



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 11:05 pm GMT

PDB ID : 2FSG  
Title : Complex SecA:ATP from Escherichia coli  
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.  
Deposited on : 2006-01-23  
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

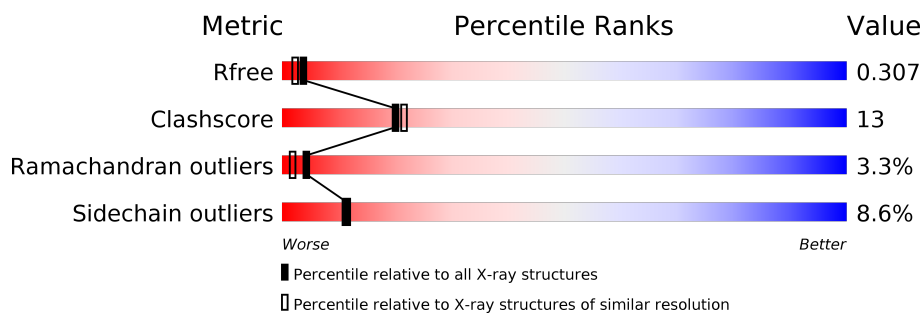
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	853	
1	B	853	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11809 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	Se	0	0	0
			5401	3392	953	1030	1	25			
1	B	743	Total	C	N	O	S	Se	0	0	0
			5915	3712	1045	1128	1	29			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	31	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	35	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	81	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	92	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	102	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	161	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	191	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	235	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	292	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	305	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	307	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	344	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	390	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	418	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	429	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	506	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	590	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	595	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	606	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	607	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	612	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	700	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	758	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	759	MSE	MET	MODIFIED RESIDUE	UNP P10408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	767	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	782	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	810	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	814	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	833	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	846	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	854	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	21	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	31	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	35	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	81	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	92	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	102	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	161	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	191	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	235	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	292	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	305	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	307	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	344	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	390	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	418	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	429	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	506	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	590	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	595	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	606	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	607	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	612	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	700	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	758	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	759	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	767	MSE	MET	MODIFIED RESIDUE	UNP P10408
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B	814	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	833	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	846	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	854	MSE	MET	MODIFIED RESIDUE	UNP P10408

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

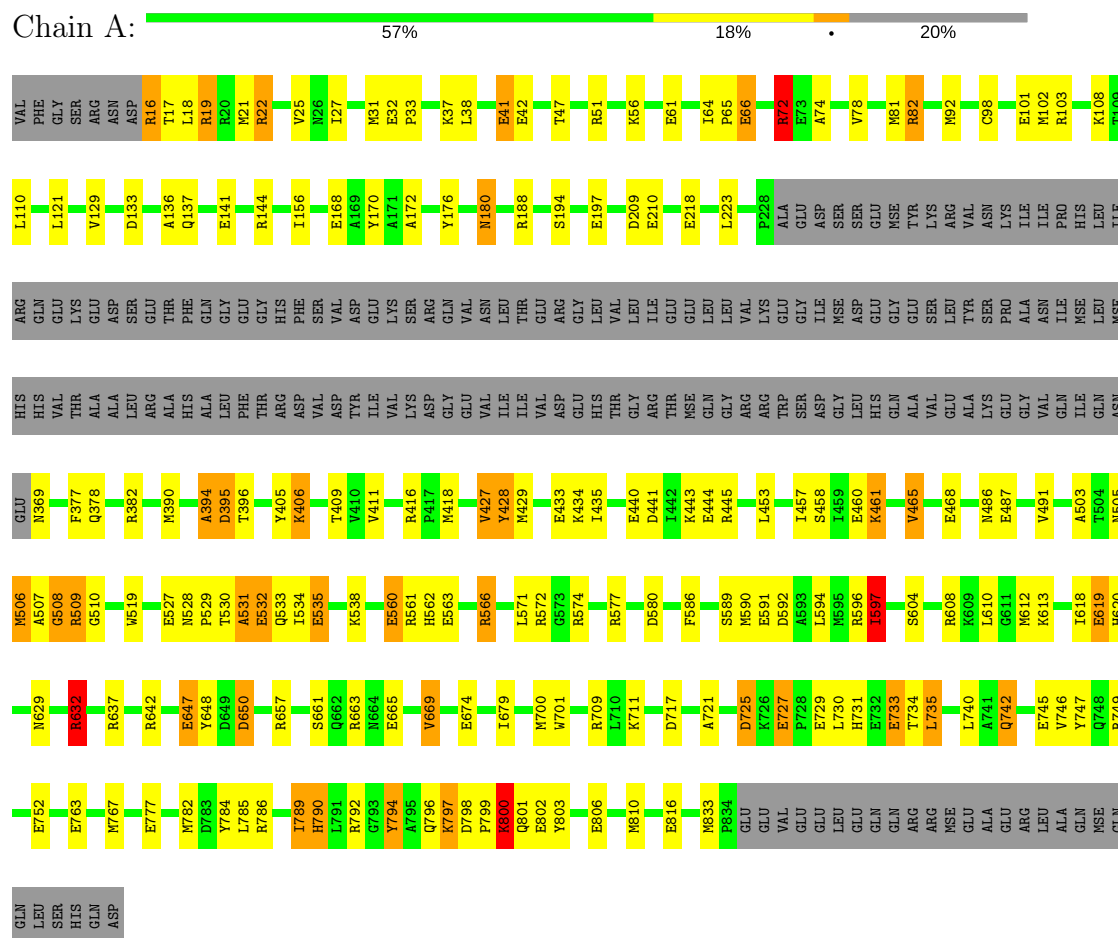
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	233	Total	O	0	0
			233	233		

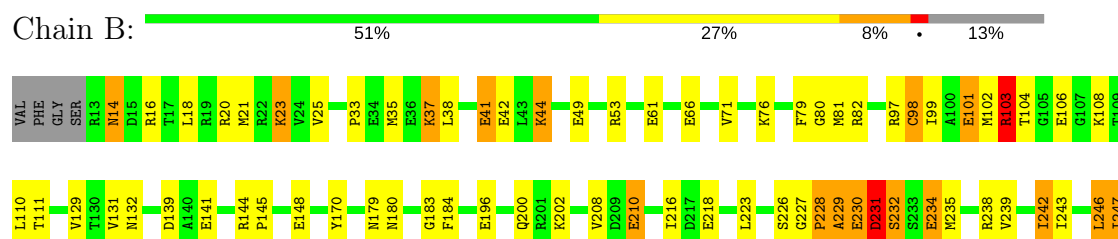
### 3 Residue-property plots

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. 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. 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: Preprotein translocase secA subunit



