Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 04:23 PM EDT

PDB ID	:	2FSI
Title	:	Complex SecA:ADP from Escherichia coli
Authors	:	Papanikolau, Y.; Petratos, K.; Economou, A.
Deposited on	:	2006-01-23
Resolution	:	2.11 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

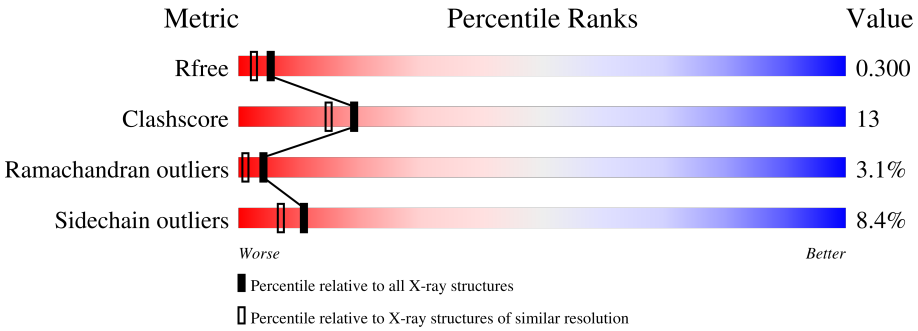
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	60% 18% • 19%
1	B	853	52% 27% 7% • 12%

2 Entry composition

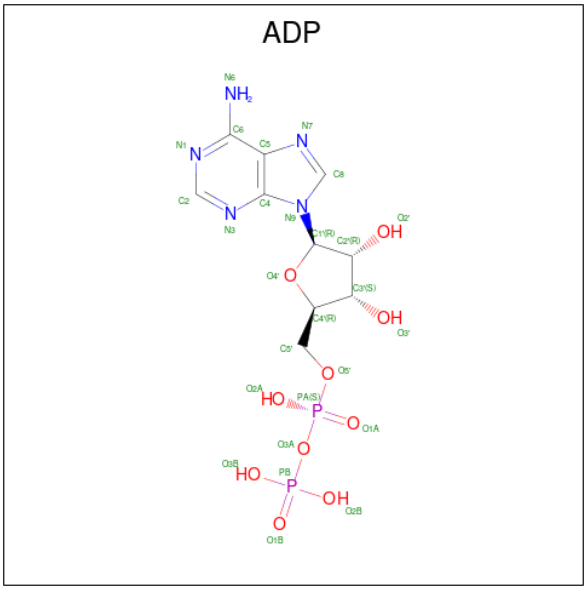
There are 3 unique types of molecules in this entry. The entry contains 11936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	691	Total	C	N	O	S	0	0	0
			5500	3445	971	1058	26			
1	B	748	Total	C	N	O	S	0	0	0
			5948	3730	1050	1138	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

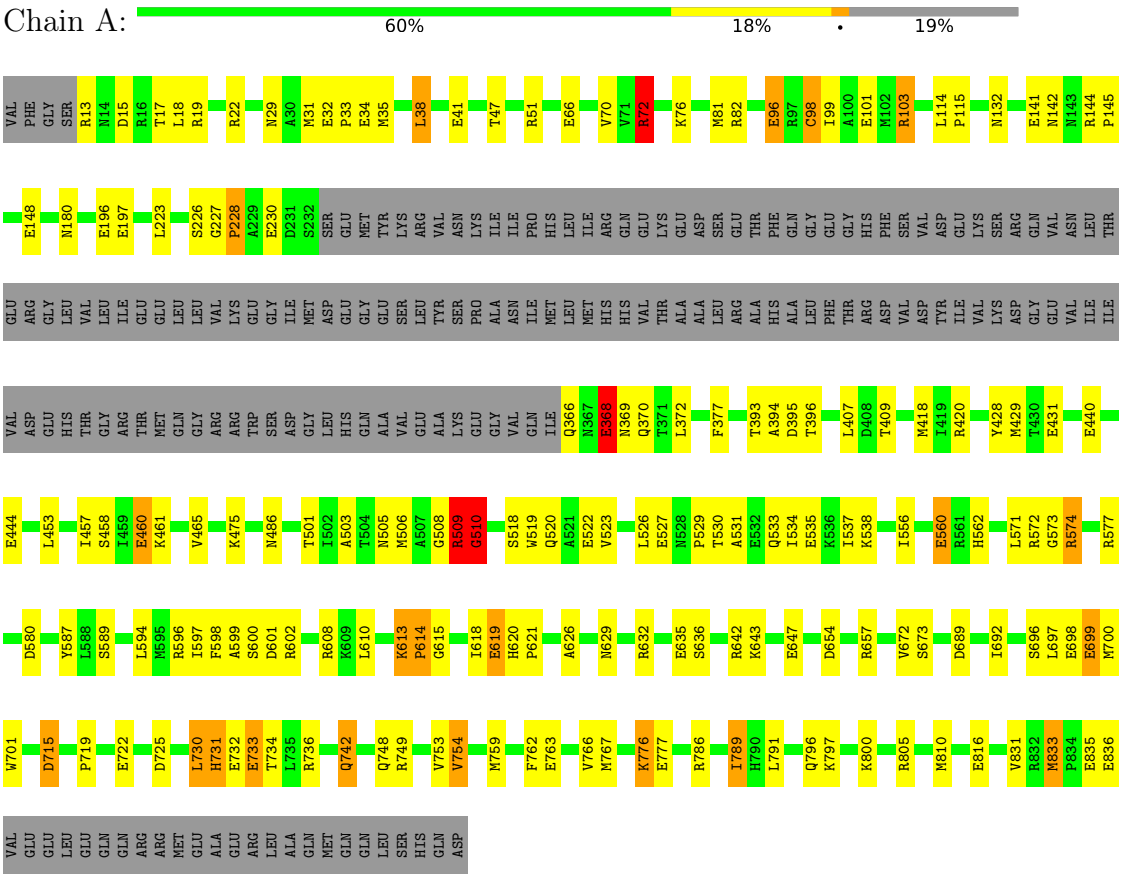
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	179	Total O 179 179	0	0
3	B	255	Total O 255 255	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

