



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:28 am GMT

PDB ID : 4NH0  
Title : Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC  
Authors : Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.  
Deposited on : 2013-11-03  
Resolution : 2.90 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 : trunk28620  
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) : recalc28949

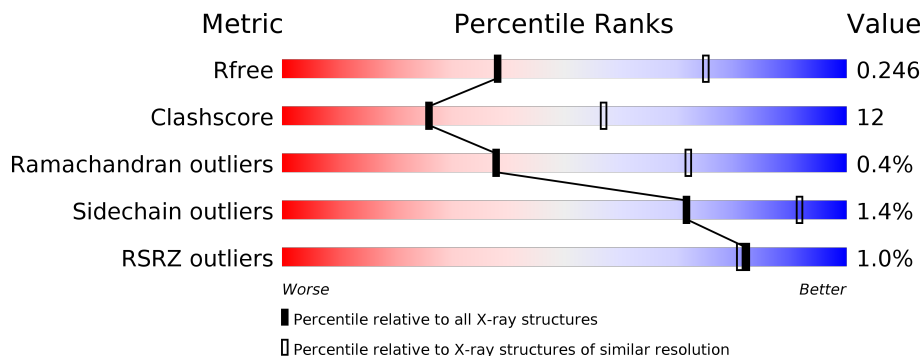
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	1147	
1	B	1147	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	0	0
			6663	4212	1181	1249	21			
1	B	859	Total	C	N	O	S	0	0	0
			6626	4186	1175	1244	21			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	EXPRESSION TAG	UNP D1A4G7
A	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	180	SER	-	EXPRESSION TAG	UNP D1A4G7
A	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	183	SER	-	EXPRESSION TAG	UNP D1A4G7
A	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
A	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
A	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	188	SER	-	EXPRESSION TAG	UNP D1A4G7
A	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
A	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	193	PHE	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
A	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	197	SER	-	EXPRESSION TAG	UNP D1A4G7
A	198	SER	-	EXPRESSION TAG	UNP D1A4G7
A	199	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	169	MET	-	EXPRESSION TAG	UNP D1A4G7
B	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	180	SER	-	EXPRESSION TAG	UNP D1A4G7
B	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	183	SER	-	EXPRESSION TAG	UNP D1A4G7
B	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
B	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
B	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	188	SER	-	EXPRESSION TAG	UNP D1A4G7
B	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
B	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	193	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
B	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	197	SER	-	EXPRESSION TAG	UNP D1A4G7
B	198	SER	-	EXPRESSION TAG	UNP D1A4G7
B	199	PRO	-	EXPRESSION TAG	UNP D1A4G7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

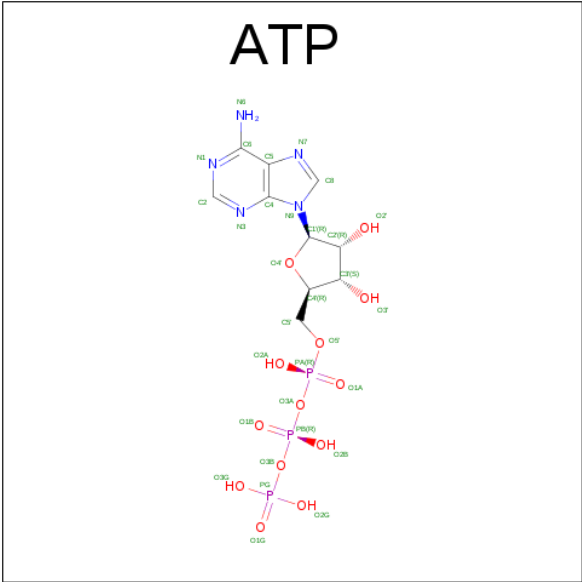


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

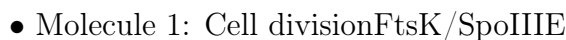
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