#### • Molecule 1: Preprotein translocase secA subunit



M810	E727	E647		K461	Q378				R248
E816	F728	Y648	S564	S462					GLN
I823	E729	V651	I567	E463	R382				GLU
L826	L730		B572	E468	E385				LYS
	H731	D654	B575	A481	A388				GLU
V829	E732	Q655	S576	P483	M390				ASP
Q830	E733	R656	B577	E487	T391				THR
R736	L734	R657	B585	V491	T393				PHE
R737	T735	Y660	B586	A492	D396				GLN
R738	R736		B587	Q493	T396				GLY
R832	E737	E665	L588	Y496	F399				GLY
M833	R738	L666	L589	P497	F401				ASP
P834	Q742	V669	M590	V500	I404				VAL
GLU	S743	D670	L594	T504	Y405				LYS
GLU	I744	S671	M595	M505	K406				ILE
VAL	E745	V672	M596	M506	L407				SER
GLU	R749	D674	S600	A507	D408				GLN
GLU	K750	E673	B601	G508	T409				VAL
GLN	V754	E674	S604	R509	V410				ASN
ARG	E757	I679	M605	G510	V411				LEU
ARG	M758	R680	M606	D512	T511				THR
MSE	H759	E681	B608	S518	R416				GLY
GLU	R760	D682	R609	M519	P417				ARG
ALA	R763	V683	L610	Q520	M413				GLY
GLU	E764	A690	M612	A521	D425				LEU
ARG	K764	Y691	M613	E522	V427				L280
LEU	L779	I692	P614	V523	M429				L281
ALA	A780	P693	A617	M528	E433				L282
GLN	A781	S696	L618	P529	K434				E283
MSE	A781	L697	B619	T530	I435				E284
GLN	M782	E698	E623	A531	Q436				L285
GLN	L785	F699	V623	E532	A437				E286
LEU	R786	M700	K625	B535	I438				K287
SER	Q787	W701	A626	K536	I439				K288
HIS	G788	D702	L627	I537	E440				E289
GLN	I789	I703	A628	K538	E444				
ASP	H790	L706	M629	A539	E445				
	L791	Q707	B632	D540	T446				
	R792	E708	B635	Q542	Q450				
	G793	K711	E636	R543	V454				A302
	Y794	N712	B637	H545	I457				Q366
	Q796	L716	E721	G553	S458				N367
	K797	D717	K723	T559	I459				E368
	D798	L718	E725	E560	E460				K305
	P799	L719	K726						L306
	K800	P719							
	Q801	I720							
	E802	A721							
	Y803	E722							
	K804	K723							
	R805	L724							
	E806	K726							
	S807								

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.38Å 89.48Å 163.35Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.61 – 2.20 19.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.61-2.20) 96.9 (19.84-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.208 , 0.270 0.262 , 0.307	Depositor DCC
$R_{free}$ test set	5245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: 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	1.52	46/5466 (0.8%)	1.22	27/7334 (0.4%)
1	B	1.59	70/5983 (1.2%)	1.22	36/8023 (0.4%)
All	All	1.55	116/11449 (1.0%)	1.22	63/15357 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	7
All	All	0	10

