



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:36 AM 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 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/ValidationPDFNotes.html>

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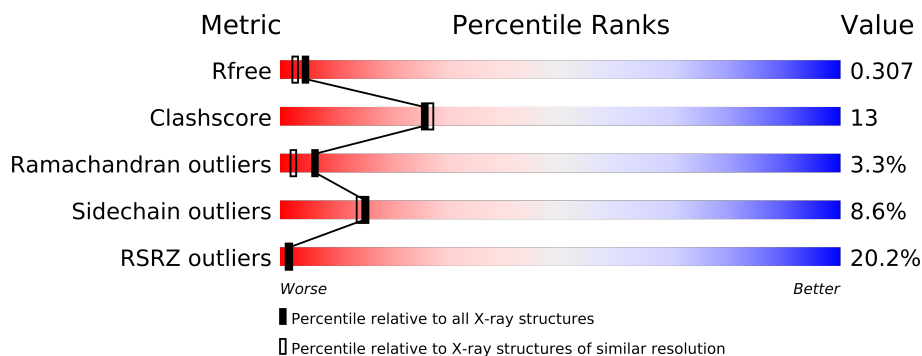
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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:

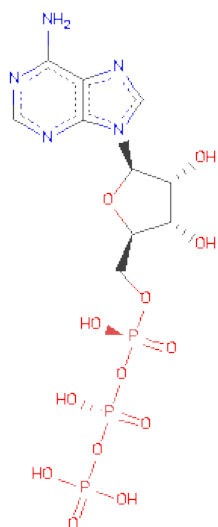
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	31	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	35	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	81	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	92	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	102	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	161	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
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B	782	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	810	MSE	MET	MODIFIED RESIDUE	UNP P10408
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<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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.

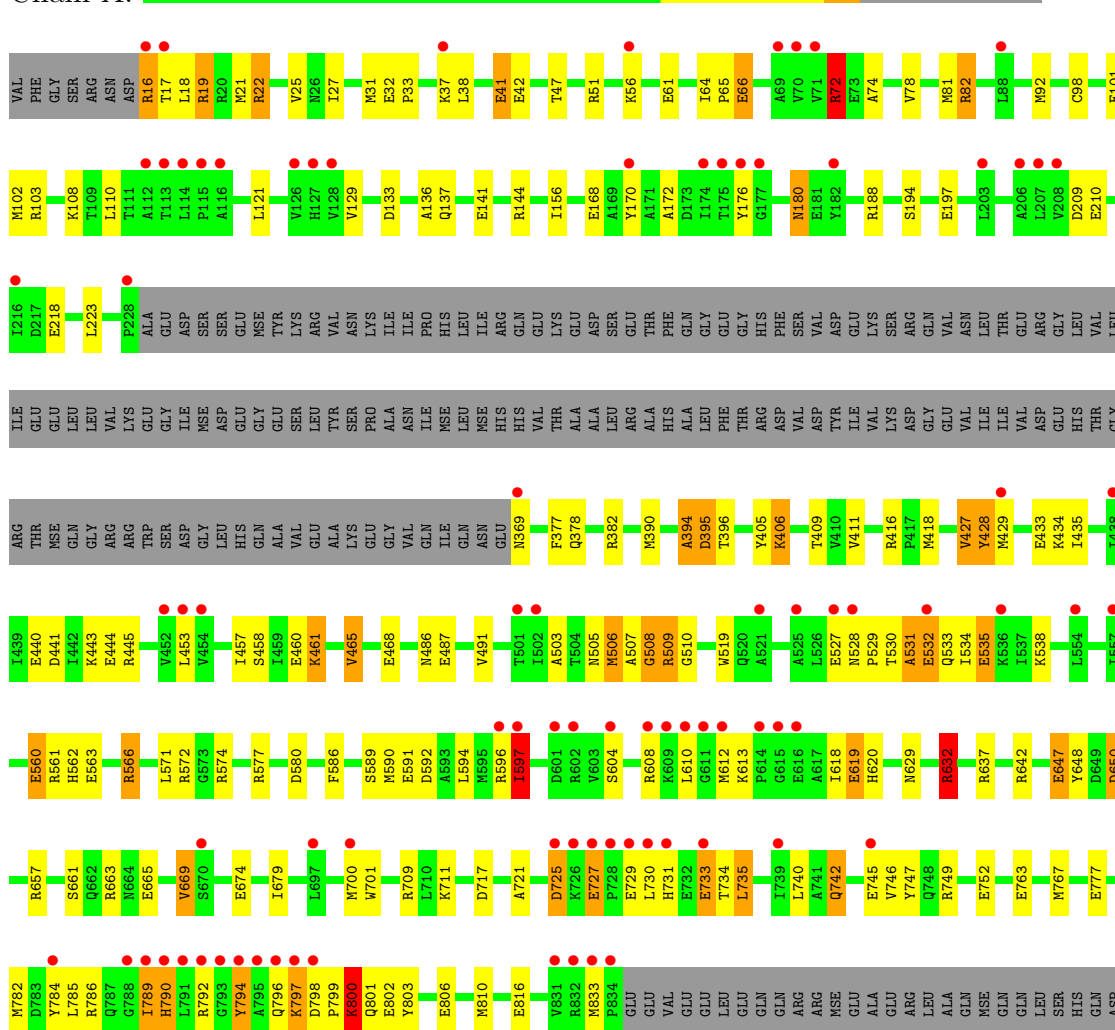
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	233	Total	O	0	0
			233	233		