- Molecule 1: Cell divisionFtsK/SpoIIIE



V1176	R1177	K1180	M1183	L1187	P1188	P1189	L1192	R1200	S1201	W1202	P1227	R1236	D1237	I1238	L1242	I1243	I1244	M1248	G1275	G1294	F1298	I1308	T1310	S1315																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
Y1001	E1002	D1006	K1009	V1013	R1020	G1021	F1029	L1030	L1033	P1034	R1035	I1036	D1037	G1038	D1039	T1040	T1044	G1048	T1051	T1052	V1053	K1054	E1058	A1059	W1060	A1065	P1066	L1071	P1072	D1095	E1096	D1117	C1120	G1121	K1122	D1148	S1152	L1153	A1166	L1175																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L850	L851	H852	T853	P854	F859	D863	F864	G867	L872	L875	V878	T883	R884	R891	E905	Q906	E910	R920	R923	F933	G934	D935	D941	N942	Y950	L953	S956	R963	S975	E980	L989	E994	L995	R996	L997																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
ARG	ALA	GLU	GLU	ASN	LYS	SER	SER	E741	S742	L743	F744	D745	V746	V747	P756	E757	P758	P764	P765	L766	P769	L772	S782	A783	G796	R797	L798	H799	L804	V805	D806	R807	P808	F809	D810	Q811	R812	R813	D819	G822	G823	A824	G828	G832	P833	Q834	K837																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S655	R656	R657	V658	L659	G660	V661	Y665	E666	L667	P668	Y675	R685	A679	Y690	V691	S692	G693	P694	V695	D696	E697	GLU	PRO	GLN	THR	ARG	SER	GLY	PRO	GLN	VAL	ARG	GLN	VAL	TYR	ILE	ARG	PRO	GLN	VAL	GLU	GLN	PRO	GLU	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L589	R590	H591	S592	Y595	Y596	Y597	E572	R575	N576	E577	G578	P580	L581	P585	D592	E593	F594	S595	K601	L607	R613	L614	A625	S626	Q627	R628	L629	E630	E631	G632	K633	L634	R635	G636	L637	D638	T639	H640	L641	S642	Y643	R644	L647	F650	M653	E654																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
GLU	GLU	ASP	VAL	LEU	S414	A415	K416	L419	L422	Y429	D432	P433	A434	V435	Q442	R445	L446	P449	D453	R457	D462	I463	K464	Q468	M471	G475	L476	S483	E487	T491	E503	L524	L534	V541	D542	Y545	R555																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
ASN	GLU	ALA	THR	THR	LEU	ARG	LEU	ARG	VAL	THR	GLY	ARG	VAL	TYR	VAL	VAL	LYS	ARG	ASP	GLU	VAL	VAL	ILE	SER	VAL	GLY	ARG	PRO	GLN	ALA	ALA	GLY	LEU	ALA	ARG	THR	THR	SER	ALA	ALA	ASP	GLU	PRO	PRO	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
GLU	SER	MET	LEU	MET	GLY	PRO	GLY	ASP	PHE	GLY	ALA	SER	ARG	THR	ALA	VAL	LYS	ALA	PRO	ALA	GLU	PRO	PHE	GLY	LEU	VAL	GLN	ILE	ALA	GLY	THR	ASP	GLY	ILE	ASP	ALA	ALA	GLY	VAL	CYS	VAL	ILE	ARG	LEU	LEU	THR	HIS	SER	GLY	VAL	LEU	VAL	ALA	GLU	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
LEU	ALA	ALA	ALA	HIS	HIS	GLY	HIS	PHE	ASP	VAL	ARG	ILE	ASP	GLY	GLY	SER	GLY	LEU	GLU	VAL	GLN	PRO	GLY	PRO	LEU	PRO	VAL	ALA	ILE	SER	LEU	HIS	PRO	ARG	SER	SER	GLU	TYR	ALA	ARG	ILE	LEU	PRO	ASP	GLN	ASP	GLY	VAL	GLY	VAL	ARG	PRO	LYS	VAL	VAL	THR	ALA	GLY	VAL	GLY	VAL	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.226 , 0.246 0.225 , 0.246	Depositor DCC
$R_{free}$ test set	1514 reflections (1.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: MG, SO4, ATP

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	0.25	0/6813	0.41	1/9264 (0.0%)
1	B	0.27	0/6774	0.47	2/9215 (0.0%)
All	All	0.26	0/13587	0.44	3/18479 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	807	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	579	ALA	C-N-CD	6.66	142.39	128.40
1	A	563	GLY	N-CA-C	-5.68	98.91	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6663	0	6636	118	0
1	B	6626	0	6588	196	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	314	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 12.