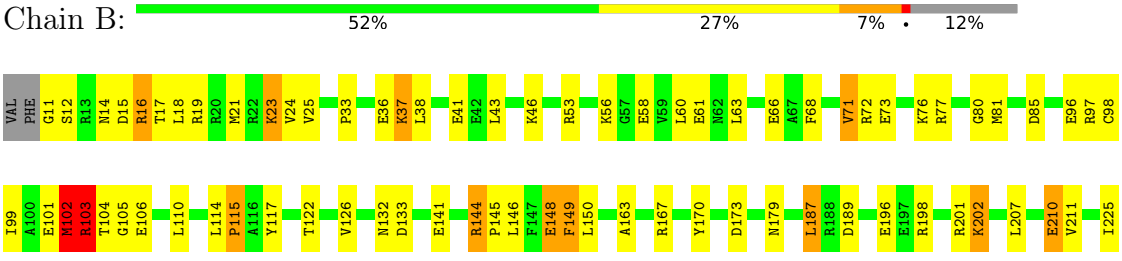
• Molecule 1: Preprotein translocase secA subunit

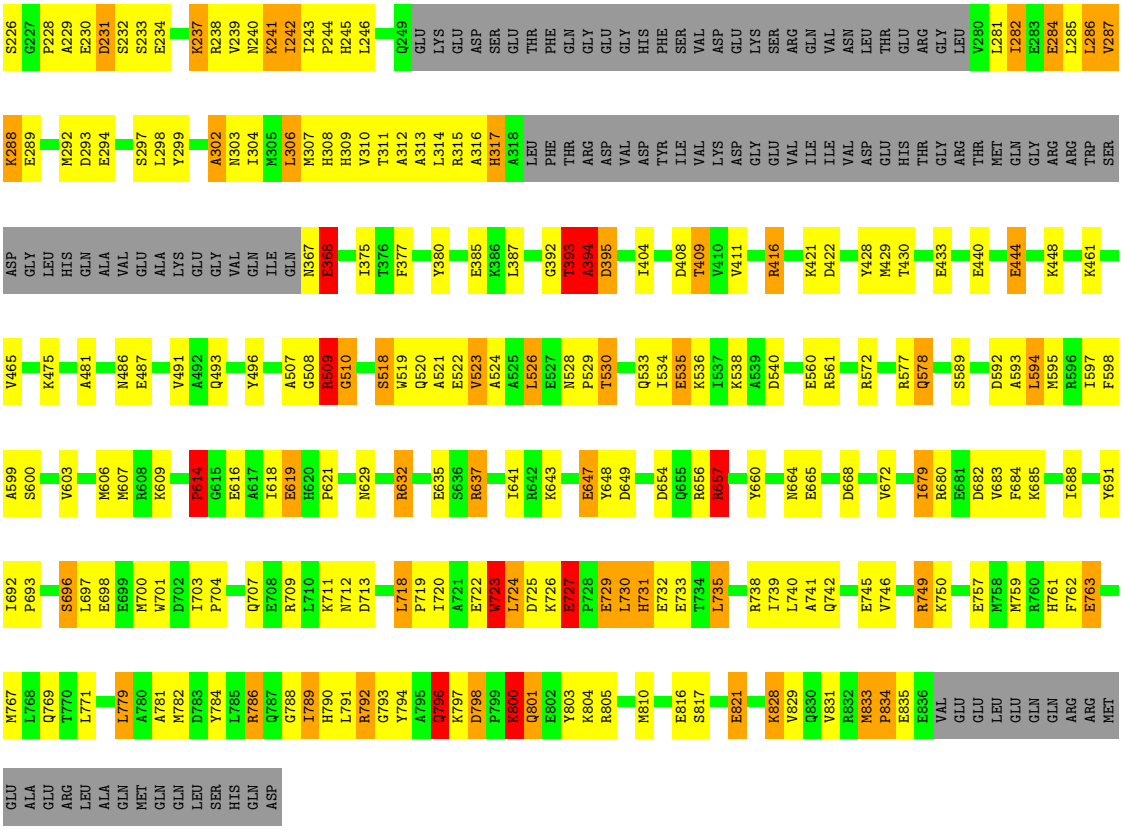
Chain A:



• Molecule 1: Preprotein translocase secA subunit

Chain B:




S226 G227 P228 A229 E230 D231 S232 S233 E234 K237 R238 V239 N240 K241 I242 I243 P244 H245 L246 Q249 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 S297 L298 Y299 A302 N303 I304 M305 L306 M307 H308 H309 V310 T311 A312 A313 L314 R315 A316 H317 A318 LEU PHE THR ARG ASP VAL ASP TYR ILE VAL LYS ASP GLY GLU VAL ILE ILE VAL ASP GLU HIS THR GLY ARG THR MET GLN GLY ARG ARG TRP SER
ASP GLY LEU HIS GLN ALA VAL GLU ALA LYS GLU GLY VAL GLN ILE GLN N367 E368 I375 T376 F377 Y380 E385 K386 L387 G392 T393 A394 D395 I404 D408 T409 V410 V411 R416 K421 D422 Y428 M429 T430 E433 E440 E444 K448 K461
V465 K475 A481 N486 E487 V491 A492 Q493 Y496 A507 G508 R509 G510 S518 W519 Q520 A521 E522 V523 A524 A525 L526 E527 N528 P529 T530 Q533 I534 E535 K536 I537 K538 A539 D540 E560 R561 R572 R577 Q578 S589 D592 A593 L594 M595 R596 I597 F598
A599 S600 V603 M606 M607 R608 K609 P614 Q615 E616 A617 I618 E619 H620 P621 M629 R632 E635 S636 R637 I641 R642 K643 E647 Y648 D649 D654 Q655 R656 R657 Y660 N664 E665 D668 V672 I679 R680 E681 D682 V683 F684 K685 I688 Y691
I692 P693 S696 L697 E698 E699 M700 W701 D702 I703 P704 Q707 E708 R709 L710 K711 N712 D713 L718 P719 I720 A721 E722 W723 L724 D725 K726 E727 P728 E729 L730 H731 E732 E733 T734 L735 R738 I739 L740 A741 Q742 E745 V746 R749 K750 E757 M758 M759 R760 H761 F762 E763
M767 L768 Q769 T770 L771 L779 A780 A781 M782 D783 Y784 L785 R786 Q787 G788 I789 H790 L791 R792 G793 Y794 A795 Q796 K797 D798 P799 K800 Q801 E802 Y803 K804 R805 M810 E816 S817 E821 K828 V829 Q830 V831 R832 M833 P834 E835 E836 VAL GLU GLU LEU GLU GLN GLN ARG ARG MET
GLU ALA GLU ARG LEU ALA GLN MET 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	75.56Å 90.43Å 163.29Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.85 – 2.11 19.84 – 2.11	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.85-2.11) 90.6 (19.84-2.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.263 0.256 , 0.300	Depositor DCC
R_{free} test set	5666 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11936	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ADP