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

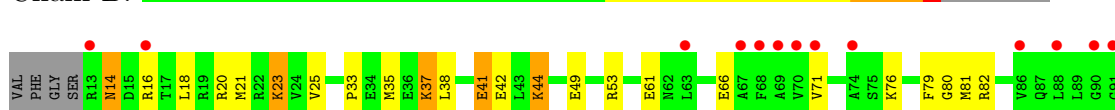
- Molecule 1: Preprotein translocase secA subunit

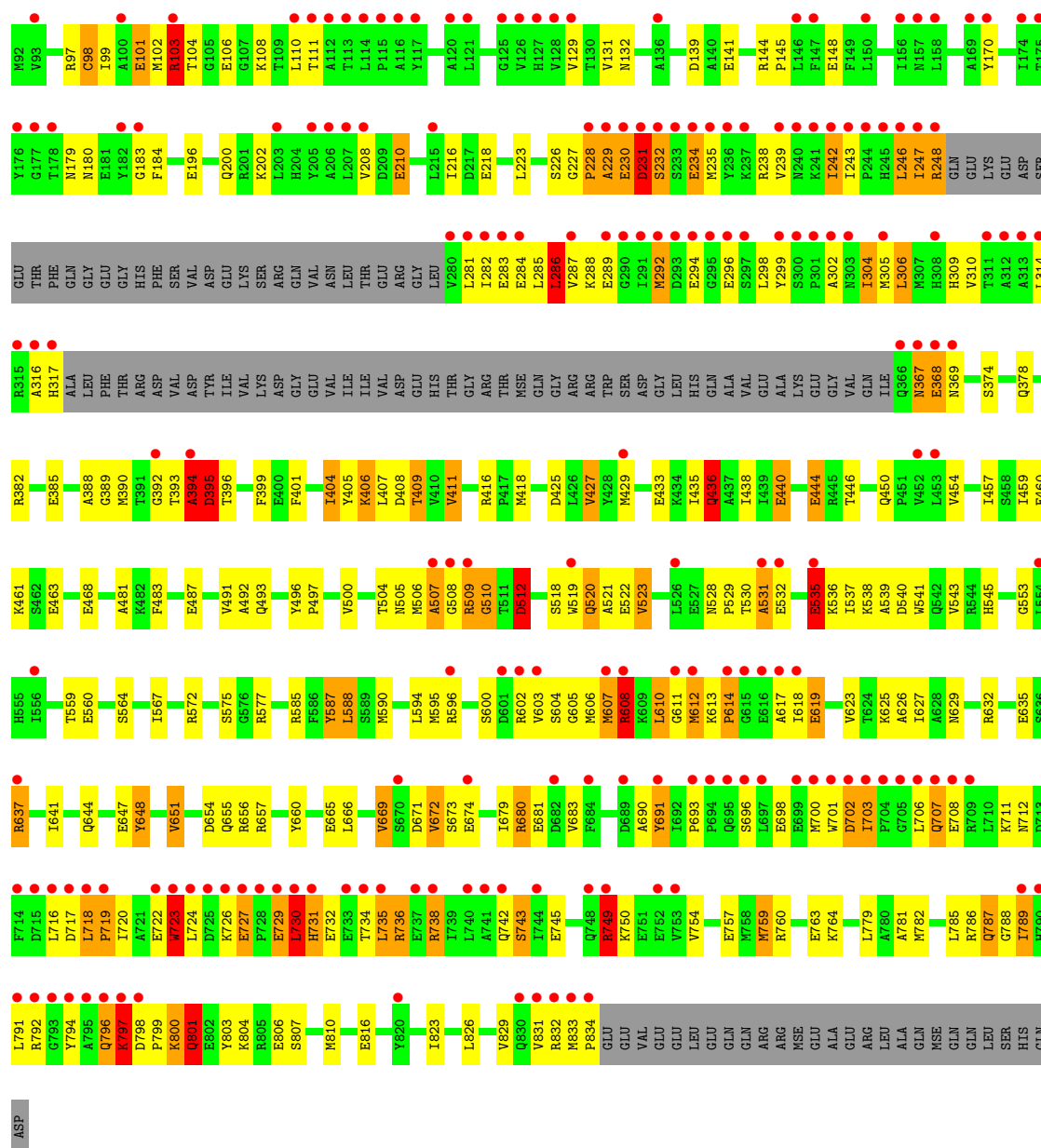
Chain A:



- Molecule 1: Preprotein translocase secA subunit

Chain B:





## 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	5246 reflections (5.00%)	DCC
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 , 20.0	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 104944 reflections	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.



## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (306) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:LYS:CE	1:B:44:LYS:NZ	1.67	1.55

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Atom-1	Atom-2	Distance(Å)	Clash(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:B:35:MSE:CE	1:B:35:MSE:SE	2.16	1.42
1:A:506:MSE:SE	1:A:506:MSE:CE	2.17	1.42
1:A:590:MSE:SE	1:A:590:MSE:CE	2.18	1.42
1:B:418:MSE:SE	1:B:418:MSE:CE	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:CE	1:A:833:MSE:SE	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:754:VAL:HG11	1:B:759:MSE:HE3	1.66	0.77
1:B:610:LEU:O	1:B:612:MSE:N	2.17	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:807:SER:HA	1:B:810:MSE:HE3	1.70	0.74
1:B:707:GLN:NE2	1:B:708:GLU:OE2	2.21	0.74
1:B:395:ASP:HA	3:B:946:HOH:O	1.88	0.74
1:B:587:TYR:C	1:B:588:LEU:HG	2.07	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:732:GLU:O	1:B:736:ARG:HG3	1.93	0.69
1:B:693:PRO:O	1:B:696:SER:HB3	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:731:HIS:CE1	1:A:734:THR:HG1	2.12	0.67
1:A:223:LEU:HD21	1:A:377:PHE:CZ	2.30	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:789:ILE:O	1:B:789:ILE:HG22	1.96	0.65
1:B:239:VAL:O	1:B:242: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:B:316:ALA:O	1:B:317:HIS:CG	2.51	0.64
1:A:529:PRO:HA	1:A:533:GLN:HE21	1.63	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:730:LEU:HG	1:B:731:HIS:H	1.67	0.59
1:B:833:MSE:HG3	1:B:834:PRO:HD2	1.83	0.59
1:A:405:TYR:O	1:A:406:LYS:HB2	2.01	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:B:14:ASN:ND2	1:B:411:VAL:H	2.00	0.58
1:A:395:ASP:HA	3:A:1028:HOH:O	2.03	0.58
1:B:564:SER:HB3	1:B:567:ILE:HD12	1.85	0.58
1:B:180:ASN:H	1:B:180:ASN:HD22	1.51	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:782:MSE:HE1	1:B:810:MSE:CE	2.35	0.57
1:B:238:ARG:NE	1:B:238:ARG:HA	2.19	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:104:THR:HG21	1:B:577:ARG:NH2	2.22	0.55
1:B:294:GLU:HG3	1:B:294:GLU:O	2.06	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:B:607:MSE:HE2	1:B:623:VAL:HG13	1.90	0.54
1:A:731:HIS:CD2	1:A:734:THR:HG1	2.25	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
1:B:292:MSE:HG2	1:B:296:GLU:HB2	1.90	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:18:LEU:HA	1:B:21:MSE:HE2	1.92	0.52
1:A:531:ALA:CB	1:A:532:GLU:OE1	2.58	0.52
1:B:651:VAL:O	1:B:655:GLN:HG3	2.10	0.52
1:B:228:PRO:C	1:B:230:GLU:N	2.63	0.51
1:A:460:GLU:N	1:A:460:GLU:OE1	2.30	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:590:MSE:HE1	1:B:604:SER:O	2.11	0.50
1:B:508:GLY:O	1:B:510:GLY:N	2.43	0.50
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:16:ARG:CB	3:B:1094:HOH:O	2.58	0.50
1:A:742:GLN:O	1:A:746:VAL:HG23	2.11	0.50
1:A:16:ARG:NH1	3:A:1005:HOH:O	2.44	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:801:GLN:HA	1:B:801:GLN:OE1	2.10	0.49
1:B:539:ALA:O	1:B:543:VAL:HG23	2.12	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:800:LYS:HD2	1:B:804:LYS:HE3	1.93	0.49
1:B:691:TYR:HD1	1:B:702:ASP:OD2	1.96	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
1:A:742:GLN:HA	1:A:745:GLU:HG2	1.94	0.48
1:A:731:HIS:HE1	1:A:733:GLU:HB3	1.78	0.48
1:A:731:HIS:CE1	1:A:733:GLU:HB3	2.48	0.48
1:A:789:ILE:O	1:A:789:ILE:CG2	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:799:PRO:O	1:A:800:LYS:HB3	2.11	0.48
1:A:747:TYR:OH	1:A:763:GLU:OE2	2.24	0.48
1:A:571:LEU:O	1:A:574:ARG:HB2	2.14	0.48
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.96	0.47
1:B:459:ILE:O	1:B:463:GLU:HG3	2.14	0.47