All (314) 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:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93
1:B:631:GLU:N	1:B:631:GLU:OE2	2.02	0.92
1:B:628:ARG:NH2	1:B:650:PHE:CG	2.38	0.91
1:B:636:GLY:O	1:B:640:HIS:HD2	1.52	0.91
1:A:1006:ASP:OD2	1:A:1009:LYS:N	2.04	0.89
1:A:442:GLN:O	1:A:464:LYS:NZ	2.07	0.86
1:B:905:GLU:OE2	1:B:963:ARG:NH1	2.08	0.86
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.38	0.85
1:A:442:GLN:HG3	1:A:445:ARG:HH12	1.42	0.82
1:A:543:ARG:NH1	1:A:806:ASP:OD2	2.13	0.81
1:B:471:MET:O	1:B:642:SER:OG	1.97	0.81
1:B:807:ARG:HG2	1:B:812:ARG:H	1.45	0.81
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ARG:HH21	1:B:650:PHE:CB	1.95	0.79
1:A:832:GLY:O	1:A:835:THR:OG1	1.99	0.79
1:A:1006:ASP:HB3	1:A:1009:LYS:HG3	1.65	0.79
1:B:561:HIS:CD2	1:B:562:SER:H	2.01	0.78
1:B:636:GLY:O	1:B:640:HIS:CD2	2.35	0.78
1:A:1006:ASP:CB	1:A:1009:LYS:HG3	2.14	0.78
1:B:644:ARG:HG3	1:B:644:ARG:NH1	1.98	0.78
1:B:807:ARG:NE	1:B:811:GLN:H	1.82	0.78
1:B:813:ARG:HG2	1:B:813:ARG:HH11	1.49	0.77
1:B:572:GLU:OE2	1:B:575:ARG:HG2	1.85	0.77
1:A:542:ASP:OD2	1:A:601:LYS:NZ	2.17	0.76
1:B:743:LEU:HD13	1:B:744:PHE:H	1.50	0.75
1:B:629:LEU:HD22	1:B:630:GLU:H	1.52	0.74
1:B:630:GLU:HG2	1:B:633:LYS:HG2	1.69	0.74
1:B:629:LEU:CD2	1:B:630:GLU:H	2.01	0.73
1:B:807:ARG:HE	1:B:811:GLN:H	1.35	0.73
1:A:555:ARG:NH2	1:A:585:PRO:O	2.21	0.73
1:B:629:LEU:HD23	1:B:633:LYS:HG3	1.71	0.73
1:B:575:ARG:HH11	1:B:575:ARG:HG2	1.52	0.72
1:B:837:LYS:NZ	4:B:1405:ATP:O2B	2.20	0.72
1:B:891:ARG:NH1	1:B:1096:GLU:OE2	2.24	0.71
1:B:629:LEU:CD2	1:B:633:LYS:CG	2.68	0.71
1:B:637:LEU:O	1:B:641:LEU:HG	1.90	0.71
1:B:743:LEU:HD13	1:B:744:PHE:N	2.05	0.71
1:B:629:LEU:HD11	1:B:634:LEU:HD21	1.71	0.71
1:B:691:VAL:HG23	1:B:692:SER:H	1.55	0.69
1:B:1033:LEU:O	1:B:1035:ARG:N	2.26	0.69
1:B:629:LEU:CD2	1:B:633:LYS:CB	2.58	0.68
1:B:807:ARG:HD2	1:B:807:ARG:C	2.14	0.68
1:B:807:ARG:HD2	1:B:808:PRO:N	2.08	0.68
1:B:464:LYS:NZ	1:B:468:GLN:O	2.27	0.68
1:A:1001:TYR:HD1	1:A:1002:GLU:H	1.39	0.68
1:B:807:ARG:HE	1:B:810:ASP:N	1.93	0.67
1:A:904:ARG:NE	1:A:931:ASP:OD2	2.23	0.67
1:B:692:SER:OG	1:B:693:GLY:N	2.26	0.66
1:B:1200:ARG:HH21	1:B:1236:ARG:HG2	1.60	0.66
1:B:487:GLU:OE2	1:B:692:SER:N	2.29	0.66
1:B:432:ASP:HB3	1:B:435:VAL:HG22	1.78	0.65
1:B:655:SER:OG	1:B:661:VAL:O	2.14	0.65
1:B:804:LEU:HD11	1:B:813:ARG:HB3	1.78	0.65
1:A:432:ASP:HB3	1:A:435:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:SER:OG	1:A:980:GLU:OE1	2.16	0.64
1:B:975:SER:OG	1:B:980:GLU:OE1	2.15	0.64
1:B:629:LEU:CD2	1:B:633:LYS:HG3	2.28	0.64
1:A:573:LYS:O	1:A:577:GLU:N	2.30	0.63
1:B:766:LEU:H	1:B:813:ARG:HH22	1.47	0.63
1:A:658:VAL:HG23	1:A:659:LEU:HG	1.81	0.62
1:A:681:GLU:N	1:A:681:GLU:OE1	2.33	0.62
1:A:442:GLN:HG3	1:A:445:ARG:NH1	2.12	0.62
1:B:743:LEU:HA	1:B:746:VAL:HB	1.80	0.62
1:B:1177:ARG:HH11	1:B:1177:ARG:HG2	1.65	0.62
1:B:813:ARG:NH1	1:B:813:ARG:HG2	2.12	0.62
1:B:805:VAL:HA	1:B:1029:PHE:HA	1.82	0.62
1:A:543:ARG:NH2	1:A:763:LEU:O	2.33	0.61
1:A:1006:ASP:CG	1:A:1009:LYS:HG3	2.21	0.61
1:A:645:ILE:HG12	1:A:676:LEU:HD23	1.83	0.61
1:A:1189:PRO:HD2	1:A:1192:LEU:HD11	1.83	0.61
1:B:542:ASP:HA	1:B:545:TYR:HB3	1.82	0.61
1:A:920:ARG:NH1	1:A:935:ASP:OD2	2.34	0.60
1:B:1036:ILE:HG12	1:B:1052:THR:HG22	1.82	0.60
1:B:628:ARG:NH2	1:B:650:PHE:CD2	2.68	0.60
1:B:1020:ARG:CG	1:B:1030:LEU:HA	2.32	0.60
1:B:810:ASP:HB3	1:B:812:ARG:NH1	2.17	0.60
1:B:644:ARG:CG	1:B:644:ARG:HH11	2.12	0.60
1:A:1006:ASP:OD2	1:A:1008:LYS:N	2.34	0.59
