0.42
4:Y:4:DC:H2"	4:Y:5:DA:C8	2.54	0.42
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.83	0.42
1:B:288:TRP:NE1	1:B:309:PRO:HD3	2.34	0.42
1:B:337:ARG:HH12	1:B:361:GLU:HG3	1.85	0.42
1:B:349:ILE:HG21	1:B:349:ILE:HD13	1.82	0.42
1:B:541:LEU:HB2	1:B:579:GLN:HE22	1.85	0.42
1:B:653:GLN:O	1:B:656:ARG:HB3	2.20	0.42
1:B:201:GLU:O	1:B:204:THR:OG1	2.37	0.42
1:B:635:HIS:CE1	1:B:691:LEU:HD21	2.55	0.42
1:A:167:LEU:HD22	1:A:172:LEU:HD12	2.02	0.42
1:A:411:ARG:O	1:A:415:GLN:N	2.52	0.42
1:B:230:THR:O	1:B:234:LEU:HD12	2.20	0.42
1:A:318:ILE:HD11	1:A:353:LEU:CD1	2.49	0.41
1:B:413:HIS:CE1	1:B:552:LEU:HB2	2.55	0.41
1:B:438:CYS:HB3	1:B:478:CYS:SG	2.60	0.41
1:A:136:LYS:HA	1:A:139:GLN:HG2	2.01	0.41
1:A:257:THR:HG22	1:A:259:GLN:H	1.83	0.41
1:B:666:ASP:OD1	1:B:667:GLU:N	2.52	0.41
1:A:186:ARG:HH22	1:A:294:GLY:C	2.23	0.41
1:B:364:HIS:ND1	1:B:631:PRO:HB2	2.35	0.41
1:A:648:ALA:HA	1:A:720:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:MET:HG3	1:B:318:ILE:HG12	2.02	0.41
1:A:257:THR:C	1:A:259:GLN:N	2.71	0.41
1:A:634:SER:O	1:A:693:GLN:HA	2.20	0.41
1:B:567:PHE:HZ	1:B:630:PRO:HG2	1.86	0.41
1:B:642:ASP:OD1	1:B:686:TRP:HB2	2.20	0.41
1:A:451:TYR:HB3	1:A:460:LEU:HD23	2.01	0.41
1:A:469:ARG:HD3	1:A:469:ARG:HA	1.88	0.41
1:A:656:ARG:O	1:A:660:GLN:HG3	2.20	0.41
1:B:34:VAL:HB	1:B:35:PRO:HD2	2.02	0.41
1:B:161:GLU:HA	1:B:164:LEU:HB3	2.01	0.41
1:B:388:GLN:HA	1:B:593:VAL:O	2.21	0.41
1:A:30:CYS:O	1:A:45:VAL:HG12	2.20	0.41
1:A:542:ALA:HB3	1:A:545:HIS:HB3	2.02	0.41
1:A:553:VAL:HG23	1:A:593:VAL:HG12	2.03	0.41
1:B:716:GLU:C	1:B:718:ARG:H	2.23	0.41
1:A:102:MET:HE3	1:A:107:LYS:HD2	2.03	0.41
1:A:131:LEU:CD1	1:A:134:SER:OG	2.68	0.41
1:A:260:THR:O	1:A:264:PHE:HD1	2.04	0.41
1:B:347:GLU:HB2	1:B:349:ILE:CG2	2.51	0.41
1:B:421:ILE:HD13	1:B:421:ILE:HG21	1.85	0.41
1:A:625:GLN:HB2	1:A:632:TRP:CE2	2.56	0.41
1:B:10:VAL:HA	1:B:11:PRO:HD3	1.87	0.41
1:B:464:HIS:CE1	1:B:672:LEU:HD21	2.56	0.41
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.94	0.40
1:A:424:LEU:HD23	1:A:556:LEU:HB2	2.03	0.40
1:A:19:LEU:HD11	1:A:59:LEU:HB2	2.02	0.40
1:A:667:GLU:OE1	1:A:667:GLU:HA	2.22	0.40
4:Y:3:DG:H2''	4:Y:4:DC:OP1	2.20	0.40
1:A:229:LYS:HB2	1:A:229:LYS:HE2	1.92	0.40
1:A:316:ILE:HG13	1:A:351:ILE:HD13	2.03	0.40
1:A:542:ALA:HB3	1:A:545:HIS:CB	2.51	0.40
1:B:33:ARG:HG3	1:B:42:ILE:HD13	2.04	0.40
1:A:5:HIS:HB3	1:A:15:THR:HG21	2.03	0.40
1:A:251:VAL:HB	1:A:252:PRO:CD	2.52	0.40
1:A:265:ARG:HE	1:A:272:VAL:CG2	2.35	0.40
1:A:414:LEU:CD2	1:A:532:ALA:HB1	2.52	0.40
1:B:288:TRP:CE2	1:B:309:PRO:HG3	2.56	0.40
1:A:421:ILE:HA	1:A:535:LEU:O	2.22	0.40
1:B:341:VAL:HG22	1:B:351:ILE:HD13	2.04	0.40
1:B:489:GLY:O	1:B:493:LEU:HB2	2.22	0.40
1:B:546:HIS:CD2	1:B:583:ARG:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:GLU:HA	1:B:686:TRP:O	2.21	0.40