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	1.32	29/5590 (0.5%)	1.07	15/7542 (0.2%)
1	B	1.56	68/6045 (1.1%)	1.27	48/8154 (0.6%)
All	All	1.45	97/11635 (0.8%)	1.17	63/15696 (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	1
1	B	0	5
All	All	0	6

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	GLU	CD-OE1	14.09	1.41	1.25
1	A	699	GLU	CD-OE2	12.11	1.39	1.25
1	A	697	LEU	C-O	11.52	1.45	1.23
1	A	98	CYS	CB-SG	-11.41	1.62	1.82
1	B	23	LYS	CE-NZ	11.33	1.77	1.49
1	B	71	VAL	CB-CG2	10.78	1.75	1.52
1	B	210	GLU	CG-CD	9.82	1.66	1.51
1	B	98	CYS	CB-SG	-8.88	1.67	1.82
1	B	385	GLU	CD-OE2	8.81	1.35	1.25
1	A	698	GLU	C-O	8.81	1.40	1.23
1	B	96	GLU	CD-OE1	8.61	1.35	1.25
1	B	385	GLU	CD-OE1	8.35	1.34	1.25
1	A	587	TYR	CE2-CZ	-8.13	1.27	1.38
1	B	117	TYR	CD2-CE2	-7.68	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	CD-OE2	7.56	1.33	1.25
1	B	801	GLN	N-CA	7.45	1.61	1.46
1	A	431	GLU	CD-OE1	7.45	1.33	1.25
1	B	103	ARG	CG-CD	7.37	1.70	1.51
1	B	380	TYR	CE2-CZ	-7.32	1.29	1.38
1	B	61	GLU	CD-OE1	7.28	1.33	1.25
1	B	68	PHE	CD2-CE2	7.23	1.53	1.39
1	B	635	GLU	CD-OE1	7.23	1.33	1.25
1	B	803	TYR	CD2-CE2	7.19	1.50	1.39
1	B	560	GLU	CG-CD	7.01	1.62	1.51
1	B	385	GLU	CG-CD	6.89	1.62	1.51
1	A	560	GLU	CD-OE1	6.78	1.33	1.25
1	A	696	SER	CB-OG	6.74	1.51	1.42
1	B	141	GLU	CG-CD	6.68	1.61	1.51
1	B	73	GLU	N-CA	6.57	1.59	1.46
1	B	394	ALA	CA-CB	6.57	1.66	1.52
1	A	141	GLU	CG-CD	6.55	1.61	1.51
1	B	56	LYS	CD-CE	6.54	1.67	1.51
1	B	46	LYS	CB-CG	-6.53	1.34	1.52
1	A	460	GLU	CB-CG	6.41	1.64	1.52
1	B	122	THR	C-O	-6.36	1.11	1.23
1	B	163	ALA	CA-CB	6.31	1.65	1.52
1	A	572	ARG	CB-CG	-6.29	1.35	1.52
1	B	572	ARG	CB-CG	-6.28	1.35	1.52
1	B	722	GLU	CD-OE1	6.28	1.32	1.25
1	B	76	LYS	CE-NZ	6.21	1.64	1.49
1	B	196	GLU	CB-CG	-6.15	1.40	1.52
1	B	202	LYS	CD-CE	6.10	1.66	1.51
1	A	460	GLU	CG-CD	6.09	1.61	1.51
1	A	626	ALA	CA-CB	-6.03	1.39	1.52
1	A	816	GLU	CB-CG	6.03	1.63	1.52
1	B	115	PRO	CG-CD	6.02	1.70	1.50
1	B	24	VAL	CB-CG2	5.98	1.65	1.52
1	B	560	GLU	CD-OE1	5.98	1.32	1.25
1	B	126	VAL	C-O	-5.98	1.11	1.23
1	B	665	GLU	CG-CD	5.96	1.60	1.51
1	B	106	GLU	CD-OE1	5.96	1.32	1.25
1	B	148	GLU	CG-CD	5.94	1.60	1.51
1	B	41	GLU	CG-CD	5.91	1.60	1.51
1	A	560	GLU	CG-CD	5.89	1.60	1.51
1	B	616	GLU	CB-CG	5.82	1.63	1.52
1	B	36	GLU	CB-CG	-5.79	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLU	CG-CD	5.76	1.60	1.51
1	B	80	GLY	C-O	-5.75	1.14	1.23
1	B	173	ASP	CB-CG	5.75	1.63	1.51
1	B	578	GLN	CB-CG	5.73	1.68	1.52
1	A	503	ALA	CA-CB	-5.67	1.40	1.52
1	A	431	GLU	CD-OE2	5.66	1.31	1.25
1	B	444	GLU	CG-CD	5.62	1.60	1.51
1	A	96	GLU	CG-CD	-5.60	1.43	1.51
1	B	421	LYS	CE-NZ	5.57	1.62	1.49
1	B	656	ARG	CB-CG	5.55	1.67	1.52
1	B	149	PHE	CD2-CE2	-5.53	1.28	1.39
1	B	56	LYS	CE-NZ	5.53	1.62	1.49
1	B	496	TYR	CB-CG	-5.51	1.43	1.51
1	B	660	TYR	CD2-CE2	5.48	1.47	1.39
1	B	763	GLU	CG-CD	5.46	1.60	1.51
1	B	647	GLU	CD-OE2	5.43	1.31	1.25
1	B	58	GLU	CD-OE1	5.40	1.31	1.25
1	A	101	GLU	CD-OE2	5.39	1.31	1.25
1	A	560	GLU	CD-OE2	5.38	1.31	1.25
1	B	72	ARG	CZ-NH1	-5.35	1.26	1.33
1	B	106	GLU	CD-OE2	5.34	1.31	1.25
1	B	416	ARG	N-CA	5.34	1.57	1.46
1	B	170	TYR	CD1-CE1	5.33	1.47	1.39
1	B	723	TRP	CB-CG	5.29	1.59	1.50
1	A	465	VAL	CB-CG1	-5.27	1.41	1.52
1	B	141	GLU	CD-OE1	5.27	1.31	1.25
1	B	665	GLU	CD-OE2	5.25	1.31	1.25
1	A	777	GLU	CG-CD	5.20	1.59	1.51
1	B	828	LYS	CE-NZ	5.20	1.62	1.49
1	B	816	GLU	CB-CG	5.19	1.62	1.52
1	A	41	GLU	CG-CD	5.14	1.59	1.51
1	B	727	GLU	CD-OE1	5.11	1.31	1.25
1	A	673	SER	CB-OG	-5.07	1.35	1.42
1	B	654	ASP	CG-OD1	5.06	1.36	1.25
1	A	196	GLU	CD-OE2	5.04	1.31	1.25
1	B	821	GLU	CG-CD	-5.04	1.44	1.51
1	B	37	LYS	N-CA	5.03	1.56	1.46
1	A	816	GLU	CG-CD	5.03	1.59	1.51
1	B	43	LEU	C-O	5.02	1.32	1.23
1	A	501	THR	C-O	-5.02	1.13	1.23
1	B	25	VAL	C-O	-5.01	1.13	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	B	167	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	657	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	A	72	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	A	657	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	B	786	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	B	23	LYS	CD-CE-NZ	8.43	131.09	111.70