1:A:642:ARG:NH1	3:A:1000:HOH:O	2.46	0.47
1:A:731:HIS:HB3	3:A:1026:HOH:O	2.14	0.47
1:A:594:LEU:O	1:A:597:ILE:HG12	2.15	0.47
1:A:727:GLU:HG3	1:A:730:LEU:CB	2.44	0.47
1:A:531:ALA:O	1:A:534:ILE:HB	2.14	0.47
1:A:487:GLU:O	1:A:491:VAL:HG23	2.14	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:64:ILE:N	1:A:65:PRO:CD	2.78	0.47
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.95	0.47
1:A:66:GLU:HG3	3:A:957:HOH:O	2.13	0.47
1:A:535:GLU:HA	1:A:535:GLU:OE1	2.15	0.47
1:B:504:THR:O	1:B:505:ASN:C	2.53	0.47
1:B:446:THR:HG21	1:B:500:VAL:CG2	2.45	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:520:GLN:C	1:B:522:GLU:N	2.69	0.47
1:B:493:GLN:HG2	3:B:1047:HOH:O	2.14	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
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:749:ARG:HD3	1:B:833:MSE:HE3	1.97	0.46
1:B:760:ARG:HB3	3:B:1124:HOH:O	2.16	0.46
1:B:613:LYS:HA	1:B:614:PRO:HD2	1.71	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:396:THR:N	3:B:1016:HOH:O	2.48	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: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:133:ASP:O	1:A:137:GLN:HG3	2.15	0.46
1:A:428:TYR:O	1:A:589:SER:HA	2.15	0.45
1:A:47:THR:O	1:A:51:ARG:HG3	2.15	0.45
1:A:434:LYS:NZ	1:A:560:GLU:HG3	2.31	0.45
1:A:590:MSE:HG3	1:A:608:ARG:CG	2.46	0.45
1:B:588:LEU:HD13	1:B:627:ILE:HD13	1.98	0.45
1:B:99:ILE:HA	1:B:389:GLY:O	2.16	0.45
1:B:457:ILE:O	1:B:505:ASN:ND2	2.49	0.45
1:A:650:ASP:OD2	3:A:1068:HOH:O	2.20	0.45
1:B:144:ARG:N	1:B:145:PRO:HD2	2.32	0.45
1:B:716:LEU:HG	1:B:718:LEU:HD11	1.99	0.45
1:A:409:THR:HG23	3:A:1007:HOH:O	2.17	0.45
1:B:727:GLU:O	1:B:730:LEU:HD22	2.16	0.45
1:B:281:LEU:HA	1:B:284:GLU:HG2	1.98	0.45
1:B:787:GLN:C	1:B:789:ILE:N	2.71	0.44
1:B:520:GLN:HA	3:B:1121:HOH:O	2.17	0.44
1:B:644:GLN:NE2	1:B:800:LYS:HE3	2.31	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: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:B:796:GLN:HB3	1:B:797:LYS:H	1.73	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: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:A:101:GLU:HB2	1:A:411:VAL:HA	2.00	0.44
1:B:742:GLN:O	1:B:745:GLU:HG2	2.18	0.44
1:B:243:ILE:HG21	1:B:317:HIS:NE2	2.33	0.44
1:B:227:GLY:C	1:B:229:ALA:N	2.71	0.44
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:B:789:ILE:HG13	1:B:792:ARG:HB2	1.99	0.43
1:A:101:GLU:OE1	1:A:411:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:ILE:O	1:A:31:MSE:HG3	2.19	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: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:A:629:ASN:HD22	1:A:632:ARG:HE	1.65	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:792:ARG:NH2	3:B:1023:HOH:O	2.52	0.41
1:B:399:PHE:HZ	1:B:635:GLU:HG3	1.84	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:B:170:TYR:CE2	1:B:200:GLN:HG2	2.55	0.41
1:A:81:MSE:HE3	1:A:110:LEU:HD13	2.03	0.41
1:B:231:ASP:OD1	1:B:232:SER:HB2	2.20	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:731:HIS:O	1:A:735:LEU:HB2	2.21	0.41
1:A:566:ARG:CD	3:A:1093:HOH:O	2.65	0.41
1:A:486:ASN:ND2	1:B:132:ASN:HD21	2.19	0.41
1:A:701:TRP:CD1	1:A:701:TRP:N	2.86	0.41
1:B:316:ALA:O	1:B:317:HIS:CD2	2.74	0.41
1:A:16:ARG:HH21	1:A:19:ARG:HD2	1.86	0.41
1:B:378:GLN:O	1:B:382:ARG:HG3	2.21	0.41
1:B:666:LEU:O	1:B:764:LYS:HE3	2.21	0.41
1:A:797:LYS:NZ	3:A:1079:HOH:O	2.50	0.41
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: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:B:519:TRP:CZ2	1:B:538:LYS:HE3	2.57	0.40
1:A:785:LEU:HD11	1:A:806:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:698:GLU:HA	1:B:701:TRP:CD2	2.56	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:32:GLU:OE2	1:A:82:ARG:HD2	2.20	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:B:247:ILE:O	1:B:248:ARG:HG2	2.22	0.40
1:A:632:ARG:HB2	1:A:632:ARG:NH1	2.36	0.40
1:B:541:TRP:CZ2	1:B:545:HIS:CD2	3.09	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