1:A:543:ARG:NH1	1:A:765:PRO:HA	2.18	0.59
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.34	0.59
1:B:628:ARG:NH2	1:B:650:PHE:CB	2.62	0.59
1:A:568:LEU:HD13	1:A:619:GLY:HA3	1.84	0.59
1:B:1006:ASP:OD2	1:B:1009:LYS:HG3	2.02	0.59
1:B:772:LEU:HD23	1:B:850:LEU:HD12	1.83	0.59
1:B:923:ARG:NH1	1:B:933:PHE:O	2.35	0.59
1:B:807:ARG:NE	1:B:811:GLN:N	2.49	0.59
1:B:764:PRO:O	1:B:766:LEU:N	2.36	0.59
1:B:575:ARG:CG	1:B:575:ARG:HH11	2.16	0.58
1:A:508:VAL:HG23	1:A:587:LEU:HD11	1.83	0.58
1:A:525:ARG:NH1	1:A:755:GLY:O	2.37	0.58
1:B:1037:ASP:OD1	1:B:1038:GLY:N	2.36	0.58
1:B:629:LEU:HD22	1:B:630:GLU:N	2.18	0.58
1:B:996:ARG:HD3	1:B:1013:VAL:HG22	1.85	0.58
1:A:476:LEU:HB2	1:A:641:LEU:HD13	1.86	0.58
1:B:422:LEU:HD23	1:B:449:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:VAL:HG11	1:B:601:LYS:HG3	1.86	0.57
1:A:1001:TYR:CD1	1:A:1002:GLU:N	2.69	0.57
1:B:804:LEU:O	1:B:1030:LEU:N	2.37	0.57
1:A:838:SER:OG	4:A:1405:ATP:O1B	2.23	0.57
1:A:837:LYS:O	1:A:840:MET:N	2.38	0.57
1:B:572:GLU:O	1:B:575:ARG:HB3	2.05	0.57
1:B:613:ARG:NH1	1:B:614:LEU:HD21	2.20	0.57
1:B:654:GLU:H	1:B:654:GLU:CD	2.07	0.56
1:B:859:PHE:HB2	1:B:878:VAL:HG12	1.86	0.56
1:B:810:ASP:HB3	1:B:812:ARG:HH12	1.70	0.56
1:B:1117:ASP:O	1:B:1122:LYS:HE2	2.05	0.56
1:B:1120:CYS:SG	1:B:1122:LYS:HE3	2.45	0.56
1:B:475:GLY:HA3	1:B:643:TYR:CZ	2.41	0.56
1:B:1020:ARG:HD3	1:B:1030:LEU:HA	1.88	0.56
1:B:561:HIS:HD2	1:B:562:SER:H	1.53	0.56
1:B:804:LEU:HD21	1:B:813:ARG:HD3	1.88	0.56
1:B:864:PHE:H	1:B:941:ASP:HB3	1.71	0.55
1:A:1035:ARG:HH12	1:A:1044:THR:HG23	1.71	0.55
1:A:462:ASP:OD2	1:A:464:LYS:HE2	2.07	0.55
1:B:442:GLN:HA	1:B:445:ARG:NH1	2.22	0.55
1:B:1117:ASP:O	1:B:1122:LYS:CE	2.54	0.55
1:B:757:GLU:HG2	1:B:758:PRO:HD2	1.90	0.54
1:A:573:LYS:O	1:A:577:GLU:HB2	2.07	0.54
1:B:822:GLY:O	1:B:824:ALA:N	2.38	0.54
1:B:483:SER:HB2	1:B:647:LEU:HB3	1.88	0.54
1:B:1054:LYS:NZ	1:B:1058:GLU:OE2	2.38	0.54
1:B:628:ARG:HH21	1:B:650:PHE:HB3	1.71	0.54
1:A:1134:ILE:HG12	1:A:1159:THR:HG21	1.90	0.54
1:B:432:ASP:OD1	1:B:434:ALA:N	2.41	0.53
1:B:631:GLU:HA	1:B:657:VAL:HG21	1.89	0.53
1:A:1126:LEU:HD21	1:A:1245:ALA:HB2	1.90	0.53
1:A:807:ARG:HD3	1:A:1027:TYR:CE2	2.43	0.53
1:B:807:ARG:HE	1:B:809:PHE:C	2.12	0.53
1:A:1144:LEU:HD23	1:A:1209:PHE:HB2	1.90	0.53
1:A:1277:LYS:H	1:A:1277:LYS:HD2	1.73	0.53
1:B:631:GLU:OE1	1:B:653:MET:SD	2.67	0.53
1:B:561:HIS:O	1:B:562:SER:OG	2.26	0.53
1:B:593:GLU:OE2	1:B:627:GLN:CG	2.57	0.53
1:B:643:TYR:C	1:B:644:ARG:HD3	2.29	0.52
1:B:693:GLY:O	1:B:743:LEU:HD12	2.09	0.52
1:A:1126:LEU:HD12	1:A:1211:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:TYR:HD1	1:B:692:SER:HB3	1.73	0.52
1:B:561:HIS:CD2	1:B:562:SER:N	2.75	0.52
1:B:595:SER:OG	1:B:633:LYS:NZ	2.42	0.52
1:B:629:LEU:HD23	1:B:633:LYS:CG	2.36	0.52
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.43	0.52
1:B:629:LEU:HD11	1:B:634:LEU:CD2	2.40	0.52
1:A:1023:THR:HG22	1:A:1025:ASP:H	1.74	0.51
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.43	0.51
1:B:1001:TYR:CD2	1:B:1002:GLU:HG3	2.44	0.51
1:B:1071:LEU:HD12	1:B:1072:PRO:HD2	1.91	0.51
1:B:572:GLU:HA	1:B:572:GLU:OE2	2.09	0.51
1:B:593:GLU:OE2	1:B:627:GLN:HG3	2.10	0.51
1:A:1035:ARG:HA	1:A:1052:THR:HG21	1.93	0.51
1:B:1048:GLY:O	1:B:1051:THR:OG1	2.26	0.51
1:A:572:GLU:O	1:A:575:ARG:HB3	2.11	0.51
1:B:1183:MET:HB3	1:B:1238:ILE:HD12	1.93	0.51
1:A:1143:ARG:HE	1:A:1163:ILE:HD11	1.76	0.50
1:B:419:LEU:HD22	1:B:491:THR:HG23	1.93	0.50
1:A:759:HIS:NE2	1:A:811:GLN:OE1	2.42	0.50