All (1) 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:A:24:MET:CE	1:A:446:ARG:O[4_565]	2.15	0.05

## 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	698/751 (93%)	655 (94%)	42 (6%)	1 (0%)	51 80
1	B	693/751 (92%)	646 (93%)	47 (7%)	0	100 100
All	All	1391/1502 (93%)	1301 (94%)	89 (6%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ARG

### 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	550/617 (89%)	536 (98%)	14 (2%)	47 78
1	B	508/617 (82%)	492 (97%)	16 (3%)	40 72
All	All	1058/1234 (86%)	1028 (97%)	30 (3%)	43 76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	136	LYS
1	A	177	CYS
1	A	189	TYR
1	A	248	LEU
1	A	267	ARG
1	A	411	ARG
1	A	438	CYS
1	A	451	TYR
1	A	454	HIS
1	A	478	CYS
1	A	549	ASP
1	A	606	GLN
1	A	693	GLN
1	B	72	PHE
1	B	107	LYS
1	B	118	PHE
1	B	151	ARG
1	B	189	TYR
1	B	235	SER
1	B	250	MET
1	B	333	ARG
1	B	403	SER
1	B	408	SER
1	B	434	LEU
1	B	438	CYS
1	B	477	SER
1	B	583	ARG
1	B	605	LEU
1	B	699	ARG

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	139	GLN
1	A	146	GLN
1	A	365	ASN
1	A	619	GLN
1	B	399	GLN
1	B	412	GLN
1	B	463	HIS
1	B	602	HIS