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CG-CD	11.27	1.68	1.51
1	B	23	LYS	CE-NZ	11.05	1.76	1.49
1	B	385	GLU	CD-OE1	9.99	1.36	1.25
1	B	66	GLU	CD-OE2	9.65	1.36	1.25
1	B	665	GLU	CG-CD	9.55	1.66	1.51
1	B	101	GLU	CB-CG	-9.44	1.34	1.52
1	B	803	TYR	CD2-CE2	9.28	1.53	1.39
1	B	61	GLU	CG-CD	9.23	1.65	1.51
1	A	777	GLU	CD-OE1	9.20	1.35	1.25
1	B	98	CYS	CB-SG	-9.08	1.66	1.82
1	B	405	TYR	CD1-CE1	9.02	1.52	1.39
1	B	61	GLU	CD-OE1	8.31	1.34	1.25
1	B	406	LYS	CE-NZ	8.24	1.69	1.49
1	B	385	GLU	CB-CG	7.74	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	GLU	CG-CD	7.63	1.63	1.51
1	A	802	GLU	CB-CG	7.46	1.66	1.52
1	B	626	ALA	CA-CB	-7.46	1.36	1.52
1	B	44	LYS	CE-NZ	7.37	1.67	1.49
1	A	141	GLU	CG-CD	7.33	1.62	1.51
1	B	41	GLU	CG-CD	7.30	1.62	1.51
1	B	648	TYR	CD2-CE2	7.29	1.50	1.39
1	B	572	ARG	CZ-NH2	-7.24	1.23	1.33
1	A	41	GLU	CB-CG	7.19	1.65	1.52
1	B	560	GLU	CG-CD	7.14	1.62	1.51
1	B	572	ARG	CB-CG	-7.06	1.33	1.52
1	B	512	ASP	CB-CG	7.05	1.66	1.51
1	B	651	VAL	CB-CG1	6.91	1.67	1.52
1	A	669	VAL	CB-CG2	-6.88	1.38	1.52
1	A	41	GLU	CG-CD	6.86	1.62	1.51
1	B	76	LYS	CE-NZ	6.86	1.66	1.49
1	A	172	ALA	CA-CB	-6.84	1.38	1.52
1	B	208	VAL	CB-CG1	-6.83	1.38	1.52
1	A	98	CYS	CB-SG	-6.76	1.70	1.82
1	A	443	LYS	CD-CE	6.60	1.67	1.51
1	A	647	GLU	CB-CG	6.58	1.64	1.52
1	B	66	GLU	CD-OE1	6.56	1.32	1.25
1	A	632	ARG	CG-CD	6.54	1.68	1.51
1	A	657	ARG	CZ-NH2	6.53	1.41	1.33
1	A	777	GLU	CG-CD	6.43	1.61	1.51
1	A	665	GLU	CD-OE2	6.37	1.32	1.25
1	A	210	GLU	CG-CD	6.33	1.61	1.51
1	B	148	GLU	CD-OE2	6.31	1.32	1.25
1	A	802	GLU	CG-CD	6.25	1.61	1.51
1	A	66	GLU	CB-CG	-6.24	1.40	1.52
1	A	180	ASN	CB-CG	-6.23	1.36	1.51
1	A	572	ARG	CB-CG	-6.23	1.35	1.52
1	B	816	GLU	CD-OE2	6.22	1.32	1.25
1	B	406	LYS	CD-CE	6.18	1.66	1.51
1	A	560	GLU	CD-OE1	6.14	1.32	1.25
1	B	625	LYS	CE-NZ	6.11	1.64	1.49
1	A	136	ALA	CA-CB	5.99	1.65	1.52
1	A	428	TYR	CE1-CZ	5.98	1.46	1.38
1	B	460	GLU	CB-CG	5.98	1.63	1.52
1	A	61	GLU	CD-OE1	5.96	1.32	1.25
1	B	681	GLU	CD-OE2	5.92	1.32	1.25
1	B	757	GLU	CD-OE1	5.89	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	VAL	CB-CG2	-5.88	1.40	1.52
1	A	740	LEU	C-O	5.88	1.34	1.23
1	B	444	GLU	CG-CD	5.86	1.60	1.51
1	A	586	PHE	CE2-CZ	5.86	1.48	1.37
1	B	141	GLU	CD-OE1	5.85	1.32	1.25
1	A	170	TYR	CE1-CZ	-5.83	1.30	1.38
1	B	444	GLU	CD-OE1	5.80	1.32	1.25
1	A	752	GLU	CB-CG	5.79	1.63	1.52
1	B	202	LYS	CD-CE	5.79	1.65	1.51
1	B	806	GLU	C-O	-5.78	1.12	1.23
1	B	763	GLU	CD-OE2	-5.78	1.19	1.25
1	A	176	TYR	CD1-CE1	5.73	1.48	1.39
1	B	44	LYS	CD-CE	5.71	1.65	1.51
1	B	587	TYR	CE2-CZ	-5.69	1.31	1.38
1	B	42	GLU	CD-OE2	-5.63	1.19	1.25
1	B	14	ASN	CB-CG	5.60	1.64	1.51
1	B	49	GLU	CD-OE1	5.59	1.31	1.25
1	A	784	TYR	CE2-CZ	5.59	1.45	1.38
1	B	25	VAL	CB-CG1	5.58	1.64	1.52
1	B	141	GLU	CG-CD	5.58	1.60	1.51
1	B	427	VAL	CB-CG2	-5.58	1.41	1.52
1	B	492	ALA	CA-CB	5.57	1.64	1.52
1	B	71	VAL	CB-CG1	-5.57	1.41	1.52
1	A	168	GLU	CB-CG	-5.55	1.41	1.52
1	B	436	GLN	CG-CD	5.55	1.63	1.51
1	A	591	GLU	CD-OE1	5.52	1.31	1.25
1	B	648	TYR	CD1-CE1	5.52	1.47	1.39
1	B	660	TYR	C-O	-5.50	1.12	1.23
1	A	752	GLU	CG-CD	5.50	1.60	1.51
1	A	560	GLU	CG-CD	5.49	1.60	1.51
1	B	468	GLU	CD-OE1	5.47	1.31	1.25
1	A	591	GLU	CG-CD	5.47	1.60	1.51
1	B	803	TYR	CZ-OH	5.45	1.47	1.37
1	A	674	GLU	CG-CD	5.43	1.60	1.51
1	B	560	GLU	CD-OE1	5.41	1.31	1.25
1	B	37	LYS	CG-CD	5.39	1.70	1.52
1	A	733	GLU	CG-CD	5.37	1.60	1.51
1	B	405	TYR	CE1-CZ	5.30	1.45	1.38
1	A	527	GLU	CG-CD	5.29	1.59	1.51
1	A	440	GLU	CG-CD	5.29	1.59	1.51
1	A	197	GLU	CD-OE2	5.26	1.31	1.25
1	B	184	PHE	CE2-CZ	5.24	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLY	C-O	-5.22	1.15	1.23
1	B	202	LYS	CE-NZ	5.22	1.62	1.49
1	B	393	THR	CA-CB	5.22	1.67	1.53
1	B	454	VAL	CB-CG2	5.22	1.63	1.52
1	A	648	TYR	CD1-CE1	5.21	1.47	1.39
1	B	388	ALA	CA-CB	5.17	1.63	1.52
1	B	106	GLU	CG-CD	5.14	1.59	1.51
1	A	444	GLU	CD-OE1	5.13	1.31	1.25
1	B	129	VAL	CB-CG1	5.12	1.63	1.52
1	B	647	GLU	CD-OE2	5.09	1.31	1.25
1	A	561	ARG	CZ-NH2	-5.09	1.26	1.33
1	B	210	GLU	CD-OE2	5.08	1.31	1.25
1	B	757	GLU	CD-OE2	5.08	1.31	1.25
1	B	218	GLU	CB-CG	5.07	1.61	1.52
1	B	408	ASP	C-O	5.05	1.32	1.23
1	A	406	LYS	CD-CE	5.02	1.63	1.51
1	A	56	LYS	CE-NZ	5.01	1.61	1.49
1	B	404	ILE	C-O	5.01	1.32	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	B	23	LYS	CD-CE-NZ	10.37	135.56	111.70
1	A	72	ARG	NE-CZ-NH2	9.47	125.03	120.30
1	B	97	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A	572	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	72	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	B	786	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	A	798	ASP	CB-CG-OD1	8.57	126.01	118.30
1	B	585	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	798	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	656	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	656	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	66	GLU	OE1-CD-OE2	7.12	131.84	123.30
1	A	663	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	637	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	801	GLN	N-CA-CB	6.64	122.55	110.60
1	A	209	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	144	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	A	784	TYR	CA-CB-CG	6.53	125.81	113.40
1	A	188	ARG	NE-CZ-NH1	6.51	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	82	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	572	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	408	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	657	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	B	53	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	209	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	144	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	654	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	654	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	B	585	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	44	LYS	CD-CE-NZ	6.01	125.53	111.70
1	B	37	LYS	CB-CG-CD	6.00	127.20	111.60
1	B	607	MSE	CG-SE-CE	5.99	112.08	98.90
1	B	139	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	572	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	784	TYR	CB-CG-CD2	5.86	124.52	121.00
1	B	749	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	577	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	784	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	20	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	465	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	B	540	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	736	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	749	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	416	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	597	ILE	CB-CA-C	-5.51	100.57	111.60
1	B	786	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	218	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	A	121	LEU	CB-CG-CD2	5.47	120.30	111.00
1	B	680	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	709	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	736	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	580	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	82	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	637	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	411	VAL	CG1-CB-CG2	-5.19	102.59	110.90
1	B	286	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	650	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	723	TRP	CA-CB-CG	5.11	123.42	113.70
1	B	425	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	B	657	ARG	CG-CD-NE	5.01	122.33	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	ALA	Peptide
1	A	796	GLN	Peptide
1	A	800	LYS	Peptide
1	B	228	PRO	Peptide
1	B	246	LEU	Peptide
1	B	394	ALA	Peptide
1	B	530	THR	Peptide
1	B	719	PRO	Peptide
1	B	730	LEU	Peptide
1	B	789	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5401	0	5406	119	0
1	B	5915	0	5921	188	0
2	A	31	0	12	0	0
2	B	31	0	12	2	0
3	A	198	0	0	15	0
3	B	233	0	0	17	0
All	All	11809	0	11351	306	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 13.