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%)	18	13
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	3	1
All	All	1412/1706 (83%)	1286 (91%)	80 (6%)	46 (3%)	6	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

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Mol	Chain	Res	Type
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
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%)	25	26
1	B	632/696 (91%)	565 (89%)	67 (11%)	10	8
All	All	1207/1392 (87%)	1103 (91%)	104 (9%)	15	14

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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 chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	-	33,33,33	1.30	4 (12%)	52,52,52	2.29	16 (30%)
2	ATP	B	901	-	33,33,33	2.14	12 (36%)	52,52,52	2.60	19 (36%)

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	-	-	0/22/38/38	0/1/3/3
2	ATP	B	901	-	-	0/22/38/38	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	PB-O3A	5.03	1.69	1.59
2	B	901	ATP	O4'-C1'	4.86	1.48	1.41
2	A	900	ATP	C5-C4	3.41	1.48	1.40
2	B	901	ATP	PA-O5'	3.32	1.74	1.59
2	B	901	ATP	PG-O3B	3.26	1.65	1.60
2	A	900	ATP	PG-O3B	3.04	1.65	1.60
2	B	901	ATP	C2'-C1'	-2.90	1.49	1.53
2	B	901	ATP	C8-N9	-2.88	1.32	1.36
2	B	901	ATP	C5-C4	2.85	1.46	1.40
2	B	901	ATP	C4-N9	-2.76	1.33	1.37
2	B	901	ATP	PA-O1A	2.70	1.61	1.51
2	B	901	ATP	C5'-C4'	2.67	1.60	1.51
2	A	900	ATP	PB-O2B	-2.18	1.45	1.55
2	A	900	ATP	C2-N3	2.11	1.36	1.32
2	B	901	ATP	C5-N7	-2.06	1.32	1.40
2	B	901	ATP	PA-O3A	2.04	1.63	1.59

