Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:42 am BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

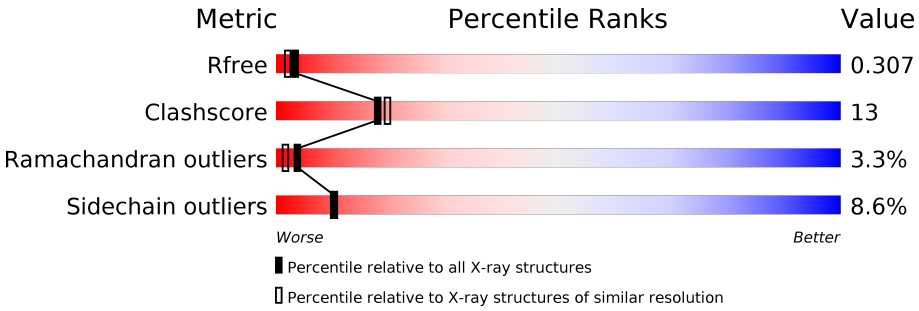
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	853	57% 18% • 20%
1	B	853	51% 27% 8% • 13%

2 Entry composition (i)

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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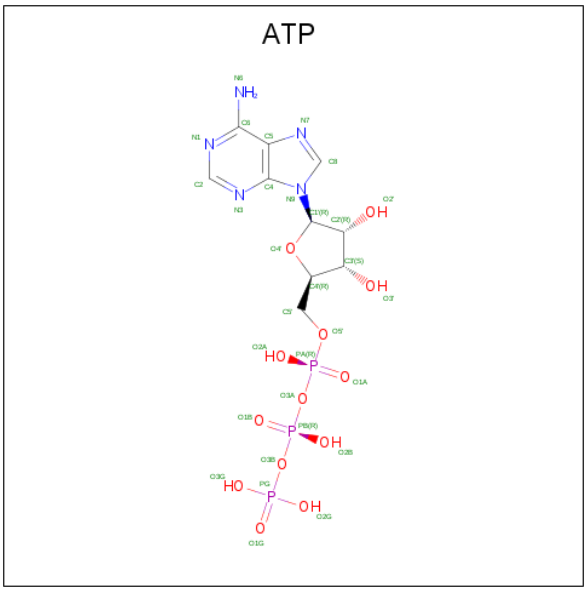
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	782	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	810	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	814	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	833	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	846	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	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
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: $C_{10}H_{16}N_5O_{13}P_3$).



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.