All (306) 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:44:LYS:CE	1:B:44:LYS:NZ	1.67	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LYS:NZ	1:B:406:LYS:CE	1.69	1.52
1:B:759:MSE:SE	1:B:759:MSE:CE	2.14	1.45
1:B:23:LYS:NZ	1:B:23:LYS:CE	1.76	1.45
1:A:429:MSE:SE	1:A:429:MSE:CE	2.14	1.45
1:B:235:MSE:SE	1:B:235:MSE:CE	2.15	1.45
1:B:607:MSE:SE	1:B:607:MSE:CE	2.17	1.43
1:A:21:MSE:SE	1:A:21:MSE:CE	2.16	1.42
1:A:506:MSE:SE	1:A:506:MSE:CE	2.17	1.42
1:B:35:MSE:CE	1:B:35:MSE:SE	2.16	1.42
1:A:590:MSE:CE	1:A:590:MSE:SE	2.18	1.42
1:B:418:MSE:CE	1:B:418:MSE:SE	2.16	1.42
1:B:506:MSE:CE	1:B:506:MSE:SE	2.18	1.41
1:B:612:MSE:SE	1:B:612:MSE:CE	2.18	1.41
1:A:418:MSE:SE	1:A:418:MSE:CE	2.20	1.39
1:B:700:MSE:SE	1:B:700:MSE:CE	2.22	1.38
1:A:833:MSE:SE	1:A:833:MSE:CE	2.23	1.37
1:A:700:MSE:SE	1:A:700:MSE:CE	2.22	1.36
1:A:782:MSE:CE	1:A:782:MSE:SE	2.23	1.35
1:B:305:MSE:HE3	3:B:1070:HOH:O	1.46	1.16
2:B:901:ATP:O3A	2:B:901:ATP:O2G	1.73	1.03
1:B:788:GLY:HA3	3:B:1023:HOH:O	1.66	0.95
1:B:782:MSE:HE1	1:B:810:MSE:SE	2.21	0.90
1:B:101:GLU:OE2	1:B:395:ASP:HB3	1.72	0.90
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.72	0.88
1:A:612:MSE:HB3	3:A:1047:HOH:O	1.74	0.87
1:A:618:ILE:O	1:A:619:GLU:HB2	1.75	0.86
1:A:731:HIS:NE2	1:A:734:THR:OG1	2.10	0.85
1:B:14:ASN:HD21	1:B:411:VAL:H	1.25	0.84
1:B:782:MSE:HG3	3:B:949:HOH:O	1.79	0.82
1:B:102:MSE:HE3	1:B:108:LYS:HG2	1.60	0.82
1:B:679:ILE:O	1:B:683:VAL:HG23	1.81	0.80
1:B:759:MSE:HA	1:B:759:MSE:CE	2.11	0.80
1:B:610:LEU:O	1:B:612:MSE:N	2.17	0.77
1:B:754:VAL:HG11	1:B:759:MSE:HE3	1.66	0.77
1:B:796:GLN:O	1:B:797:LYS:O	2.02	0.77
1:B:18:LEU:HD23	1:B:21:MSE:CE	2.15	0.76
1:A:789:ILE:O	1:A:790:HIS:CG	2.40	0.75
1:A:531:ALA:HB1	1:A:532:GLU:OE1	1.87	0.74
1:B:707:GLN:NE2	1:B:708:GLU:OE2	2.21	0.74
1:B:807:SER:HA	1:B:810:MSE:HE3	1.70	0.74
1:B:395:ASP:HA	3:B:946:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:TYR:C	1:B:588:LEU:HG	2.07	0.74
1:B:367:ASN:O	1:B:368:GLU:O	2.06	0.73
1:A:594:LEU:HG	1:A:597:ILE:HD13	1.69	0.73
1:A:786:ARG:O	1:A:789:ILE:HB	1.89	0.72
1:A:612:MSE:CB	3:A:1047:HOH:O	2.36	0.72
1:A:799:PRO:O	1:A:800:LYS:CB	2.37	0.71
1:B:409:THR:HG23	3:B:939:HOH:O	1.90	0.71
1:B:718:LEU:O	1:B:720:ILE:N	2.24	0.70
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.21	0.70
1:B:228:PRO:C	1:B:230:GLU:H	1.95	0.70
1:A:799:PRO:O	1:A:800:LYS:HG3	1.93	0.69
1:B:693:PRO:O	1:B:696:SER:HB3	1.93	0.69
1:B:732:GLU:O	1:B:736:ARG:HG3	1.93	0.69
1:B:595:MSE:HE3	1:B:604:SER:OG	1.93	0.68
1:A:530:THR:O	1:A:532:GLU:N	2.26	0.68
1:A:17:THR:O	1:A:21:MSE:HG3	1.93	0.68
1:A:620:HIS:HD2	3:A:992:HOH:O	1.75	0.68
1:A:458:SER:HB2	1:A:460:GLU:OE1	1.94	0.67
1:A:618:ILE:O	1:A:619:GLU:CB	2.42	0.67
1:A:223:LEU:HD21	1:A:377:PHE:CZ	2.30	0.67
1:A:731:HIS:CE1	1:A:734:THR:HG1	2.12	0.67
1:B:247:ILE:HG23	1:B:247:ILE:O	1.94	0.67
1:B:759:MSE:HE2	1:B:759:MSE:HA	1.76	0.66
1:B:637:ARG:HH11	1:B:641:ILE:HD11	1.59	0.66
1:B:239:VAL:O	1:B:242:ILE:HG22	1.96	0.65
1:B:789:ILE:O	1:B:789:ILE:HG22	1.96	0.65
1:B:703:ILE:HA	1:B:706:LEU:HB3	1.78	0.65
1:B:595:MSE:CE	1:B:604:SER:OG	2.45	0.65
1:B:800:LYS:O	1:B:801:GLN:HB2	1.97	0.64
1:A:102:MSE:HE1	1:A:390:MSE:SE	2.48	0.64
1:A:529:PRO:HA	1:A:533:GLN:HE21	1.63	0.64
1:B:316:ALA:O	1:B:317:HIS:CG	2.51	0.64
1:B:605:GLY:O	1:B:608:ARG:HB2	1.97	0.64
1:A:799:PRO:O	1:A:800:LYS:CG	2.46	0.64
1:B:600:SER:HB3	1:B:603:VAL:HB	1.81	0.63
1:B:519:TRP:CH2	1:B:538:LYS:HE3	2.34	0.63
1:A:435:ILE:HG21	1:A:468:GLU:HG3	1.80	0.62
1:B:629:ASN:HD22	1:B:632:ARG:HH22	1.47	0.62
1:B:102:MSE:HE1	1:B:390:MSE:SE	2.49	0.62
1:A:429:MSE:HB2	1:A:433:GLU:OE2	1.99	0.61
1:A:566:ARG:HD2	3:A:1093:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ILE:O	1:B:619:GLU:HB2	2.01	0.60
1:B:693:PRO:O	1:B:696:SER:CB	2.48	0.60
1:B:730:LEU:HG	1:B:731:HIS:H	1.67	0.59
1:A:405:TYR:O	1:A:406:LYS:HB2	2.01	0.59
1:B:833:MSE:HG3	1:B:834:PRO:HD2	1.83	0.59
1:A:730:LEU:HD12	1:A:734:THR:HB	1.85	0.59
1:B:16:ARG:HB2	3:B:1094:HOH:O	2.03	0.59
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.84	0.59
1:A:395:ASP:HA	3:A:1028:HOH:O	2.03	0.58
1:B:180:ASN:H	1:B:180:ASN:HD22	1.51	0.58
1:B:14:ASN:ND2	1:B:411:VAL:H	2.00	0.58
1:B:564:SER:HB3	1:B:567:ILE:HD12	1.85	0.58
1:B:429:MSE:HB2	1:B:433:GLU:OE2	2.02	0.58
1:A:102:MSE:HE3	1:A:108:LYS:HG2	1.86	0.58
1:B:723:TRP:O	1:B:727:GLU:HG2	2.02	0.58
1:A:507:ALA:HB3	3:A:1094:HOH:O	2.02	0.58
1:A:800:LYS:HA	1:A:803:TYR:HB3	1.86	0.57
1:B:216:ILE:HD11	1:B:401:PHE:CE1	2.39	0.57
1:B:523:VAL:HG22	3:B:1121:HOH:O	2.05	0.57
1:A:529:PRO:HA	1:A:533:GLN:NE2	2.20	0.57