1:B:1177:ARG:NH1	1:B:1177:ARG:HG2	2.27	0.50
1:A:558:HIS:ND1	1:A:562:SER:OG	2.44	0.50
1:A:591:LEU:HD21	1:A:597:LEU:HD13	1.93	0.50
1:A:999:ASP:OD1	1:A:1001:TYR:N	2.44	0.50
1:B:1180:LYS:HD2	1:B:1227:PRO:HB2	1.93	0.50
1:B:1242:LEU:HD23	1:B:1244:ILE:HD11	1.94	0.50
1:B:572:GLU:HA	1:B:575:ARG:HB3	1.93	0.50
1:B:828:GLY:HA3	1:B:989:LEU:HD13	1.94	0.50
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.47	0.49
1:B:807:ARG:HD3	1:B:810:ASP:H	1.76	0.49
1:A:1193:THR:HG23	1:A:1196:GLN:H	1.77	0.49
1:B:832:GLY:O	1:B:837:LYS:NZ	2.46	0.49
1:B:782:SER:OG	1:B:783:ALA:N	2.44	0.49
1:B:872:LEU:HB3	1:B:875:LEU:HD12	1.95	0.49
1:A:638:ASP:CG	1:A:644:ARG:HH22	2.16	0.49
1:B:565:TYR:CD2	1:B:571:TYR:HA	2.47	0.48
1:B:592:ASP:HA	1:B:625:ALA:HB3	1.95	0.48
1:B:654:GLU:O	1:B:658:VAL:HG13	2.13	0.48
1:B:691:VAL:O	1:B:743:LEU:HD11	2.13	0.48
1:A:866:GLY:H	1:A:884:ARG:HH22	1.60	0.48
1:B:1035:ARG:HA	1:B:1052:THR:HG21	1.96	0.48
1:A:522:GLU:HG3	1:A:530:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:GLY:HA3	1:A:989:LEU:HD13	1.94	0.48
1:B:1020:ARG:HG3	1:B:1029:PHE:O	2.12	0.48
1:A:1191:ASP:N	1:A:1191:ASP:OD1	2.42	0.48
1:B:641:LEU:HD23	1:B:641:LEU:N	2.27	0.48
1:B:1148:ASP:OD2	1:B:1153:LEU:N	2.44	0.48
1:B:807:ARG:HE	1:B:811:GLN:N	2.07	0.48
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.47	0.48
1:A:443:ARG:HA	1:A:464:LYS:HZ1	1.79	0.48
1:A:657:VAL:HG23	1:A:658:VAL:HG13	1.95	0.48
1:A:794:TRP:HA	1:A:797:ARG:HG3	1.96	0.48
1:B:690:TYR:CD1	1:B:692:SER:HB3	2.49	0.47
1:B:769:PRO:HA	1:B:1030:LEU:HD23	1.95	0.47
1:A:1095:ASP:HA	1:A:1308:ILE:HA	1.96	0.47
1:A:1151:ARG:HB3	1:A:1154:LEU:HD21	1.95	0.47
1:A:419:LEU:HD21	1:A:495:ALA:HB2	1.96	0.47
1:B:416:ASN:HB3	1:B:690:TYR:CE2	2.49	0.47
1:B:629:LEU:CD2	1:B:630:GLU:N	2.73	0.47
1:B:545:TYR:CE1	1:B:607:LEU:HB2	2.49	0.47
1:B:854:PRO:HG2	1:B:1060:TRP:CD1	2.48	0.47
1:A:1218:VAL:O	1:A:1223:ASN:ND2	2.42	0.47
1:B:807:ARG:HD2	1:B:808:PRO:CA	2.44	0.47
1:B:1248:MET:HG3	1:B:1275:GLY:HA2	1.97	0.47
1:B:631:GLU:OE1	1:B:653:MET:CG	2.62	0.47
1:B:575:ARG:NH1	1:B:575:ARG:CG	2.73	0.47
1:A:558:HIS:O	1:A:562:SER:OG	2.33	0.47
1:A:593:GLU:N	1:A:625:ALA:O	2.47	0.47
1:A:810:ASP:HB3	1:A:812:ARG:NH1	2.30	0.47
1:A:442:GLN:HA	1:A:445:ARG:NH1	2.30	0.46
1:A:1178:ASP:OD1	1:A:1178:ASP:N	2.38	0.46
1:B:675:TYR:CE1	1:B:685:ARG:HD3	2.50	0.46
1:B:807:ARG:NE	1:B:810:ASP:N	2.63	0.46
1:A:1242:LEU:HD12	1:A:1244:ILE:HD11	1.96	0.46
1:B:1187:LEU:HA	1:B:1188:PRO:HD3	1.81	0.46
1:A:1014:PRO:HG2	1:A:1020:ARG:NH1	2.31	0.46
1:B:1294:GLY:O	1:B:1310:THR:OG1	2.24	0.46
1:B:629:LEU:HD23	1:B:630:GLU:H	1.80	0.46
1:B:995:LEU:HA	1:B:1021:GLY:HA3	1.98	0.46
1:A:1277:LYS:N	1:A:1277:LYS:HD2	2.31	0.46
1:B:953:LEU:HA	1:B:956:SER:HB3	1.96	0.46
1:A:837:LYS:HB2	1:A:837:LYS:HE2	1.25	0.46
1:B:1039:ASP:OD1	1:B:1040:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:TYR:HE1	1:B:685:ARG:HD3	1.81	0.46
1:A:416:ASN:ND2	1:A:687:LYS:NZ	2.63	0.45
1:B:628:ARG:CG	1:B:629:LEU:N	2.79	0.45
1:B:696:ASP:OD1	1:B:697:GLU:N	2.49	0.45
1:A:1183:MET:HB3	1:A:1238:ILE:HD12	1.98	0.45
1:B:1122:LYS:NZ	4:B:1404:ATP:O1G	2.49	0.45
1:B:462:ASP:OD1	1:B:464:LYS:HE3	2.17	0.45
1:B:693:GLY:C	1:B:743:LEU:HD12	2.37	0.45
1:B:1020:ARG:CD	1:B:1030:LEU:HA	2.47	0.45
1:B:476:LEU:HB2	1:B:641:LEU:HD13	1.99	0.45
1:A:837:LYS:O	1:A:839:THR:N	2.49	0.45
1:B:1200:ARG:HA	1:B:1202:TRP:CZ3	2.52	0.45
1:A:1001:TYR:O	1:A:1002:GLU:HB2	2.17	0.45
1:B:1020:ARG:HD3	1:B:1030:LEU:CA	2.47	0.45