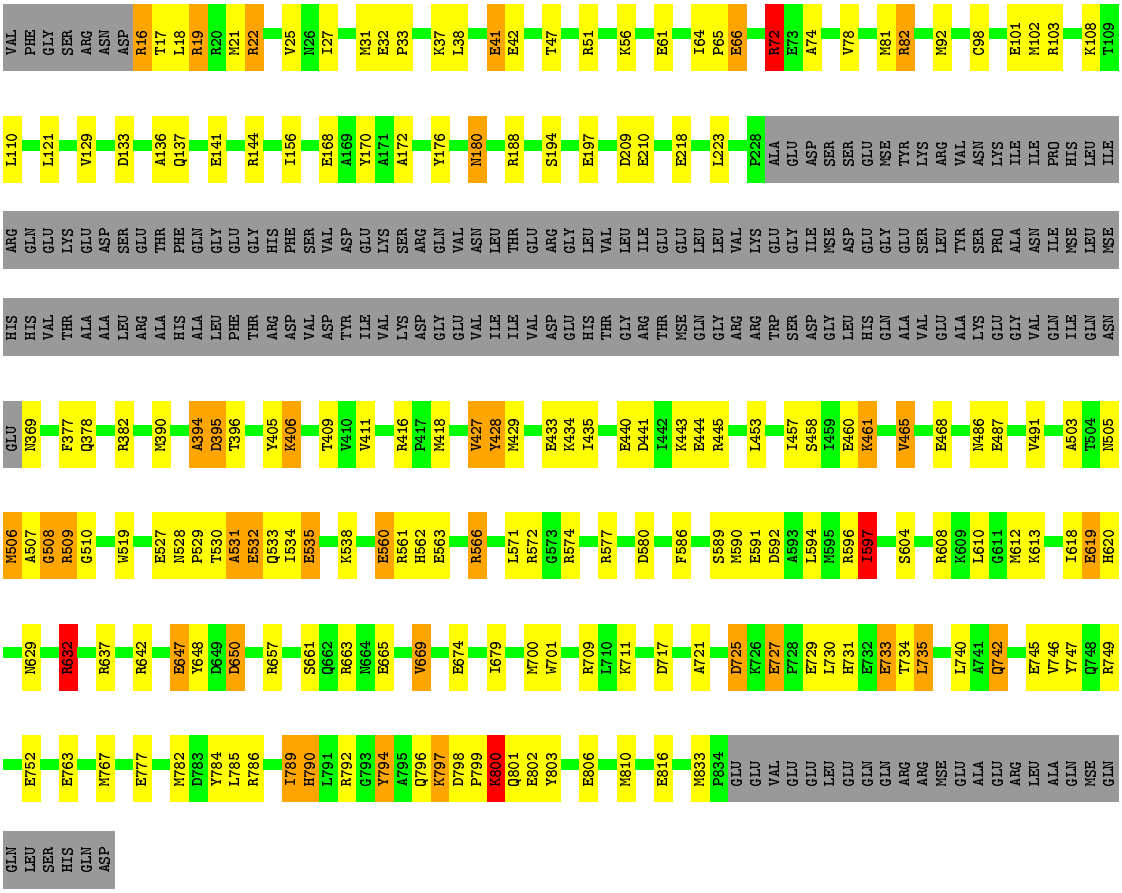
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	233	Total	O	0	0
			233	233		

3 Residue-property plots (i)

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.

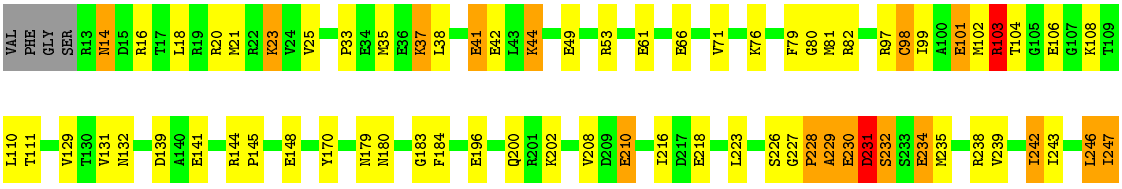
- Molecule 1: Preprotein translocase secA subunit