1	B	408	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	144	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	B	201	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	189	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	782	MET	CG-SD-CE	7.27	111.83	100.20
1	B	207	LEU	CB-CG-CD2	-7.18	98.79	111.00
1	B	801	GLN	N-CA-CB	7.09	123.36	110.60
1	B	53	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	540	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	786	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	A	72	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	97	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	102	MET	CG-SD-CE	-6.58	89.68	100.20
1	B	367	ASN	CB-CA-C	6.55	123.51	110.40
1	B	408	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	572	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	821	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	B	187	LEU	CB-CG-CD1	-6.33	100.24	111.00
1	B	723	TRP	CA-CB-CG	6.26	125.59	113.70
1	B	133	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	367	ASN	N-CA-CB	-5.98	99.83	110.60
1	B	167	ARG	CD-NE-CZ	5.89	131.85	123.60
1	B	540	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	367	ASN	N-CA-C	5.86	126.83	111.00
1	B	103	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	A	509	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	B	387	LEU	CA-CB-CG	5.79	128.60	115.30
1	A	654	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	689	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	810	MET	CG-SD-CE	-5.72	91.04	100.20
1	B	801	GLN	CB-CA-C	-5.70	99.00	110.40
1	A	805	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	173	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	805	ARG	CB-CA-C	-5.55	99.30	110.40
1	B	821	GLU	CB-CA-C	-5.53	99.35	110.40
1	A	657	ARG	NE-CZ-NH1	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	800	LYS	C-N-CA	-5.43	108.11	121.70
1	B	572	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	77	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	85	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	656	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	779	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	418	MET	CG-SD-CE	5.21	108.54	100.20
1	A	38	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	189	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	475	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	B	77	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	81	MET	CG-SD-CE	-5.14	91.98	100.20
1	B	682	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	420	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	649	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	53	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	805	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	801	GLN	CA-CB-CG	5.03	124.47	113.40
1	B	422	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	580	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	GLY	Peptide
1	B	393	THR	Peptide
1	B	394	ALA	Peptide
1	B	791	LEU	Peptide
1	B	793	GLY	Peptide
1	B	794	TYR	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	5500	0	5481	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5948	0	5946	203	0
2	A	27	0	12	0	0
2	B	27	0	12	4	0
3	A	179	0	0	11	0
3	B	255	0	0	34	0
All	All	11936	0	11451	298	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 (298) 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:71:VAL:CB	1:B:71:VAL:CG2	1.75	1.59
1:B:23:LYS:CE	1:B:23:LYS:NZ	1.77	1.44
1:A:538:LYS:HZ3	1:B:528:ASN:ND2	1.28	1.27
1:A:538:LYS:NZ	1:B:528:ASN:HD22	1.48	1.10
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.59	1.00
1:A:538:LYS:NZ	1:B:528:ASN:ND2	2.07	0.96
1:B:493:GLN:HG2	3:B:1068:HOH:O	1.66	0.96
1:B:395:ASP:HB2	3:B:1109:HOH:O	1.63	0.96
1:B:519:TRP:CH2	1:B:538:LYS:NZ	2.35	0.94
1:B:519:TRP:CZ2	1:B:538:LYS:NZ	2.37	0.92
1:A:577:ARG:HD3	3:A:1000:HOH:O	1.73	0.89
1:B:297:SER:O	1:B:303:ASN:ND2	2.06	0.87
1:B:800:LYS:O	1:B:801:GLN:HB2	1.75	0.86
1:B:17:THR:HG22	1:B:21:MET:HE2	1.58	0.85
1:B:598:PHE:O	1:B:600:SER:N	2.09	0.84
1:B:647:GLU:OE2	1:B:800:LYS:HE2	1.78	0.83
1:B:17:THR:HG22	1:B:21:MET:CE	2.09	0.82
1:A:732:GLU:OE2	1:A:736:ARG:NH1	2.12	0.82
1:A:531:ALA:O	1:A:534:ILE:HG13	1.80	0.81
1:B:33:PRO:O	1:B:37:LYS:HD3	1.81	0.81
1:B:518:SER:HA	3:B:1001:HOH:O	1.79	0.80