1:B:503:GLU:HB2	1:B:756:PRO:HG2	1.98	0.45
1:A:518:PHE:HB3	1:A:521:MET:HG3	1.99	0.44
1:A:693:GLY:O	1:A:743:LEU:N	2.46	0.44
1:B:1166:ALA:HB2	1:B:1175:LEU:HD12	1.98	0.44
1:B:667:LEU:HA	1:B:668:PRO:HD3	1.86	0.44
1:A:1111:HIS:ND1	1:A:1242:LEU:HB2	2.33	0.44
1:B:1188:PRO:HB3	1:B:1192:LEU:HD12	2.00	0.44
1:A:1202:TRP:CE2	1:A:1203:TRP:HD1	2.35	0.44
1:B:994:GLU:OE2	1:B:997:LEU:HD21	2.18	0.44
1:B:799:HIS:NE2	1:B:819:ASP:OD1	2.51	0.44
1:A:992:LYS:HD2	1:A:1004:GLU:HG2	1.99	0.43
1:B:883:THR:OG1	1:B:884:ARG:N	2.52	0.43
1:B:442:GLN:O	1:B:464:LYS:HE2	2.18	0.43
1:B:691:VAL:HG23	1:B:692:SER:N	2.30	0.43
1:B:542:ASP:HA	1:B:545:TYR:CB	2.47	0.43
1:B:654:GLU:O	1:B:657:VAL:HG12	2.18	0.43
1:A:443:ARG:HA	1:A:464:LYS:NZ	2.33	0.43
1:A:652:ALA:O	1:A:656:ARG:HG3	2.18	0.43
1:B:446:LEU:HD23	1:B:463:ILE:HG13	2.01	0.43
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.53	0.43
1:A:1230:GLU:HG2	1:A:1230:GLU:H	1.57	0.43
1:B:432:ASP:HB3	1:B:435:VAL:CG2	2.47	0.43
1:B:593:GLU:OE2	1:B:627:GLN:HG2	2.19	0.43
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	2.00	0.43
1:B:462:ASP:O	1:B:471:MET:HB2	2.19	0.43
1:B:864:PHE:HB2	1:B:942:ASN:HB3	2.01	0.43
1:A:1110:PRO:HG2	1:A:1111:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:THR:O	1:A:843:THR:HG23	2.18	0.43
1:B:834:GLN:HB3	4:B:1405:ATP:H5'1	2.01	0.43
1:B:632:GLY:O	1:B:633:LYS:C	2.57	0.43
1:B:741:GLU:HB2	1:B:742:SER:HB3	2.01	0.43
1:B:476:LEU:HB2	1:B:641:LEU:CD1	2.49	0.42
1:A:1148:ASP:OD2	1:A:1153:LEU:N	2.52	0.42
1:A:1302:ARG:O	1:A:1303:SER:OG	2.33	0.42
1:A:422:LEU:HD23	1:A:449:PRO:HB2	2.00	0.42
1:A:1035:ARG:NH2	1:A:1037:ASP:OD2	2.49	0.42
1:A:543:ARG:HH12	1:A:765:PRO:HA	1.84	0.42
1:B:1298:PHE:HB2	1:B:1308:ILE:HD13	2.02	0.42
1:B:1095:ASP:HA	1:B:1308:ILE:HA	2.01	0.42
1:B:453:ASP:OD1	1:B:457:ARG:N	2.52	0.42
1:B:580:PRO:C	1:B:581:LEU:HD12	2.40	0.42
1:A:906:GLN:O	1:A:910:GLU:HG3	2.19	0.42
1:A:1143:ARG:NE	1:A:1163:ILE:HD11	2.34	0.42
1:A:1223:ASN:HA	1:A:1224:PRO:HD3	1.85	0.42
1:A:884:ARG:H	1:A:884:ARG:HG2	1.61	0.42
1:A:1014:PRO:HB3	1:A:1017:ARG:HG3	2.01	0.42
1:A:471:MET:HA	1:A:678:PHE:CD1	2.55	0.42
1:A:1048:GLY:O	1:A:1052:THR:HG23	2.20	0.41
1:B:555:ARG:NH2	1:B:585:PRO:O	2.51	0.41
1:B:798:LEU:HD11	1:B:920:ARG:NH1	2.35	0.41
1:B:863:ASP:OD2	1:B:867:GLY:HA2	2.19	0.41
1:A:1148:ASP:CG	1:A:1152:SER:H	2.17	0.41
1:A:1179:ILE:O	1:A:1183:MET:HG2	2.20	0.41
1:A:1189:PRO:HA	1:A:1190:PRO:HD3	1.87	0.41
1:A:613:ARG:HE	1:A:614:LEU:CD1	2.33	0.41
1:B:743:LEU:O	1:B:747:VAL:N	2.43	0.41
1:A:949:ASP:N	1:A:949:ASP:OD1	2.54	0.41
1:A:1036:ILE:HG13	1:A:1052:THR:HG22	2.02	0.41
1:B:429:TYR:HE1	1:B:695:VAL:HG21	1.85	0.41
1:A:1187:LEU:HA	1:A:1188:PRO:HD3	1.81	0.41
1:B:630:GLU:OE2	1:B:633:LYS:NZ	2.33	0.41
1:A:484:GLY:N	2:A:1401:SO4:O4	2.54	0.41
1:A:954:GLU:O	1:A:958:THR:OG1	2.27	0.41
1:A:818:LEU:HG	1:A:991:THR:HG21	2.03	0.41
1:A:437:TRP:CZ2	1:A:751:LEU:HD12	2.56	0.41
1:A:571:TYR:CE1	1:A:581:LEU:HD13	2.56	0.41
1:B:1020:ARG:HG2	1:B:1030:LEU:HD12	2.03	0.41
1:B:629:LEU:HD22	1:B:630:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:PHE:HD2	1:A:1153:LEU:HD23	1.85	0.40
1:A:551:GLU:OE1	1:A:555:ARG:NH1	2.53	0.40
1:A:679:ALA:HB3	1:A:681:GLU:OE1	2.21	0.40
1:A:638:ASP:CG	1:A:644:ARG:NH2	2.75	0.40
1:A:864:PHE:H	1:A:941:ASP:HB3	1.86	0.40
1:B:950:TYR:HB3	1:B:953:LEU:HD13	2.03	0.40
1:A:1302:ARG:C	1:A:1304:GLY:H	2.22	0.40
1:B:1065:ALA:HA	1:B:1066:PRO:HD3	1.97	0.40
1:A:864:PHE:HB2	1:A:942:ASN:H	1.86	0.40
1:B:906:GLN:O	1:B:910:GLU:HG3	2.20	0.40