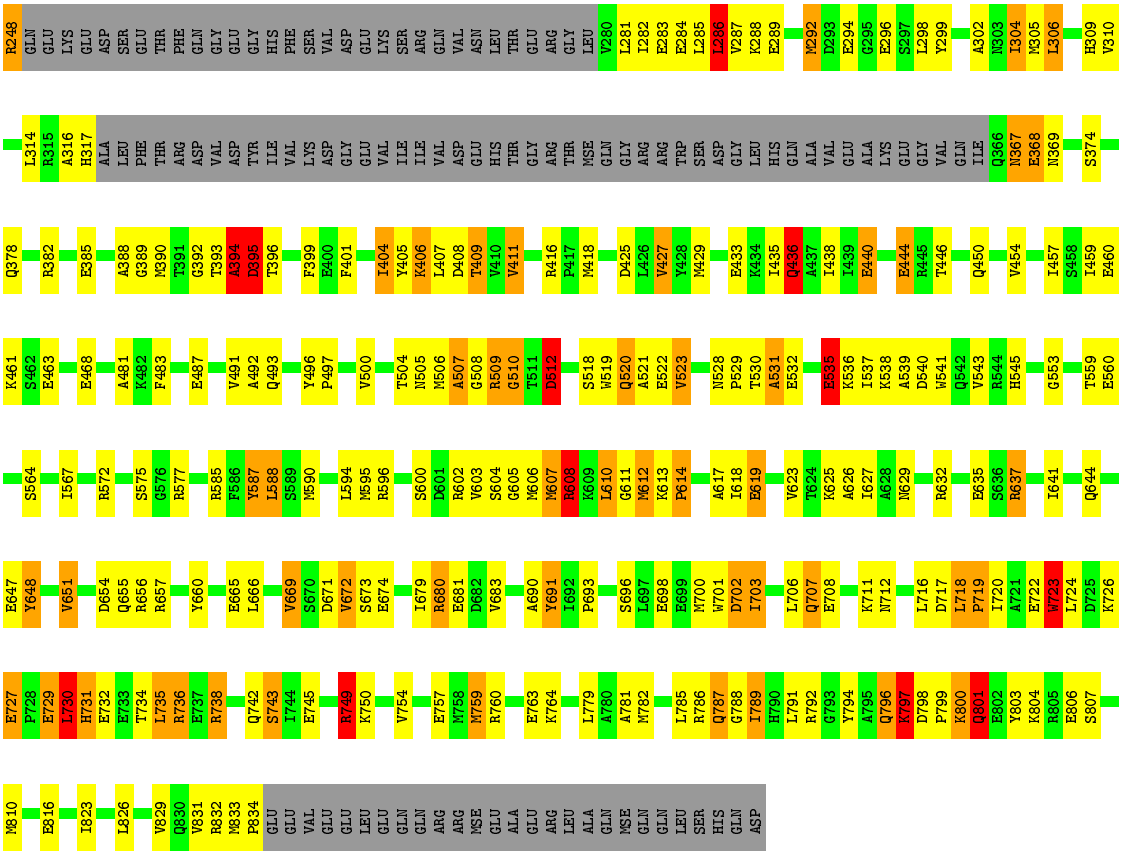
Chain A:



- Molecule 1: Preprotein translocase secA subunit

Chain B:




R248 GLN GLU LYS GLU ASP SER GLU THR PHE GLN GLY GLU GLY HIS PHE SER VAL ASP GLU LYS SER ARG GLN VAL ASN LEU THR GLU ARG GLY LEU V280 L281 I282 E283 E284 L285 L286 V287 K288 E289 M292 D293 E294 G295 E296 S297 L298 Y299 A302 N303 I304 M305 L306 H309 V310
L314 R315 A316 H317 ALA LEU PHE THR ARG ASP VAL ASP TYR ILE VAL LYS ASP GLY GLU VAL ILE ILE VAL ASP GLU LYS GLY ARG THR MSE GLN GLY ARG ARG TRP SER ASP GLY LEU HIS GLN ALA VAL GLU ALA LYS GLU GLY VAL GLN ILE Q366 N367 E368 N369 S374
Q378 R382 E385 A388 G389 M390 T391 G392 T393 A394 D395 T396 F399 E400 F401 I404 Y405 K406 L407 D408 T409 V410 V411 R416 P417 M418 D425 L426 V427 Y428 M429 E433 K434 I435 Q436 A437 I438 I439 E440 E444 R445 T446 Q450 V454 I457 S458 I459 E460
K461 S462 E463 E468 A481 K482 F483 E487 V491 A492 Q493 Y496 P497 V500 T504 N505 M506 A507 G508 R509 G510 T511 D512 S518 W519 Q520 A521 E522 V523 N528 P529 T530 A531 E532 E535 K536 I537 K538 A539 D540 W541 Q542 V543 R544 H545 G553 T559 E560
S564 I567 R572 S575 G576 R577 R585 F586 V587 L588 S589 M590 L594 M595 R596 S600 D601 R602 V603 S604 G605 M606 M607 R608 K609 L610 G611 M612 K613 P614 A617 I618 E619 V623 T624 K625 A626 I627 A628 M629 R632 E635 S636 R637 I641 Q644
E647 V648 V651 D654 Q655 R656 R657 Y660 E665 L666 V669 S670 D671 V672 S673 E674 I679 R680 E681 D682 V683 A690 Y691 I692 P693 S696 L697 E698 E699 M700 W701 D702 I703 L706 Q707 E708 K711 N712 L716 D717 L718 P719 I720 A721 E722 W723 L724 D725 K726
E727 P728 E729 L730 H731 E732 E733 T734 L735 R736 E737 R738 Q742 S743 I744 E745 R749 K750 V754 E757 M758 M759 R760 E763 K764 L779 A780 A781 M782 L785 R786 Q787 G788 I789 H790 L791 R792 G793 Y794 A795 Q796 K797 D798 P799 K800 Q801 E802 Y803 K804 R805 E806 S807
M810 E816 I823 L826 V829 Q830 V831 R832 M833 P834 GLU GLU VAL GLU GLU LEU GLU GLN GLN ARG ARG MSE GLU ALA GLU ARG LEU ALA GLN MSE GLN GLN LEU SER HIS GLN ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	34.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	675/853 (79%)	635 (94%)	31 (5%)	9 (1%)	12 9
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	2 0
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	575/696 (83%)	538 (94%)	37 (6%)	17 20
1	B	632/696 (91%)	565 (89%)	67 (11%)	6 6
All	All	1207/1392 (87%)	1103 (91%)	104 (9%)	10 10