1:B:79:PHE:HB3	1:B:81:MSE:HE2	1.85	0.57
1:B:671:ASP:OD1	1:B:673:SER:HB2	2.04	0.57
1:B:238:ARG:NE	1:B:238:ARG:HA	2.19	0.57
1:B:782:MSE:HE1	1:B:810:MSE:CE	2.35	0.57
1:B:18:LEU:HD23	1:B:21:MSE:HE3	1.86	0.56
1:B:826:LEU:O	1:B:829:VAL:HG12	2.05	0.56
1:B:679:ILE:HG13	1:B:823:ILE:HD11	1.87	0.56
1:B:512:ASP:OD1	1:B:577:ARG:HD3	2.06	0.56
1:B:787:GLN:C	1:B:789:ILE:H	2.08	0.55
1:B:785:LEU:O	1:B:789:ILE:HB	2.06	0.55
1:A:441:ASP:O	1:A:445:ARG:HG3	2.06	0.55
1:B:294:GLU:HG3	1:B:294:GLU:O	2.06	0.55
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.22	0.55
1:B:457:ILE:HA	1:B:505:ASN:OD1	2.06	0.55
1:A:461:LYS:O	1:A:465:VAL:HG12	2.07	0.55
1:B:648:TYR:OH	1:B:800:LYS:HB3	2.06	0.54
1:B:789:ILE:O	1:B:789:ILE:CG2	2.55	0.54
1:A:731:HIS:CD2	1:A:734:THR:HG1	2.25	0.54
1:B:607:MSE:HE2	1:B:623:VAL:HG13	1.90	0.54
1:B:247:ILE:CG2	1:B:247:ILE:O	2.56	0.54
1:B:722:GLU:O	1:B:723:TRP:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TRP:CZ3	1:A:538:LYS:HD3	2.43	0.53
1:B:170:TYR:CZ	1:B:200:GLN:HG2	2.43	0.53
1:B:292:MSE:HG2	1:B:296:GLU:HB2	1.90	0.53
1:A:711:LYS:HG2	1:A:717:ASP:HB2	1.90	0.53
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.07	0.53
1:B:507:ALA:HB3	3:B:1043:HOH:O	2.08	0.53
1:B:785:LEU:HD11	1:B:810:MSE:HE1	1.89	0.53
1:B:760:ARG:CB	3:B:1124:HOH:O	2.56	0.53
1:B:637:ARG:NH1	1:B:641:ILE:HD11	2.24	0.52
1:B:228:PRO:O	1:B:230:GLU:N	2.40	0.52
1:B:531:ALA:O	1:B:535:GLU:HB2	2.10	0.52
1:A:531:ALA:CB	1:A:532:GLU:OE1	2.58	0.52
1:B:18:LEU:HA	1:B:21:MSE:HE2	1.92	0.52
1:B:651:VAL:O	1:B:655:GLN:HG3	2.10	0.52
1:A:460:GLU:N	1:A:460:GLU:OE1	2.30	0.51
1:B:228:PRO:C	1:B:230:GLU:N	2.63	0.51
1:B:716:LEU:HG	1:B:718:LEU:CD1	2.40	0.51
1:A:427:VAL:HB	1:A:612:MSE:HE2	1.92	0.51
1:A:590:MSE:HG3	1:A:608:ARG:HG2	1.93	0.51
1:A:763:GLU:O	1:A:767:MSE:HG3	2.10	0.51
1:B:435:ILE:O	1:B:436:GLN:C	2.47	0.50
1:B:438:ILE:HD13	1:B:559:THR:HG22	1.93	0.50
1:B:508:GLY:O	1:B:510:GLY:N	2.43	0.50
1:B:590:MSE:HE1	1:B:604:SER:O	2.11	0.50
1:A:16:ARG:NH1	3:A:1005:HOH:O	2.44	0.50
1:A:742:GLN:O	1:A:746:VAL:HG23	2.11	0.50
1:B:16:ARG:CB	3:B:1094:HOH:O	2.58	0.50
1:A:727:GLU:HB2	1:A:729:GLU:HB2	1.93	0.50
2:B:901:ATP:PA	2:B:901:ATP:O2G	2.70	0.50
1:B:587:TYR:O	1:B:588:LEU:HG	2.11	0.50
1:B:79:PHE:HB3	1:B:81:MSE:CE	2.41	0.50
1:B:539:ALA:O	1:B:543:VAL:HG23	2.12	0.49
1:B:801:GLN:HA	1:B:801:GLN:OE1	2.10	0.49
1:B:782:MSE:CE	1:B:810:MSE:SE	3.05	0.49
1:B:102:MSE:CE	1:B:390:MSE:SE	3.10	0.49
1:A:727:GLU:HG3	1:A:730:LEU:HB3	1.93	0.49
1:B:691:TYR:HD1	1:B:702:ASP:OD2	1.96	0.49
1:B:800:LYS:HD2	1:B:804:LYS:HE3	1.93	0.49
1:B:648:TYR:CZ	1:B:800:LYS:HB3	2.47	0.49
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.53	0.49
1:B:680:ARG:HD2	1:B:743:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:GLN:HA	1:A:745:GLU:HG2	1.94	0.48
1:A:731:HIS:CE1	1:A:733:GLU:HB3	2.48	0.48
1:A:731:HIS:HE1	1:A:733:GLU:HB3	1.78	0.48
1:A:789:ILE:O	1:A:789:ILE:CG2	2.61	0.48
1:B:246:LEU:HD13	1:B:314:LEU:HD21	1.94	0.48
1:A:503:ALA:HB1	1:A:506:MSE:HG2	1.95	0.48
1:A:538:LYS:NZ	1:B:528:ASN:ND2	2.61	0.48
1:B:179:ASN:OD1	3:B:1055:HOH:O	2.20	0.48
1:B:99:ILE:HD11	1:B:407:LEU:HD13	1.95	0.48
1:B:730:LEU:HG	1:B:731:HIS:N	2.28	0.48
1:B:708:GLU:O	1:B:712:ASN:N	2.37	0.48
1:A:789:ILE:O	1:A:790:HIS:ND1	2.46	0.48
1:A:571:LEU:O	1:A:574:ARG:HB2	2.14	0.48
1:A:747:TYR:OH	1:A:763:GLU:OE2	2.24	0.48
1:A:799:PRO:O	1:A:800:LYS:HB3	2.11	0.48
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.96	0.47
1:A:642:ARG:NH1	3:A:1000:HOH:O	2.46	0.47
1:B:459:ILE:O	1:B:463:GLU:HG3	2.14	0.47
1:A:594:LEU:O	1:A:597:ILE:HG12	2.15	0.47
1:A:731:HIS:HB3	3:A:1026:HOH:O	2.14	0.47
1:A:487:GLU:O	1:A:491:VAL:HG23	2.14	0.47
1:A:531:ALA:O	1:A:534:ILE:HB	2.14	0.47
1:A:727:GLU:HG3	1:A:730:LEU:CB	2.44	0.47
1:A:64:ILE:N	1:A:65:PRO:CD	2.78	0.47
1:B:367:ASN:O	1:B:368:GLU:HG3	2.15	0.47
1:B:520:GLN:O	1:B:522:GLU:N	2.48	0.47
1:A:535:GLU:HA	1:A:535:GLU:OE1	2.15	0.47
1:A:66:GLU:HG3	3:A:957:HOH:O	2.13	0.47
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.95	0.47
1:B:446:THR:HG21	1:B:500:VAL:CG2	2.45	0.47
1:B:504:THR:O	1:B:505:ASN:C	2.53	0.47
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.97	0.47
1:A:785:LEU:HD22	1:A:810:MSE:HE1	1.97	0.47
1:B:239:VAL:O	1:B:242:ILE:CG2	2.61	0.47
1:B:493:GLN:HG2	3:B:1047:HOH:O	2.14	0.47
1:B:520:GLN:C	1:B:522:GLU:N	2.69	0.47
1:B:131:VAL:HG11	1:B:210:GLU:HG2	1.97	0.46
1:B:440:GLU:O	1:B:444:GLU:HG3	2.15	0.46
1:B:131:VAL:CG1	1:B:210:GLU:HG2	2.45	0.46
1:B:404:ILE:O	1:B:404:ILE:HG22	2.16	0.46