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	O3A-PB-O3B	-8.93	83.50	101.66
2	A	900	ATP	N3-C2-N1	-8.48	121.62	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	N3-C4-N9	6.33	136.87	125.43
2	A	900	ATP	N3-C4-N9	6.28	136.78	125.43
2	B	901	ATP	N3-C2-N1	-6.02	123.68	128.71
2	B	901	ATP	O4'-C1'-N9	-4.80	103.97	108.44
2	B	901	ATP	C2'-C3'-C4'	4.35	111.32	102.65
2	B	901	ATP	O2B-PB-O3A	4.17	124.94	105.14
2	B	901	ATP	O5'-C5'-C4'	3.89	123.22	108.94
2	A	900	ATP	PB-O3B-PG	-3.58	121.17	131.68
2	B	901	ATP	O3'-C3'-C2'	-3.56	100.27	111.83
2	A	900	ATP	C5-C4-N3	-3.51	118.07	125.70
2	A	900	ATP	O3A-PA-O5'	-3.16	89.28	103.41
2	A	900	ATP	O3A-PB-O3B	-3.12	95.32	101.66
2	B	901	ATP	O4'-C4'-C3'	-3.03	99.03	105.17
2	B	901	ATP	C5-C4-N3	-3.03	119.11	125.70
2	A	900	ATP	C2-N3-C4	3.00	122.54	114.01
2	A	900	ATP	O4'-C1'-N9	-2.89	105.75	108.44
2	B	901	ATP	O5'-PA-O1A	2.88	120.67	109.37
2	A	900	ATP	O5'-PA-O1A	2.72	120.02	109.37
2	B	901	ATP	C2-N1-C6	2.63	123.52	118.77
2	B	901	ATP	C4'-O4'-C1'	2.61	112.58	109.75
2	A	900	ATP	C4-C5-N7	-2.60	107.30	109.52
2	A	900	ATP	C4'-O4'-C1'	2.58	112.55	109.75
2	A	900	ATP	N6-C6-N1	2.58	124.44	119.36
2	A	900	ATP	C8-N9-C4	2.57	108.86	106.90
2	B	901	ATP	PA-O5'-C5'	2.41	139.32	122.03
2	B	901	ATP	O4'-C4'-C5'	2.38	117.87	109.36
2	A	900	ATP	O2G-PG-O1G	2.35	118.12	110.44
2	B	901	ATP	O3A-PA-O5'	-2.33	92.96	103.41
2	A	900	ATP	O2'-C2'-C3'	2.22	119.07	111.83
2	B	901	ATP	C5-C4-N9	-2.22	103.95	107.16
2	A	900	ATP	O2A-PA-O3A	2.18	115.50	105.14
2	B	901	ATP	C5'-C4'-C3'	2.09	123.58	115.21
2	B	901	ATP	O2G-PG-O3B	-2.08	95.25	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	679/853 (79%)	0.70	86 (12%) 4 4	5, 19, 44, 63	0
1	B	743/853 (87%)	1.39	202 (27%) 1 1	3, 21, 47, 66	0
All	All	1422/1706 (83%)	1.06	288 (20%) 2 1	3, 20, 45, 66	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	LEU	11.0
1	A	794	TYR	10.7
1	A	793	GLY	10.6
1	B	233	SER	10.6
1	B	794	TYR	9.8
1	B	287	VAL	9.8
1	B	314	LEU	9.6
1	A	790	HIS	8.6
1	B	791	LEU	8.5
1	B	793	GLY	8.3
1	B	228	PRO	8.2
1	B	728	PRO	8.1
1	B	299	TYR	7.9
1	B	704	PRO	7.8
1	B	247	ILE	7.8
1	B	789	ILE	7.7
1	B	315	ARG	7.7
1	A	795	ALA	7.7
1	B	696	SER	7.6
1	B	366	GLN	7.6
1	B	290	GLY	7.3
1	B	700	MSE	7.1
1	B	702	ASP	7.0
1	A	792	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	615	GLY	6.9
1	B	792	ARG	6.8
1	B	294	GLU	6.7