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	B	901	-	26,33,33	2.01	7 (26%)	31,52,52	2.16	12 (38%)
2	ATP	A	900	-	26,33,33	1.24	3 (11%)	31,52,52	1.82	8 (25%)

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	B	901	-	-	6/18/38/38	0/3/3/3
2	ATP	A	900	-	-	3/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	O4'-C1'	5.54	1.48	1.41
2	B	901	ATP	PA-O5'	3.68	1.74	1.59
2	B	901	ATP	PA-O1A	3.04	1.61	1.50
2	B	901	ATP	C2'-C1'	-2.92	1.49	1.53
2	B	901	ATP	C5'-C4'	2.80	1.60	1.51
2	A	900	ATP	C5-C4	2.75	1.48	1.40
2	A	900	ATP	C2-N3	2.64	1.36	1.32
2	B	901	ATP	C5-C4	2.26	1.46	1.40
2	B	901	ATP	C2-N3	2.14	1.35	1.32
2	A	900	ATP	PB-O2B	-2.13	1.45	1.55

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	ATP	N3-C2-N1	-4.52	121.62	128.68
2	B	901	ATP	C2'-C3'-C4'	4.46	111.32	102.64
2	B	901	ATP	O5'-C5'-C4'	4.13	123.22	108.99
2	B	901	ATP	O3'-C3'-C2'	-3.57	100.27	111.82
2	A	900	ATP	PB-O3B-PG	-3.40	121.17	132.83
2	B	901	ATP	N3-C2-N1	-3.20	123.68	128.68
2	B	901	ATP	O4'-C4'-C3'	-3.08	99.03	105.11
2	B	901	ATP	PA-O5'-C5'	3.01	139.32	121.68
2	B	901	ATP	O5'-PA-O1A	2.97	120.67	109.07
2	A	900	ATP	N6-C6-N1	2.82	124.44	118.57
2	A	900	ATP	O5'-PA-O1A	2.80	120.02	109.07
2	B	901	ATP	O2G-PG-O3B	-2.80	95.25	104.64
2	B	901	ATP	C2-N1-C6	2.78	123.52	118.75
2	B	901	ATP	O4'-C4'-C5'	2.58	117.87	109.37
2	B	901	ATP	O3G-PG-O3B	2.57	113.24	104.64
2	A	900	ATP	C5-C6-N6	-2.55	116.47	120.35
2	B	901	ATP	C5'-C4'-C3'	2.24	123.58	115.18
2	A	900	ATP	O2'-C2'-C3'	2.24	119.07	111.82
2	A	900	ATP	PA-O5'-C5'	2.17	134.39	121.68
2	A	900	ATP	C4-C5-N7	-2.02	107.30	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	ATP	C5'-O5'-PA-O3A
2	B	901	ATP	C4'-C5'-O5'-PA
2	B	901	ATP	O4'-C4'-C5'-O5'
2	B	901	ATP	C3'-C4'-C5'-O5'
2	B	901	ATP	PB-O3A-PA-O5'
2	A	900	ATP	PB-O3A-PA-O2A
2	B	901	ATP	C5'-O5'-PA-O1A
2	A	900	ATP	PB-O3A-PA-O1A
2	A	900	ATP	C4'-C5'-O5'-PA