1:A:395:ASP:HA	3:A:927:HOH:O	1.83	0.79
1:A:598:PHE:O	1:A:600:SER:N	2.16	0.78
1:B:526:LEU:HD21	1:B:533:GLN:HE22	1.49	0.76
1:B:637:ARG:NH1	1:B:641:ILE:HD11	2.00	0.76
1:B:518:SER:CA	3:B:1001:HOH:O	2.33	0.76
1:A:753:VAL:HG21	1:A:833:MET:HE2	1.67	0.76
1:B:316:ALA:O	1:B:317:HIS:CG	2.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:HD3	3:B:914:HOH:O	1.86	0.74
1:B:395:ASP:CB	3:B:1109:HOH:O	2.25	0.74
1:B:521:ALA:O	1:B:524:ALA:N	2.18	0.73
1:A:618:ILE:O	1:A:619:GLU:HB2	1.88	0.72
1:B:800:LYS:O	1:B:801:GLN:CB	2.29	0.72
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.38	0.71
1:A:103:ARG:NH1	1:A:573:GLY:O	2.24	0.70
1:B:621:PRO:HG2	3:B:966:HOH:O	1.93	0.69
1:A:395:ASP:CG	1:A:396:THR:N	2.46	0.69
1:A:731:HIS:CE1	1:A:734:THR:HG23	2.28	0.69
1:B:71:VAL:CG2	1:B:71:VAL:CA	2.67	0.68
1:B:600:SER:HB3	1:B:603:VAL:HB	1.76	0.68
1:B:685:LYS:HE3	3:B:1135:HOH:O	1.93	0.68
1:B:395:ASP:CA	3:B:1109:HOH:O	2.41	0.67
1:B:788:GLY:CA	3:B:1137:HOH:O	2.43	0.66
1:A:530:THR:H	1:A:533:GLN:HE21	1.43	0.66
1:B:647:GLU:OE2	1:B:800:LYS:CE	2.44	0.65
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.27	0.65
1:B:614:PRO:HA	3:B:1115:HOH:O	1.95	0.65
1:B:311:THR:O	1:B:315:ARG:HB2	1.96	0.64
1:B:238:ARG:NE	1:B:238:ARG:HA	2.12	0.64
1:B:282:ILE:CD1	1:B:286:LEU:HD13	2.28	0.64
1:A:508:GLY:O	1:A:510:GLY:N	2.31	0.63
1:B:37:LYS:CD	3:B:1125:HOH:O	2.47	0.63
1:B:71:VAL:CG2	1:B:71:VAL:CG1	2.72	0.63
1:A:742:GLN:HA	1:A:742:GLN:HE21	1.65	0.62
1:B:304:ILE:HG21	1:B:781:ALA:HB1	1.80	0.62
1:A:508:GLY:C	1:A:510:GLY:H	2.02	0.62
1:A:395:ASP:CG	1:A:396:THR:H	2.04	0.62
1:B:198:ARG:HH21	1:B:664:ASN:HD22	1.47	0.62
1:A:531:ALA:O	1:A:534:ILE:CG1	2.47	0.61
1:A:699:GLU:OE2	1:A:700:MET:CE	2.49	0.61
1:A:15:ASP:OD1	1:A:19:ARG:NH2	2.34	0.61
1:B:817:SER:O	1:B:821:GLU:CG	2.49	0.61
1:B:804:LYS:HE2	3:B:954:HOH:O	2.00	0.61
1:A:144:ARG:O	1:A:148:GLU:HG3	2.01	0.61
1:B:668:ASP:OD1	3:B:1147:HOH:O	2.16	0.61
1:A:520:GLN:CD	3:A:1029:HOH:O	2.39	0.60
1:A:29:ASN:OD1	1:A:72:ARG:NH1	2.32	0.60
1:B:114:LEU:HB2	1:B:115:PRO:HD3	1.84	0.60
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HD22	1:A:377:PHE:HZ	1.49	0.60
1:A:534:ILE:HD13	1:B:529:PRO:HG2	1.84	0.60
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.32	0.60
1:B:11:GLY:O	1:B:16:ARG:HB2	2.02	0.59
1:B:228:PRO:O	1:B:230:GLU:HB2	2.02	0.59
1:B:657:ARG:HD3	3:B:1144:HOH:O	2.02	0.59
1:A:510:GLY:HA2	1:A:574:ARG:HH11	1.67	0.59
1:B:287:VAL:O	1:B:288:LYS:HG2	2.02	0.59
1:A:594:LEU:HG	1:A:597:ILE:HD13	1.84	0.59
1:B:742:GLN:O	1:B:745:GLU:HG2	2.02	0.59
1:B:316:ALA:O	1:B:317:HIS:CD2	2.55	0.59
1:B:657:ARG:HH21	1:B:657:ARG:HG3	1.68	0.58
1:B:233:SER:O	1:B:234:GLU:HB2	2.04	0.58
1:A:629:ASN:HD22	1:A:632:ARG:HH21	1.51	0.58
1:B:786:ARG:O	1:B:789:ILE:HB	2.04	0.58
1:B:198:ARG:HH21	1:B:664:ASN:ND2	2.02	0.58
1:B:395:ASP:HA	3:B:1109:HOH:O	2.01	0.58
1:B:392:GLY:O	1:B:394:ALA:HB3	2.03	0.58
1:B:509:ARG:O	1:B:577:ARG:NH2	2.35	0.58
1:A:519:TRP:CH2	1:A:538:LYS:HD3	2.39	0.58
1:A:227:GLY:HA3	1:A:372:LEU:HD21	1.85	0.57
1:B:146:LEU:O	1:B:149:PHE:HB3	2.04	0.57
1:B:304:ILE:CG2	1:B:781:ALA:HB1	2.34	0.57
1:B:394:ALA:HA	3:B:1002:HOH:O	2.05	0.57
1:B:16:ARG:NE	1:B:19:ARG:HH21	2.03	0.57
1:A:18:LEU:O	1:A:22:ARG:HG3	2.05	0.57
1:A:510:GLY:CA	1:A:574:ARG:NH1	2.68	0.56
1:B:81:MET:CE	2:B:901:ADP:C4	2.88	0.56
1:B:81:MET:HE2	2:B:901:ADP:C4	2.40	0.56
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.86	0.56
1:B:245:HIS:HB2	3:B:1098:HOH:O	2.04	0.56
1:B:409:THR:HG23	3:B:912:HOH:O	2.03	0.56
1:B:817:SER:O	1:B:821:GLU:HG2	2.06	0.56
1:A:395:ASP:N	3:A:927:HOH:O	2.38	0.56
1:A:519:TRP:O	1:A:522:GLU:HB2	2.05	0.56
1:B:102:MET:O	1:B:392:GLY:HA2	2.06	0.56
1:B:763:GLU:O	1:B:767:MET:HG3	2.06	0.56
1:B:37:LYS:HD2	3:B:1125:HOH:O	2.05	0.56
1:B:81:MET:HE2	2:B:901:ADP:N3	2.20	0.56
1:B:282:ILE:HD13	1:B:286:LEU:HD13	1.87	0.56
1:A:715:ASP:CG	1:A:715:ASP:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLU:OE2	1:B:395:ASP:N	2.39	0.55
1:B:518:SER:N	3:B:1049:HOH:O	2.39	0.55
1:B:691:TYR:O	1:B:693:PRO:HD3	2.06	0.55
1:B:738:ARG:O	1:B:742:GLN:HG2	2.06	0.55
1:A:754:VAL:CG1	1:A:759:MET:HG2	2.36	0.55
1:B:561:ARG:HB2	1:B:594:LEU:HD22	1.89	0.55
1:B:700:MET:HE3	3:B:1134:HOH:O	2.07	0.55
1:A:618:ILE:O	1:A:619:GLU:CB	2.55	0.55
1:B:11:GLY:O	1:B:16:ARG:CB	2.55	0.55