1:A:731:HIS:CD2	1:A:734:THR:OG1	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ALA:HB3	3:B:1054:HOH:O	2.15	0.46
1:B:228:PRO:HG3	1:B:369:ASN:HB3	1.96	0.46
1:B:396:THR:N	3:B:1016:HOH:O	2.48	0.46
1:B:613:LYS:HA	1:B:614:PRO:HD2	1.71	0.46
1:B:760:ARG:HB3	3:B:1124:HOH:O	2.16	0.46
1:B:749:ARG:HD3	1:B:833:MSE:HE3	1.97	0.46
1:A:103:ARG:NE	3:A:1082:HOH:O	2.35	0.46
1:A:563:GLU:HA	1:A:594:LEU:HD11	1.96	0.46
1:A:133:ASP:O	1:A:137:GLN:HG3	2.15	0.46
1:A:395:ASP:OD2	1:A:396:THR:N	2.49	0.46
1:B:520:GLN:C	1:B:522:GLU:H	2.19	0.46
1:A:428:TYR:O	1:A:589:SER:HA	2.15	0.45
1:A:434:LYS:NZ	1:A:560:GLU:HG3	2.31	0.45
1:A:47:THR:O	1:A:51:ARG:HG3	2.15	0.45
1:A:590:MSE:HG3	1:A:608:ARG:CG	2.46	0.45
1:B:99:ILE:HA	1:B:389:GLY:O	2.16	0.45
1:B:588:LEU:HD13	1:B:627:ILE:HD13	1.98	0.45
1:A:650:ASP:OD2	3:A:1068:HOH:O	2.20	0.45
1:B:457:ILE:O	1:B:505:ASN:ND2	2.49	0.45
1:B:144:ARG:N	1:B:145:PRO:HD2	2.32	0.45
1:A:409:THR:HG23	3:A:1007:HOH:O	2.17	0.45
1:B:716:LEU:HG	1:B:718:LEU:HD11	1.99	0.45
1:B:281:LEU:HA	1:B:284:GLU:HG2	1.98	0.45
1:B:727:GLU:O	1:B:730:LEU:HD22	2.16	0.45
1:B:520:GLN:HA	3:B:1121:HOH:O	2.17	0.44
1:B:787:GLN:C	1:B:789:ILE:N	2.71	0.44
1:A:38:LEU:HG	1:A:42:GLU:HB3	1.97	0.44
1:A:74:ALA:O	1:A:78:VAL:HG23	2.17	0.44
1:B:644:GLN:NE2	1:B:800:LYS:HE3	2.31	0.44
1:B:282:ILE:HD11	1:B:286:LEU:HD21	1.99	0.44
1:A:486:ASN:HD21	1:B:132:ASN:HD21	1.65	0.44
1:B:483:PHE:O	1:B:487:GLU:HG3	2.18	0.44
1:A:32:GLU:N	1:A:33:PRO:CD	2.81	0.44
1:B:735:LEU:HA	1:B:738:ARG:HB2	1.99	0.44
1:B:796:GLN:HB3	1:B:797:LYS:H	1.73	0.44
1:A:101:GLU:HB2	1:A:411:VAL:HA	2.00	0.44
1:A:800:LYS:O	1:A:801:GLN:HB2	2.18	0.44
1:B:33:PRO:O	1:B:37:LYS:HD3	2.16	0.44
1:B:742:GLN:O	1:B:745:GLU:HG2	2.18	0.44
1:B:227:GLY:C	1:B:229:ALA:N	2.71	0.44
1:B:243:ILE:HG21	1:B:317:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG23	1:A:92:MSE:HE1	2.00	0.44
1:A:507:ALA:O	1:A:508:GLY:O	2.36	0.44
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.53	0.44
1:B:487:GLU:O	1:B:491:VAL:HG23	2.18	0.44
1:A:27:ILE:O	1:A:31:MSE:HG3	2.19	0.43
1:A:101:GLU:OE1	1:A:411:VAL:HG22	2.18	0.43
1:B:789:ILE:HG13	1:B:792:ARG:HB2	1.99	0.43
1:B:223:LEU:O	1:B:374:SER:HA	2.19	0.43
1:B:711:LYS:HE2	1:B:717:ASP:HA	2.00	0.43
1:B:183:GLY:HA3	1:B:223:LEU:CD1	2.48	0.43
1:B:299:TYR:CD1	1:B:299:TYR:O	2.71	0.43
1:B:304:ILE:HG21	1:B:781:ALA:HB1	2.00	0.43
1:A:18:LEU:O	1:A:22:ARG:HG3	2.18	0.43
1:A:629:ASN:HD22	1:A:632:ARG:HE	1.65	0.43
1:B:298:LEU:HD13	1:B:306:LEU:HD13	2.00	0.43
1:B:103:ARG:NH2	1:B:575:SER:O	2.52	0.43
1:B:669:VAL:HG12	1:B:672:VAL:HG23	2.01	0.43
1:B:306:LEU:O	1:B:309:HIS:HB2	2.19	0.43
1:B:230:GLU:HB3	1:B:367:ASN:ND2	2.33	0.42
1:A:378:GLN:O	1:A:382:ARG:HG3	2.19	0.42
1:A:721:ALA:O	1:A:725:ASP:HB3	2.19	0.42
1:A:792:ARG:O	1:A:794:TYR:CD1	2.73	0.42
1:B:110:LEU:O	1:B:111:THR:C	2.58	0.41
1:B:798:ASP:HA	1:B:799:PRO:HD2	1.52	0.41
1:B:399:PHE:HZ	1:B:635:GLU:HG3	1.84	0.41
1:B:792:ARG:NH2	3:B:1023:HOH:O	2.52	0.41
1:A:453:LEU:HD21	1:A:506:MSE:SE	2.70	0.41
1:A:589:SER:H	1:A:592:ASP:CG	2.24	0.41
1:A:81:MSE:HE3	1:A:110:LEU:HD13	2.03	0.41
1:B:170:TYR:CE2	1:B:200:GLN:HG2	2.55	0.41
1:B:231:ASP:OD1	1:B:232:SER:HB2	2.20	0.41
1:A:566:ARG:CD	3:A:1093:HOH:O	2.65	0.41
1:A:731:HIS:O	1:A:735:LEU:HB2	2.21	0.41
1:B:406:LYS:NZ	1:B:406:LYS:HG2	2.36	0.41
1:B:427:VAL:O	1:B:612:MSE:HG2	2.20	0.41
1:A:701:TRP:CD1	1:A:701:TRP:N	2.86	0.41
1:A:486:ASN:ND2	1:B:132:ASN:HD21	2.19	0.41
1:A:16:ARG:HH21	1:A:19:ARG:HD2	1.86	0.41
1:A:797:LYS:NZ	3:A:1079:HOH:O	2.50	0.41
1:B:316:ALA:O	1:B:317:HIS:CD2	2.74	0.41
1:B:378:GLN:O	1:B:382:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LEU:O	1:B:764:LYS:HE3	2.21	0.41
1:A:519:TRP:CE3	1:A:538:LYS:HD3	2.57	0.40
1:A:679:ILE:HG21	1:A:679:ILE:HD13	1.92	0.40
1:A:800:LYS:H	1:A:803:TYR:H	1.68	0.40
1:B:693:PRO:HG2	1:B:696:SER:OG	2.21	0.40
1:A:785:LEU:HD11	1:A:806:GLU:OE2	2.21	0.40
1:B:519:TRP:CZ2	1:B:538:LYS:HE3	2.57	0.40
1:B:698:GLU:HA	1:B:701:TRP:CD2	2.56	0.40
1:A:32:GLU:OE2	1:A:82:ARG:HD2	2.20	0.40
1:B:102:MSE:O	1:B:392:GLY:HA2	2.20	0.40
1:B:644:GLN:HE22	1:B:800:LYS:CE	2.34	0.40
1:A:457:ILE:HD13	1:A:457:ILE:HG21	1.81	0.40
1:A:745:GLU:HG3	1:A:746:VAL:N	2.36	0.40
1:A:632:ARG:HB2	1:A:632:ARG:NH1	2.36	0.40
1:B:247:ILE:O	1:B:248:ARG:HG2	2.22	0.40
1:B:450:GLN:HG3	1:B:553:GLY:O	2.22	0.40
1:B:496:TYR:O	1:B:497:PRO:C	2.60	0.40
1:B:541:TRP:CZ2	1:B:545:HIS:CD2	3.09	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	675/853 (79%)	635 (94%)	31 (5%)	9 (1%)	13	10
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	2	1
All	All	1412/1706 (83%)	1286 (91%)	80 (6%)	46 (3%)	4	2