There are no symmetry-related clashes.

## 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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	51 82
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	32 68
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	38 72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO
1	B	693	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	709/953 (74%)	704 (99%)	5 (1%)	87	97
1	B	703/953 (74%)	688 (98%)	15 (2%)	59	86
All	All	1412/1906 (74%)	1392 (99%)	20 (1%)	71	91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	LYS
1	A	816	TYR
1	A	837	LYS
1	A	838	SER
1	A	1023	THR
1	B	534	LEU
1	B	560	ARG
1	B	575	ARG
1	B	576	MET
1	B	577	GLU
1	B	629	LEU
1	B	630	GLU
1	B	631	GLU
1	B	638	ASP
1	B	644	ARG
1	B	658	VAL
1	B	742	SER
1	B	743	LEU
1	B	807	ARG
1	B	1020	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS

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Mol	Chain	Res	Type
1	B	640	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z  > 2$
2	SO4	A	1401	-	4,4,4	0.13	0	6,6,6	0.06	0
4	ATP	A	1404	3	27,33,33	0.94	1 (3%)	25,52,52	1.63	2 (8%)
4	ATP	A	1405	3	27,33,33	0.95	1 (3%)	25,52,52	1.61	2 (8%)
2	SO4	B	1401	-	4,4,4	0.13	0	6,6,6	0.06	0
4	ATP	B	1404	3	27,33,33	0.95	1 (3%)	25,52,52	1.61	2 (8%)
4	ATP	B	1405	3	27,33,33	0.96	1 (3%)	25,52,52	1.65	2 (8%)