1:B:243:ILE:HD11	1:B:313:ALA:HB1	1.88	0.55
1:B:307:MET:O	1:B:311:THR:HG23	2.07	0.54
1:A:529:PRO:HA	1:A:533:GLN:NE2	2.21	0.54
1:A:730:LEU:O	1:A:731:HIS:HB3	2.07	0.54
1:A:614:PRO:HA	3:A:1064:HOH:O	2.08	0.53
1:B:308:HIS:CE1	1:B:784:TYR:CZ	2.97	0.53
1:B:727:GLU:HG2	1:B:730:LEU:HB3	1.90	0.53
1:A:180:ASN:ND2	1:A:377:PHE:HZ	2.05	0.53
1:A:526:LEU:HD12	1:A:529:PRO:HB3	1.90	0.53
1:B:518:SER:O	1:B:521:ALA:HB3	2.09	0.53
1:B:12:SER:HB2	1:B:15:ASP:OD2	2.09	0.53
1:B:392:GLY:O	1:B:394:ALA:CA	2.57	0.53
1:A:429:MET:SD	1:A:608:ARG:HG2	2.49	0.52
1:A:519:TRP:CZ2	1:A:538:LYS:HD3	2.45	0.52
1:A:731:HIS:NE2	1:A:733:GLU:HB3	2.25	0.52
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.44	0.52
1:B:17:THR:HG22	1:B:21:MET:HE1	1.89	0.52
1:B:99:ILE:HD12	1:B:211:VAL:HG11	1.92	0.52
1:B:789:ILE:HG22	1:B:789:ILE:O	2.10	0.52
1:B:14:ASN:HD21	1:B:411:VAL:H	1.58	0.51
1:A:535:GLU:OE1	1:A:535:GLU:HA	2.09	0.51
1:B:526:LEU:HD21	1:B:533:GLN:NE2	2.22	0.51
1:A:835:GLU:HG2	1:A:836:GLU:N	2.25	0.51
1:A:394:ALA:HB3	3:A:1006:HOH:O	2.10	0.51
1:B:757:GLU:HG3	3:B:1141:HOH:O	2.10	0.51
1:B:37:LYS:HD3	3:B:1125:HOH:O	2.07	0.51
1:B:759:MET:CE	1:B:762:PHE:HD2	2.24	0.51
1:A:731:HIS:HE1	1:A:734:THR:HG23	1.76	0.51
1:B:444:GLU:O	1:B:448:LYS:HG3	2.11	0.51
1:B:487:GLU:O	1:B:491:VAL:HG23	2.12	0.50
1:B:523:VAL:HG22	3:B:1096:HOH:O	2.11	0.50
1:B:618:ILE:O	1:B:619:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:O	1:B:230:GLU:CB	2.59	0.50
1:B:302:ALA:HA	1:B:810:MET:HE3	1.93	0.50
1:A:461:LYS:HD2	1:A:560:GLU:OE2	2.12	0.50
1:B:789:ILE:O	1:B:789:ILE:CG2	2.59	0.50
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.27	0.50
1:A:577:ARG:CD	3:A:1000:HOH:O	2.43	0.50
1:A:753:VAL:HG21	1:A:833:MET:CE	2.39	0.50
1:B:409:THR:CG2	3:B:912:HOH:O	2.59	0.50
1:B:522:GLU:HA	3:B:1003:HOH:O	2.12	0.50
1:B:771:LEU:C	1:B:771:LEU:HD23	2.32	0.50
1:A:643:LYS:O	1:A:647:GLU:HG3	2.12	0.49
1:A:786:ARG:O	1:A:789:ILE:HB	2.11	0.49
1:A:518:SER:HA	3:A:919:HOH:O	2.11	0.49
1:B:18:LEU:HD23	1:B:21:MET:HE3	1.93	0.49
1:B:691:TYR:OH	1:B:709:ARG:NH2	2.44	0.49
1:B:771:LEU:HD23	1:B:771:LEU:O	2.13	0.49
1:A:833:MET:HE2	1:A:833:MET:HA	1.94	0.49
1:B:833:MET:CB	1:B:834:PRO:HD2	2.42	0.49
1:B:657:ARG:CD	3:B:1144:HOH:O	2.59	0.49
1:B:688:ILE:HD11	1:B:739:ILE:HG21	1.95	0.49
1:A:486:ASN:HD21	1:B:132:ASN:HD21	1.61	0.49
1:B:105:GLY:O	1:B:578:GLN:NE2	2.43	0.48
1:B:712:ASN:C	1:B:828:LYS:HZ1	2.16	0.48
1:A:460:GLU:CD	1:A:460:GLU:H	2.16	0.48
1:B:428:TYR:O	1:B:589:SER:HA	2.12	0.48
1:A:223:LEU:HD21	1:A:377:PHE:CZ	2.49	0.48
1:B:759:MET:HE3	1:B:762:PHE:CD2	2.48	0.48
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.46	0.48
1:A:831:VAL:HG12	1:A:833:MET:HE3	1.96	0.48
1:B:282:ILE:HD11	1:B:298:LEU:HB3	1.95	0.48
1:B:306:LEU:O	1:B:309:HIS:HB2	2.14	0.48
1:A:76:LYS:HD2	1:A:82:ARG:HG3	1.96	0.48
1:A:132:ASN:HD21	1:B:486:ASN:HD21	1.61	0.48
1:B:648:TYR:CZ	1:B:800:LYS:HB2	2.49	0.48
1:A:372:LEU:HD22	1:A:776:LYS:NZ	2.29	0.47
1:B:237:LYS:HA	1:B:240:ASN:HB2	1.96	0.47
1:B:230:GLU:HB3	1:B:231:ASP:O	2.15	0.47
1:B:526:LEU:HD11	1:B:533:GLN:NE2	2.29	0.47
1:B:14:ASN:ND2	1:B:411:VAL:H	2.12	0.47
1:B:302:ALA:HA	1:B:810:MET:CE	2.45	0.47
1:A:47:THR:O	1:A:51:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LYS:O	1:B:465:VAL:HG12	2.15	0.47
1:B:757:GLU:O	1:B:761:HIS:HD2	1.98	0.47
1:B:237:LYS:NZ	1:B:241:LYS:HD2	2.30	0.47
1:B:713:ASP:C	1:B:828:LYS:NZ	2.69	0.47
1:B:817:SER:O	1:B:821:GLU:HG3	2.15	0.47
1:B:287:VAL:O	1:B:287:VAL:HG13	2.15	0.46
1:B:284:GLU:O	1:B:287:VAL:HB	2.15	0.46
1:A:510:GLY:HA2	1:A:574:ARG:NH1	2.29	0.46
1:A:538:LYS:HZ3	1:B:528:ASN:HD22	0.59	0.46
1:B:730:LEU:O	1:B:731:HIS:HB2	2.15	0.46
1:A:458:SER:HB2	1:A:460:GLU:OE2	2.16	0.46
1:A:132:ASN:HD21	1:B:486:ASN:ND2	2.14	0.46
1:B:81:MET:HE1	2:B:901:ADP:C4	2.51	0.46
1:B:680:ARG:O	1:B:684:PHE:HB2	2.16	0.46
1:B:720:ILE:HG22	1:B:724:LEU:HG	1.98	0.46
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.15	0.46
1:A:613:LYS:HA	1:A:614:PRO:HD2	1.84	0.46
1:B:508:GLY:O	1:B:510:GLY:N	2.48	0.46
1:A:368:GLU:CD	1:A:368:GLU:N	2.70	0.45
1:A:508:GLY:O	1:A:509:ARG:HG2	2.16	0.45
1:B:71:VAL:O	1:B:71:VAL:HG12	2.16	0.45
1:B:742:GLN:O	1:B:746:VAL:HG23	2.16	0.45
1:A:571:LEU:O	1:A:574:ARG:HB2	2.17	0.45
1:A:642:ARG:NH1	3:A:942:HOH:O	2.48	0.45