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	A	395	ASP
1	A	508	GLY
1	A	509	ARG
1	A	531	ALA
1	B	229	ALA
1	B	230	GLU
1	B	289	GLU
1	B	368	GLU
1	B	395	ASP
1	B	507	ALA
1	B	509	ARG
1	B	521	ALA
1	B	531	ALA
1	B	611	GLY
1	B	612	MSE
1	B	729	GLU
1	B	730	LEU
1	B	731	HIS
1	B	796	GLN
1	B	797	LYS
1	A	510	GLY
1	A	619	GLU
1	A	790	HIS
1	B	231	ASP
1	B	302	ALA
1	B	394	ALA
1	B	594	LEU
1	B	801	GLN
1	B	234	GLU
1	B	608	ARG
1	B	614	PRO
1	B	617	ALA
1	B	707	GLN
1	B	794	TYR
1	A	613	LYS
1	B	286	LEU
1	B	690	ALA
1	B	691	TYR
1	B	481	ALA
1	B	535	GLU
1	B	619	GLU
1	B	719	PRO

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Mol	Chain	Res	Type
1	B	703	ILE
1	B	510	GLY
1	B	287	VAL

### 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	575/696 (83%)	538 (94%)	37 (6%)	19	22
1	B	632/696 (91%)	565 (89%)	67 (11%)	7	7
All	All	1207/1392 (87%)	1103 (91%)	104 (9%)	11	11