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
2	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	A	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/18/38/38	0/3/3/3
2	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	B	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1404	ATP	C5-C4	3.04	1.47	1.40
4	B	1404	ATP	C5-C4	3.06	1.47	1.40
4	A	1405	ATP	C5-C4	3.09	1.47	1.40
4	B	1405	ATP	C5-C4	3.12	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	ATP	N3-C2-N1	-5.92	123.70	128.86
4	A	1405	ATP	N3-C2-N1	-5.89	123.73	128.86
4	A	1404	ATP	N3-C2-N1	-5.81	123.80	128.86
4	B	1404	ATP	N3-C2-N1	-5.79	123.81	128.86
4	A	1404	ATP	C4-C5-N7	-2.97	106.55	109.41
4	B	1405	ATP	C4-C5-N7	-2.88	106.62	109.41
4	B	1404	ATP	C4-C5-N7	-2.87	106.63	109.41
4	A	1405	ATP	C4-C5-N7	-2.87	106.64	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	SO4	1	0
4	A	1405	ATP	1	0
4	B	1404	ATP	2	0
4	B	1405	ATP	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	861/1147 (75%)	-0.19	4 (0%) 90 90	44, 80, 113, 151	0
1	B	859/1147 (74%)	-0.10	13 (1%) 74 72	35, 84, 128, 161	0
All	All	1720/2294 (74%)	-0.15	17 (0%) 82 81	35, 82, 125, 161	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.8
1	B	580	PRO	3.5
1	B	634	LEU	3.2
1	B	565	TYR	2.5
1	B	560	ARG	2.2
1	A	580	PRO	2.2
1	B	1001	TYR	2.2
1	B	1059	ALA	2.2
1	A	565	TYR	2.2
1	B	524	LEU	2.1
1	A	414	SER	2.1
1	B	665	TYR	2.1
1	B	581	LEU	2.1
1	B	659	LEU	2.1
1	B	559	LEU	2.1
1	B	579	ALA	2.0
1	B	1021	GLY	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	B	1404	31/31	0.97	0.16	0.19	34,63,78,97	0
4	ATP	A	1404	31/31	0.97	0.14	0.05	61,73,96,101	0
4	ATP	A	1405	31/31	0.97	0.14	-0.69	65,92,108,113	0
4	ATP	B	1405	31/31	0.96	0.14	-0.80	69,117,135,141	0
2	SO4	B	1401	5/5	0.92	0.11	-1.04	97,105,124,150	0
2	SO4	A	1401	5/5	0.96	0.11	-1.48	72,86,91,93	0
3	MG	A	1403	1/1	0.96	0.11	-	77,77,77,77	0
3	MG	A	1402	1/1	0.97	0.05	-	82,82,82,82	0
3	MG	B	1403	1/1	0.97	0.06	-	86,86,86,86	0
3	MG	B	1402	1/1	0.97	0.11	-	59,59,59,59	0

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

There are no such residues in this entry.