1:B:243:ILE:N	1:B:244:PRO:HD2	2.31	0.45
1:B:144:ARG:O	1:B:148:GLU:HB2	2.17	0.45
1:B:377:PHE:CD1	3:B:981:HOH:O	2.68	0.45
1:B:712:ASN:O	1:B:828:LYS:NZ	2.49	0.45
1:B:246:LEU:CD1	1:B:314:LEU:HD22	2.47	0.45
1:A:227:GLY:N	1:A:370:GLN:O	2.50	0.45
1:A:518:SER:CA	3:A:919:HOH:O	2.64	0.45
1:A:699:GLU:OE2	1:A:700:MET:HE1	2.17	0.45
1:B:589:SER:OG	1:B:592:ASP:OD2	2.27	0.45
1:B:732:GLU:O	1:B:735:LEU:HG	2.16	0.45
1:A:763:GLU:O	1:A:767:MET:HG3	2.17	0.45
1:B:282:ILE:HG13	1:B:299:TYR:CE2	2.52	0.45
1:B:312:ALA:O	1:B:316:ALA:HB2	2.17	0.45
1:B:718:LEU:O	1:B:720:ILE:N	2.48	0.45
1:B:230:GLU:OE1	1:B:368:GLU:O	2.36	0.44
1:B:239:VAL:O	1:B:242:ILE:HG22	2.17	0.44
1:B:430:THR:OG1	1:B:433:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:HG22	1:B:404:ILE:O	2.18	0.44
1:B:60:LEU:O	1:B:63:LEU:HB2	2.16	0.44
1:B:202:LYS:NZ	3:B:1081:HOH:O	2.50	0.44
1:B:392:GLY:O	1:B:394:ALA:CB	2.66	0.44
1:B:440:GLU:O	1:B:444:GLU:HG3	2.18	0.44
1:B:518:SER:C	3:B:1001:HOH:O	2.54	0.44
1:B:697:LEU:HD12	1:B:697:LEU:H	1.82	0.44
1:B:718:LEU:HB3	1:B:723:TRP:CZ2	2.53	0.44
1:B:693:PRO:O	1:B:696:SER:HB2	2.18	0.43
1:B:594:LEU:HG	1:B:597:ILE:HD13	2.01	0.43
1:B:718:LEU:O	1:B:720:ILE:HD12	2.19	0.43
1:B:593:ALA:O	1:B:595:MET:N	2.51	0.43
1:B:735:LEU:C	1:B:735:LEU:HD12	2.38	0.43
1:A:66:GLU:O	1:A:70:VAL:HG23	2.19	0.43
1:A:754:VAL:HG11	1:A:759:MET:HG2	2.00	0.43
1:B:11:GLY:O	1:B:16:ARG:HG2	2.19	0.43
1:B:679:ILE:O	1:B:683:VAL:HG23	2.19	0.43
1:B:796:GLN:O	1:B:798:ASP:N	2.51	0.43
1:A:620:HIS:HA	1:A:621:PRO:HD2	1.76	0.43
1:B:392:GLY:O	1:B:394:ALA:N	2.52	0.43
1:B:718:LEU:HB3	1:B:723:TRP:HZ2	1.83	0.43
1:B:311:THR:O	1:B:315:ARG:CB	2.66	0.43
1:B:745:GLU:HG3	1:B:749:ARG:NH2	2.33	0.43
1:B:788:GLY:CA	1:B:792:ARG:CG	2.97	0.43
1:A:719:PRO:HB2	1:A:722:GLU:HB2	2.01	0.42
1:B:788:GLY:O	1:B:792:ARG:CG	2.67	0.42
1:A:33:PRO:O	1:A:34:GLU:C	2.57	0.42
1:A:699:GLU:OE2	1:A:700:MET:HE2	2.18	0.42
1:B:103:ARG:HG2	1:B:393:THR:OG1	2.19	0.42
1:B:507:ALA:O	3:B:1136:HOH:O	2.22	0.42
1:A:35:MET:HA	1:A:38:LEU:HD13	2.01	0.42
1:A:519:TRP:CH2	1:A:538:LYS:HE2	2.54	0.42
1:B:12:SER:HB2	1:B:15:ASP:OD1	2.19	0.42
1:B:530:THR:HG22	1:B:533:GLN:HG3	2.00	0.42
1:A:428:TYR:O	1:A:589:SER:HA	2.19	0.42
1:A:594:LEU:O	1:A:597:ILE:HG12	2.20	0.42
1:A:114:LEU:HB2	1:A:115:PRO:CD	2.50	0.42
1:B:187:LEU:HD21	1:B:375:ILE:HB	2.01	0.42
1:B:228:PRO:O	1:B:230:GLU:N	2.53	0.42
1:B:692:ILE:HG21	1:B:732:GLU:HG3	2.01	0.42
1:A:228:PRO:O	1:A:230:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:O	1:A:145:PRO:HD2	2.20	0.41
1:A:762:PHE:O	1:A:766:VAL:HG23	2.20	0.41
1:B:114:LEU:N	1:B:115:PRO:HD2	2.35	0.41
1:B:242:ILE:HD11	1:B:246:LEU:HD21	2.02	0.41
1:A:99:ILE:HD11	1:A:407:LEU:HD13	2.02	0.41
1:B:103:ARG:HD2	1:B:104:THR:N	2.35	0.41
1:B:179:ASN:HB2	1:B:377:PHE:CE1	2.54	0.41
1:B:672:VAL:HG12	1:B:672:VAL:O	2.21	0.41
1:B:534:ILE:O	1:B:535:GLU:C	2.57	0.41
1:B:788:GLY:HA3	3:B:1137:HOH:O	2.14	0.41
1:A:31:MET:CE	1:A:66:GLU:HG2	2.51	0.41
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.95	0.41
1:B:282:ILE:CD1	1:B:286:LEU:CD1	2.98	0.41
1:A:395:ASP:CA	3:A:927:HOH:O	2.55	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.93	0.41
1:B:523:VAL:CG2	3:B:1096:HOH:O	2.69	0.41
1:A:440:GLU:O	1:A:444:GLU:HG3	2.21	0.41
1:B:750:LYS:HD2	1:B:829:VAL:HG13	2.03	0.41
1:A:598:PHE:C	1:A:600:SER:N	2.75	0.40
1:B:103:ARG:CD	1:B:104:THR:N	2.85	0.40
1:B:723:TRP:HB2	1:B:724:LEU:HD23	2.04	0.40
1:A:453:LEU:HB3	1:A:556:ILE:HD13	2.03	0.40
1:B:701:TRP:N	1:B:701:TRP:CD1	2.87	0.40
1:A:692:ILE:HG23	1:A:701:TRP:CD1	2.57	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	687/853 (80%)	639 (93%)	36 (5%)	12 (2%)	9 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	742/853 (87%)	657 (88%)	53 (7%)	32 (4%)	2 0
All	All	1429/1706 (84%)	1296 (91%)	89 (6%)	44 (3%)	4 1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	599	ALA
1	A	614	PRO
1	B	229	ALA
1	B	289	GLU
1	B	292	MET
1	B	293	ASP
1	B	368	GLU
1	B	394	ALA
1	B	599	ALA
1	B	614	PRO
1	B	729	GLU
1	B	741	ALA
1	B	797	LYS
1	B	834	PRO
1	A	509	ARG
1	A	601	ASP
1	A	602	ARG
1	B	302	ALA
1	B	509	ARG
1	B	510	GLY
1	B	594	LEU
1	B	740	LEU
1	B	796	GLN
1	A	619	GLU
1	B	317	HIS
1	B	395	ASP
1	B	481	ALA
1	B	719	PRO
1	B	731	HIS
1	A	613	LYS
1	A	789	ILE
1	B	287	VAL
1	B	835	GLU
1	A	228	PRO
1	A	510	GLY