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	ARG
1	A	22	ARG
1	A	37	LYS
1	A	41	GLU
1	A	72	ARG
1	A	156	ILE
1	A	180	ASN
1	A	194	SER
1	A	369	ASN
1	A	427	VAL
1	A	461	LYS
1	A	506	MSE
1	A	509	ARG
1	A	528	ASN
1	A	532	GLU
1	A	535	GLU
1	A	566	ARG
1	A	596	ARG
1	A	597	ILE

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Mol	Chain	Res	Type
1	A	604	SER
1	A	610	LEU
1	A	632	ARG
1	A	637	ARG
1	A	647	GLU
1	A	661	SER
1	A	669	VAL
1	A	725	ASP
1	A	727	GLU
1	A	735	LEU
1	A	742	GLN
1	A	749	ARG
1	A	789	ILE
1	A	794	TYR
1	A	797	LYS
1	A	800	LYS
1	A	816	GLU
1	B	38	LEU
1	B	41	GLU
1	B	98	CYS
1	B	103	ARG
1	B	196	GLU
1	B	226	SER
1	B	231	ASP
1	B	232	SER
1	B	234	GLU
1	B	242	ILE
1	B	247	ILE
1	B	248	ARG
1	B	283	GLU
1	B	285	LEU
1	B	288	LYS
1	B	292	MSE
1	B	304	ILE
1	B	306	LEU
1	B	310	VAL
1	B	367	ASN
1	B	395	ASP
1	B	409	THR
1	B	416	ARG
1	B	436	GLN
1	B	440	GLU

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Mol	Chain	Res	Type
1	B	461	LYS
1	B	509	ARG
1	B	512	ASP
1	B	518	SER
1	B	520	GLN
1	B	523	VAL
1	B	529	PRO
1	B	532	GLU
1	B	535	GLU
1	B	536	LYS
1	B	537	ILE
1	B	588	LEU
1	B	596	ARG
1	B	602	ARG
1	B	606	MSE
1	B	608	ARG
1	B	610	LEU
1	B	669	VAL
1	B	672	VAL
1	B	674	GLU
1	B	702	ASP
1	B	718	LEU
1	B	723	TRP
1	B	724	LEU
1	B	726	LYS
1	B	727	GLU
1	B	729	GLU
1	B	734	THR
1	B	735	LEU
1	B	738	ARG
1	B	743	SER
1	B	749	ARG
1	B	750	LYS
1	B	759	MSE
1	B	779	LEU
1	B	787	GLN
1	B	791	LEU
1	B	797	LYS
1	B	800	LYS
1	B	801	GLN
1	B	831	VAL
1	B	832	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	A	370	GLN
1	A	486	ASN
1	A	528	ASN
1	A	533	GLN
1	A	570	GLN
1	A	620	HIS
1	A	629	ASN
1	A	638	ASN
1	A	662	GLN
1	A	742	GLN
1	A	761	HIS
1	B	14	ASN
1	B	180	ASN
1	B	309	HIS
1	B	486	ASN
1	B	520	GLN
1	B	528	ASN
1	B	533	GLN
1	B	542	GLN
1	B	545	HIS
1	B	629	ASN
1	B	638	ASN
1	B	644	GLN
1	B	664	ASN
1	B	707	GLN
1	B	712	ASN
1	B	748	GLN
1	B	787	GLN
1	B	830	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z  > 2$
2	ATP	A	900	-	27,33,33	1.39	4 (14%)	27,52,52	2.38	8 (29%)
2	ATP	B	901	-	27,33,33	2.15	9 (33%)	27,52,52	2.45	11 (40%)

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	ATP	A	900	-	-	0/18/38/38	0/3/3/3
2	ATP	B	901	-	-	0/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	C8-N9	-3.82	1.32	1.36
2	A	900	ATP	PB-O2B	-2.03	1.45	1.55
2	B	901	ATP	C5-N7	-2.02	1.32	1.39
2	B	901	ATP	C2-N3	2.08	1.35	1.32
2	A	900	ATP	C2-N3	2.58	1.36	1.32
2	B	901	ATP	C5'-C4'	2.72	1.60	1.51
2	B	901	ATP	C5-C4	2.85	1.46	1.40
2	B	901	ATP	PA-O1A	2.97	1.61	1.50
2	A	900	ATP	C5-C4	3.41	1.48	1.40
2	A	900	ATP	PG-O3B	3.56	1.65	1.60
2	B	901	ATP	PA-O5'	3.68	1.74	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	PG-O3B	3.80	1.65	1.60
2	B	901	ATP	O4'-C1'	5.42	1.48	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ATP	N3-C2-N1	-8.46	121.62	128.86
2	B	901	ATP	N3-C2-N1	-6.06	123.68	128.86
2	B	901	ATP	O3'-C3'-C2'	-3.61	100.27	111.83
2	A	900	ATP	PB-O3B-PG	-3.41	121.17	132.63
2	B	901	ATP	O4'-C4'-C3'	-3.10	99.03	105.15
2	A	900	ATP	C4-C5-N7	-2.19	107.30	109.41
2	A	900	ATP	PA-O5'-C5'	2.17	134.39	121.68
2	B	901	ATP	C5'-C4'-C3'	2.20	123.58	115.29
2	A	900	ATP	O2'-C2'-C3'	2.26	119.07	111.83
2	B	901	ATP	O4'-C4'-C5'	2.55	117.87	109.39
2	A	900	ATP	C4'-O4'-C1'	2.61	112.55	109.83
2	B	901	ATP	C4'-O4'-C1'	2.64	112.58	109.83
2	A	900	ATP	O5'-PA-O1A	2.80	120.02	109.07
2	B	901	ATP	C2-N1-C6	2.80	123.52	118.75
2	A	900	ATP	N6-C6-N1	2.83	124.44	118.57
2	B	901	ATP	O5'-PA-O1A	2.97	120.67	109.07
2	B	901	ATP	PA-O5'-C5'	3.01	139.32	121.68
2	B	901	ATP	O5'-C5'-C4'	4.09	123.22	109.00
2	B	901	ATP	C2'-C3'-C4'	4.53	111.32	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.