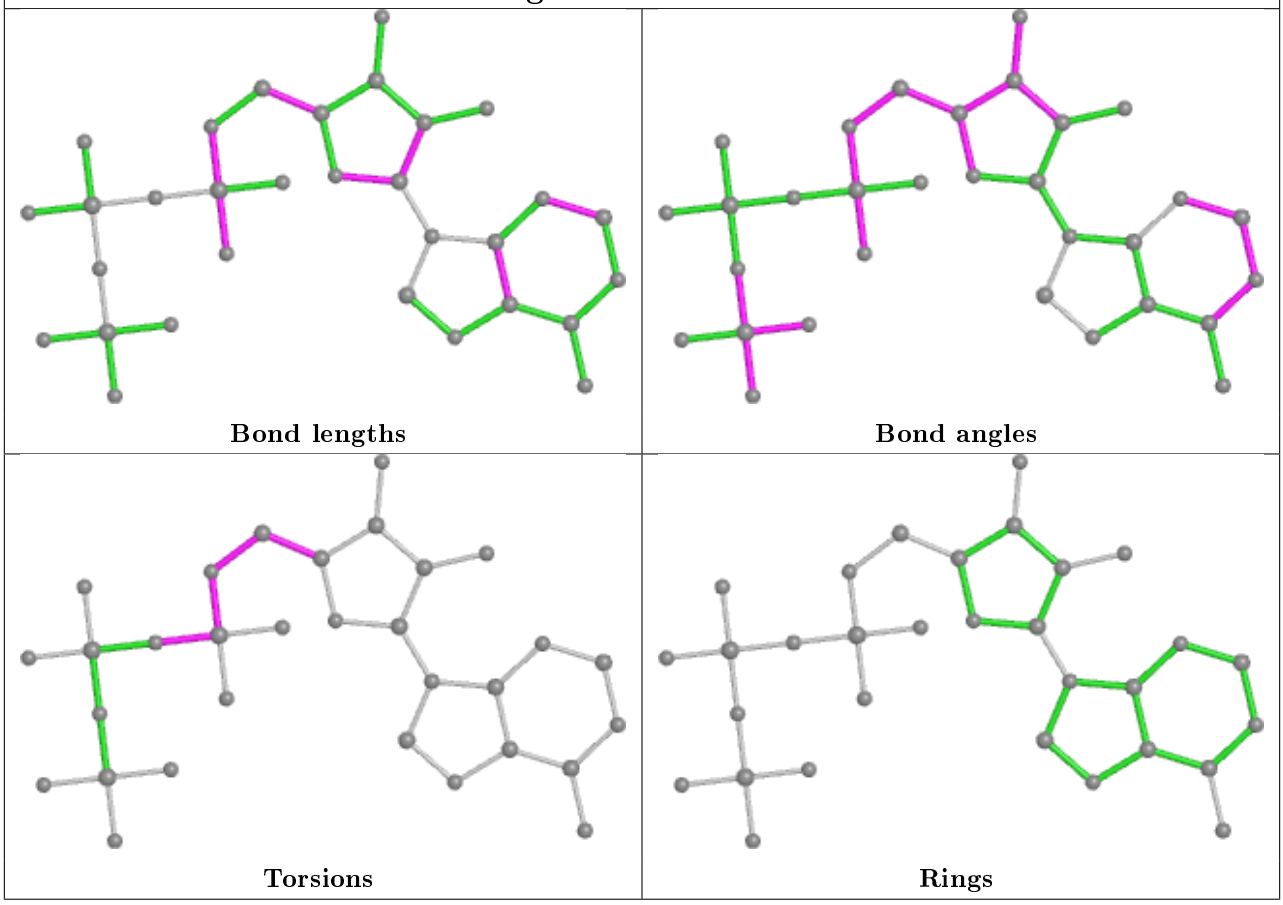
There are no ring outliers.