### 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 monosaccharides in this entry.

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

Of 17 ligands modelled in this entry, 4 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	B	803	-	4,4,4	0.14	0	6,6,6	0.12	0
6	SO4	A	807	-	4,4,4	0.15	0	6,6,6	0.08	0
6	SO4	A	808	-	4,4,4	0.17	0	6,6,6	0.19	0
6	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.12	0
6	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.08	0
6	SO4	B	804	-	4,4,4	0.15	0	6,6,6	0.05	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	810	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.16	0
6	SO4	B	807	-	4,4,4	0.13	0	6,6,6	0.16	0
6	SO4	A	804	-	4,4,4	0.13	0	6,6,6	0.19	0
6	SO4	A	803	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	A	806	-	4,4,4	0.13	0	6,6,6	0.11	0
6	SO4	A	809	-	4,4,4	0.14	0	6,6,6	0.06	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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	SO4	1	0
6	B	805	SO4	3	0
6	B	804	SO4	1	0
6	B	807	SO4	1	0
6	A	809	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, 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	704/751 (93%)	0.29	14 (1%) 65 56	76, 115, 159, 175	0
1	B	701/751 (93%)	0.44	51 (7%) 15 8	79, 123, 181, 233	0
2	W	12/12 (100%)	1.91	6 (50%) 0 0	159, 197, 248, 251	0
3	X	12/12 (100%)	1.50	6 (50%) 0 0	116, 217, 234, 237	0
3	Z	12/12 (100%)	2.20	7 (58%) 0 0	126, 222, 238, 239	0
4	Y	13/13 (100%)	2.63	7 (53%) 0 0	199, 220, 247, 250	0
All	All	1454/1551 (93%)	0.42	91 (6%) 20 12	76, 120, 182, 251	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	588	GLY	8.8
3	Z	2	DG	6.6
1	B	130	GLY	6.4
2	W	10	DG	6.0
4	Y	12	DC	5.5
1	B	149	ILE	5.2
3	Z	5	DG	4.7
4	Y	11	DA	4.6
3	X	2	DG	4.5
4	Y	1	DG	4.3
1	A	192	ALA	4.3
4	Y	13	DT	4.3
1	B	153	GLN	4.3
1	A	128	LEU	4.2
3	Z	3	DT	4.2
3	X	3	DT	4.1
2	W	11	DA	4.1
1	B	587	ALA	3.9
1	B	156	GLU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	Y	10	DG	3.8
3	Z	4	DC	3.7
1	B	174	GLU	3.6
1	B	150	TRP	3.6
1	B	23	GLY	3.4
1	B	717	ALA	3.4
1	B	175	LEU	3.4
1	B	106	GLY	3.4
1	A	552	LEU	3.4
1	B	159	PHE	3.4
1	B	19	LEU	3.3
1	B	720	VAL	3.3
2	W	13	DT	3.2
1	B	155	GLY	3.2
3	Z	6	DG	3.2
2	W	9	DC	3.2
1	B	179	ALA	3.2
1	B	552	LEU	3.1
1	B	142	ALA	3.1
2	W	12	DC	3.0
1	B	680	PRO	3.0
1	B	273	GLU	3.0
1	B	143	ALA	3.0
1	B	212	ALA	3.0
1	A	453	LEU	3.0
1	B	119	ALA	3.0
4	Y	5	DA	3.0
1	B	129	ASN	2.9
1	B	664	LEU	2.9
1	B	154	VAL	2.9
3	X	7	DC	2.8
1	B	157	LEU	2.8
1	A	173	ALA	2.7
1	A	131	LEU	2.7
1	B	146	GLN	2.6
3	X	6	DG	2.6
1	A	481	THR	2.6
1	A	509	ILE	2.6
1	B	248	LEU	2.6
1	B	547	PHE	2.5
4	Y	6	DC	2.5
1	B	140	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	2.5
1	B	161	GLU	2.5
1	B	158	GLU	2.4
1	B	219	TRP	2.4
1	B	531	GLY	2.4
1	B	374	LEU	2.4
1	A	482	HIS	2.4
3	X	8	DG	2.3
1	B	189	TYR	2.3
1	A	487	GLY	2.3
1	B	115	TRP	2.3
1	B	294	GLY	2.3
3	Z	7	DC	2.3
1	A	149	ILE	2.3
1	A	48	VAL	2.3
1	B	534	ILE	2.2
1	B	300	ILE	2.2
1	B	203	ALA	2.2
1	B	172	LEU	2.2
3	Z	8	DG	2.1
1	A	412	GLN	2.1
3	X	5	DG	2.1
1	B	352	ILE	2.1
1	B	151	ARG	2.1
1	B	453	LEU	2.1
1	A	489	GLY	2.1
1	B	259	GLN	2.1
1	B	56	LEU	2.1
2	W	8	DC	2.1
1	B	176	ALA	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	A	809	5/5	0.62	0.47	192,215,220,285	0
6	SO4	B	804	5/5	0.66	0.20	177,183,201,212	0
6	SO4	A	805	5/5	0.70	0.18	152,154,169,170	0
6	SO4	A	810	5/5	0.75	0.29	138,163,201,215	0
6	SO4	A	804	5/5	0.81	0.20	127,129,144,157	0
6	SO4	B	805	5/5	0.84	0.19	162,163,180,183	0
6	SO4	A	806	5/5	0.85	0.28	123,128,144,163	5
6	SO4	B	803	5/5	0.87	0.21	133,140,150,158	5
5	ZN	B	801	1/1	0.92	0.20	134,134,134,134	0
6	SO4	B	806	5/5	0.93	0.12	122,126,135,155	0
6	SO4	A	808	5/5	0.95	0.22	73,100,133,150	0
6	SO4	A	803	5/5	0.96	0.15	141,143,154,161	0
5	ZN	A	802	1/1	0.97	0.16	155,155,155,155	0
6	SO4	B	807	5/5	0.97	0.19	98,119,142,150	0
5	ZN	B	802	1/1	0.98	0.22	99,99,99,99	0
6	SO4	A	807	5/5	0.98	0.10	111,119,125,153	0
5	ZN	A	801	1/1	0.99	0.23	126,126,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.