1	B	707	GLN	6.5
1	B	316	ALA	6.5
1	B	703	ILE	6.5
1	B	245	HIS	6.5
1	A	611	GLY	6.3
1	B	727	GLU	6.2
1	B	795	ALA	6.2
1	B	834	PRO	6.2
1	B	244	PRO	6.1
1	B	246	LEU	6.1
1	B	301	PRO	6.1
1	B	236	TYR	6.1
1	B	614	PRO	6.0
1	B	790	HIS	6.0
1	B	229	ALA	5.9
1	A	834	PRO	5.9
1	B	695	GLN	5.9
1	B	796	GLN	5.9
1	B	248	ARG	5.9
1	A	615	GLY	5.8
1	B	697	LEU	5.8
1	B	317	HIS	5.6
1	B	694	PRO	5.5
1	B	706	LEU	5.4
1	B	725	ASP	5.4
1	B	235	MSE	5.4
1	B	730	LEU	5.4
1	B	280	VAL	5.2
1	B	729	GLU	5.2
1	B	281	LEU	5.2
1	B	243	ILE	5.1
1	B	237	LYS	5.0
1	B	833	MSE	5.0
1	A	16	ARG	5.0
1	B	705	GLY	4.9
1	B	230	GLU	4.9
1	B	232	SER	4.9
1	B	295	GLY	4.8
1	B	231	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	292	MSE	4.7
1	B	719	PRO	4.6
1	B	293	ASP	4.6
1	A	228	PRO	4.6
1	B	71	VAL	4.6
1	B	240	ASN	4.6
1	B	291	ILE	4.6
1	B	709	ARG	4.5
1	B	731	HIS	4.4
1	B	289	GLU	4.3
1	A	597	ILE	4.3
1	B	753	VAL	4.2
1	B	726	LYS	4.2
1	B	114	LEU	4.2
1	B	508	GLY	4.1
1	B	128	VAL	4.1
1	A	784	TYR	4.1
1	B	691	TYR	4.0
1	B	618	ILE	4.0
1	B	532	GLU	4.0
1	B	113	THR	4.0
1	B	242	ILE	4.0
1	B	830	GLN	4.0
1	B	283	GLU	3.9
1	B	296	GLU	3.9
1	B	312	ALA	3.9
1	B	234	GLU	3.9
1	B	608	ARG	3.9
1	A	728	PRO	3.9
1	B	175	THR	3.8
1	B	282	ILE	3.8
1	B	735	LEU	3.8
1	B	367	ASN	3.7
1	B	369	ASN	3.7
1	B	797	LYS	3.7
1	B	602	ARG	3.7
1	B	718	LEU	3.7
1	A	525	ALA	3.6
1	B	670	SER	3.6
1	A	832	ARG	3.6
1	B	117	TYR	3.5
1	B	717	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	723	TRP	3.5
1	B	150	LEU	3.5
1	B	724	LEU	3.5
1	B	699	GLU	3.5
1	A	789	ILE	3.5
1	B	368	GLU	3.5
1	A	521	ALA	3.4
1	A	614	PRO	3.4
1	B	182	TYR	3.4
1	A	527	GLU	3.4
1	B	738	ARG	3.4
1	B	701	TRP	3.4
1	B	241	LYS	3.4
1	A	730	LEU	3.3
1	B	734	THR	3.3
1	B	70	VAL	3.3
1	B	129	VAL	3.3
1	B	749	ARG	3.3
1	B	832	ARG	3.3
1	B	170	TYR	3.3
1	B	176	TYR	3.3
1	B	740	LEU	3.2
1	B	297	SER	3.2
1	B	67	ALA	3.2
1	B	157	ASN	3.2
1	B	68	PHE	3.2
1	B	601	ASP	3.2
1	B	722	GLU	3.2
1	A	610	LEU	3.1
1	B	177	GLY	3.1
1	B	693	PRO	3.1
1	B	831	VAL	3.1
1	A	127	HIS	3.1
1	A	602	ARG	3.1
1	A	369	ASN	3.1
1	B	737	GLU	3.0
1	B	136	ALA	3.0
1	B	684	PHE	3.0
1	B	596	ARG	3.0
1	A	206	ALA	3.0
1	B	127	HIS	3.0
1	A	731	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	2.9
1	A	115	PRO	2.9
1	B	116	ALA	2.9
1	B	120	ALA	2.9
1	A	608	ARG	2.9
1	B	158	LEU	2.9
1	B	111	THR	2.9
1	B	126	VAL	2.9
1	A	532	GLU	2.9
1	A	697	LEU	2.9
1	A	733	GLU	2.8
1	B	174	ILE	2.8
1	A	175	THR	2.8