1 monomer is involved in 2 short contacts:

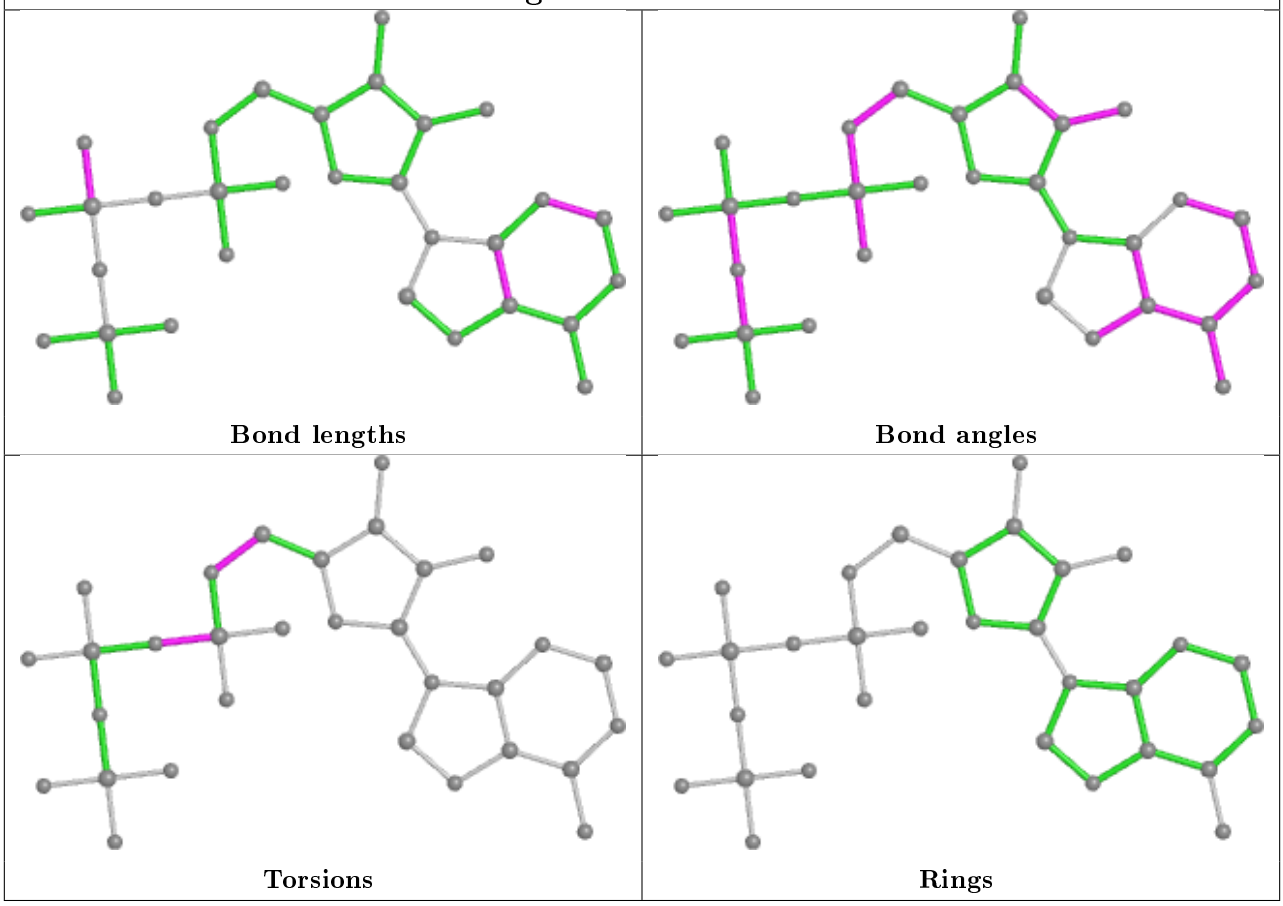
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 901



Ligand ATP A 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

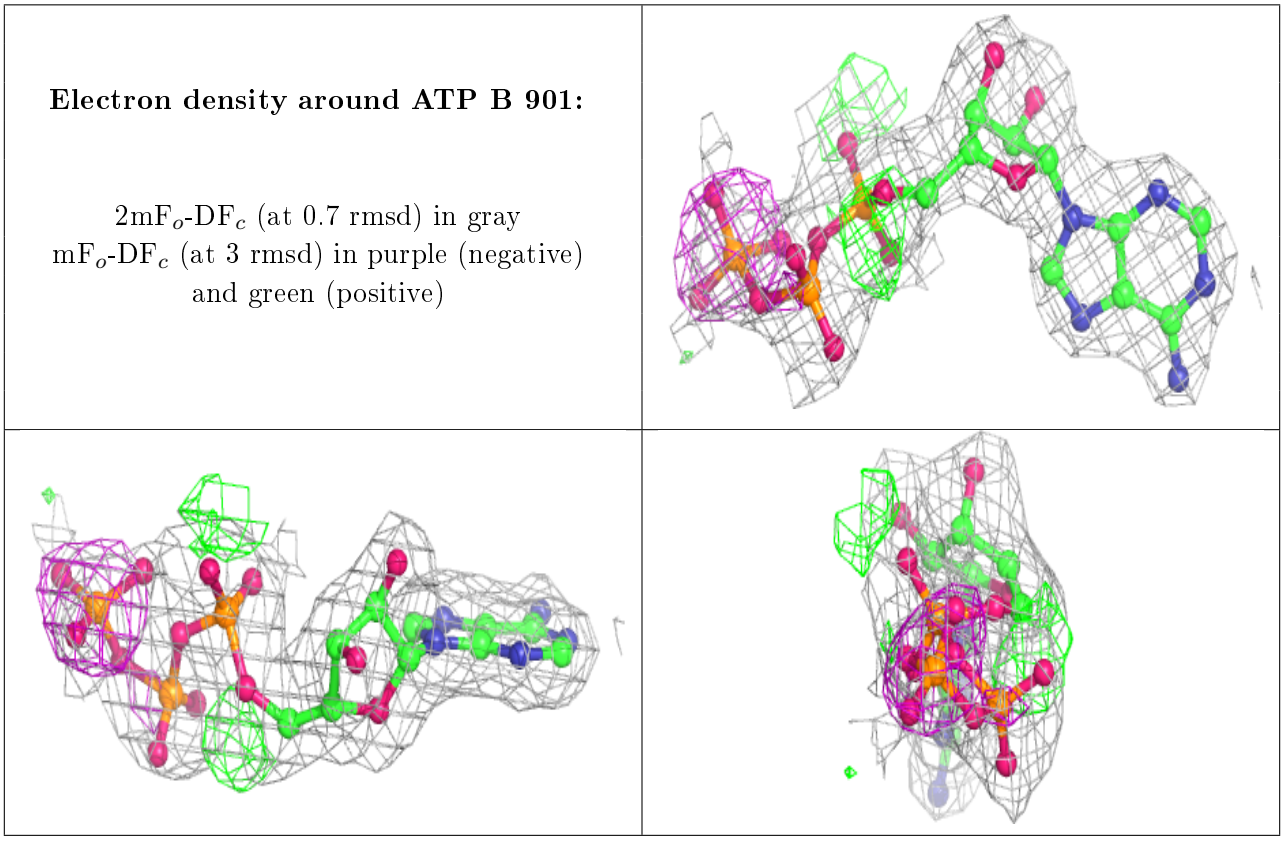
6.4 Ligands

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

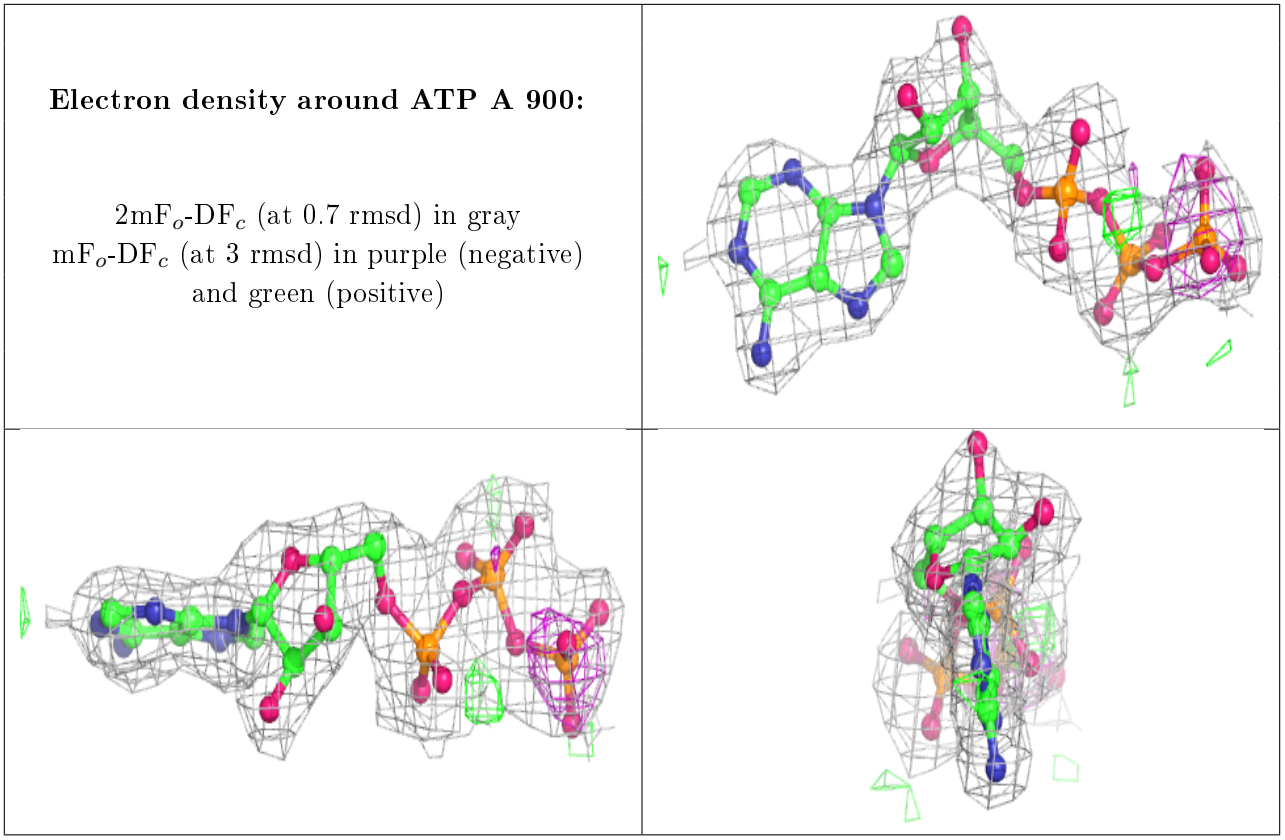
Electron density around ATP B 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ATP A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

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