1	B	91	GLY	2.8
1	B	302	ALA	2.8
1	A	596	ARG	2.8
1	A	729	GLU	2.8
1	A	601	ASP	2.8
1	B	147	PHE	2.8
1	A	182	TYR	2.8
1	B	637	ARG	2.8
1	A	116	ALA	2.7
1	B	612	MSE	2.7
1	A	17	THR	2.7
1	A	177	GLY	2.7
1	A	788	GLY	2.7
1	A	609	LYS	2.7
1	B	716	LEU	2.7
1	A	71	VAL	2.7
1	B	178	THR	2.7
1	A	831	VAL	2.7
1	A	454	VAL	2.7
1	B	616	GLU	2.6
1	A	128	VAL	2.6
1	B	146	LEU	2.6
1	B	519	TRP	2.6
1	A	174	ILE	2.6
1	B	313	ALA	2.6
1	A	797	LYS	2.6
1	A	126	VAL	2.6
1	B	526	LEU	2.6
1	A	726	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	2.6
1	B	554	LEU	2.6
1	B	69	ALA	2.6
1	B	74	ALA	2.6
1	A	208	VAL	2.6
1	A	616	GLU	2.6
1	A	727	GLU	2.6
1	B	531	ALA	2.6
1	A	170	TYR	2.6
1	A	725	ASP	2.6
1	B	392	GLY	2.6
1	A	700	MSE	2.6
1	A	833	MSE	2.6
1	A	113	THR	2.6
1	B	88	LEU	2.6
1	A	557	ILE	2.5
1	B	156	ILE	2.5
1	B	300	SER	2.5
1	B	308	HIS	2.5
1	A	745	GLU	2.5
1	A	203	LEU	2.5
1	B	303	ASN	2.5
1	B	509	ARG	2.5
1	B	284	GLU	2.4
1	B	203	LEU	2.4
1	B	206	ALA	2.4
1	B	507	ALA	2.4
1	B	741	ALA	2.4
1	A	536	LYS	2.4
1	B	121	LEU	2.4
1	B	90	GLY	2.4
1	A	796	GLN	2.4
1	A	207	LEU	2.4
1	B	603	VAL	2.4
1	A	604	SER	2.4
1	A	176	TYR	2.4
1	B	16	ARG	2.4
1	A	739	ILE	2.4
1	B	115	PRO	2.4
1	B	556	ILE	2.4
1	B	714	PHE	2.4
1	B	453	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	612	MSE	2.3
1	B	820	TYR	2.3
1	A	112	ALA	2.3
1	A	37	LYS	2.3
1	B	798	ASP	2.3
1	B	752	GLU	2.3
1	B	112	ALA	2.3
1	B	394	ALA	2.3
1	A	502	ILE	2.2
1	B	674	GLU	2.2
1	B	715	ASP	2.2
1	B	452	VAL	2.2
1	A	429	MSE	2.2
1	B	103	ARG	2.2
1	A	69	ALA	2.2
1	A	453	LEU	2.2
1	B	110	LEU	2.2
1	B	93	VAL	2.2
1	A	798	ASP	2.2
1	A	501	THR	2.2
1	B	169	ALA	2.2
1	A	70	VAL	2.2
1	A	452	VAL	2.2
1	B	239	VAL	2.2
1	A	56	LYS	2.2
1	B	617	ALA	2.2
1	B	607	MSE	2.2
1	B	611	GLY	2.2
1	B	733	GLU	2.2
1	B	63	LEU	2.1
1	B	215	LEU	2.1
1	B	125	GLY	2.1
1	B	689	ASP	2.1
1	A	554	LEU	2.1
1	B	183	GLY	2.1
1	B	682	ASP	2.1
1	B	205	TYR	2.1
1	A	216	ILE	2.1
1	B	535	GLU	2.1
1	A	528	ASN	2.1
1	A	438	ILE	2.1
1	B	744	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	2.1
1	B	86	VAL	2.1
1	B	13	ARG	2.1
1	B	742	GLN	2.1
1	B	311	THR	2.1
1	B	208	VAL	2.1
1	B	305	MSE	2.1
1	A	670	SER	2.0
1	B	429	MSE	2.0
1	B	748	GLN	2.0
1	B	100	ALA	2.0
1	B	708	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ATP	A	900	31/31	0.21	0.92	11,24,29,30	0
2	ATP	B	901	31/31	0.16	-1.18	9,19,24,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.