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Mol	Chain	Res	Type
1	B	232	SER
1	B	619	GLU
1	B	789	ILE
1	B	790	HIS
1	B	798	ASP
1	A	615	GLY
1	B	698	GLU
1	B	704	PRO

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	586/728 (80%)	548 (94%)	38 (6%)	17 14
1	B	635/728 (87%)	571 (90%)	64 (10%)	7 4
All	All	1221/1456 (84%)	1119 (92%)	102 (8%)	11 7

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	17	THR
1	A	72	ARG
1	A	96	GLU
1	A	98	CYS
1	A	103	ARG
1	A	226	SER
1	A	366	GLN
1	A	368	GLU
1	A	369	ASN
1	A	393	THR
1	A	409	THR
1	A	475	LYS
1	A	506	MET
1	A	523	VAL

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Mol	Chain	Res	Type
1	A	527	GLU
1	A	537	ILE
1	A	574	ARG
1	A	596	ARG
1	A	610	LEU
1	A	635	GLU
1	A	636	SER
1	A	672	VAL
1	A	715	ASP
1	A	725	ASP
1	A	730	LEU
1	A	731	HIS
1	A	733	GLU
1	A	742	GLN
1	A	748	GLN
1	A	749	ARG
1	A	754	VAL
1	A	776	LYS
1	A	791	LEU
1	A	796	GLN
1	A	797	LYS
1	A	800	LYS
1	A	833	MET
1	B	16	ARG
1	B	38	LEU
1	B	102	MET
1	B	103	ARG
1	B	210	GLU
1	B	225	ILE
1	B	226	SER
1	B	231	ASP
1	B	237	LYS
1	B	241	LYS
1	B	242	ILE
1	B	281	LEU
1	B	282	ILE
1	B	284	GLU
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	294	GLU
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	368	GLU
1	B	393	THR
1	B	409	THR
1	B	416	ARG
1	B	429	MET
1	B	509	ARG
1	B	518	SER
1	B	520	GLN
1	B	523	VAL
1	B	526	LEU
1	B	530	THR
1	B	535	GLU
1	B	536	LYS
1	B	606	MET
1	B	607	MET
1	B	609	LYS
1	B	614	PRO
1	B	632	ARG
1	B	637	ARG
1	B	643	LYS
1	B	657	ARG
1	B	679	ILE
1	B	696	SER
1	B	703	ILE
1	B	707	GLN
1	B	711	LYS
1	B	718	LEU
1	B	723	TRP
1	B	724	LEU
1	B	725	ASP
1	B	726	LYS
1	B	727	GLU
1	B	729	GLU
1	B	730	LEU
1	B	733	GLU
1	B	735	LEU
1	B	749	ARG
1	B	769	GLN
1	B	779	LEU
1	B	792	ARG
1	B	796	GLN

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Mol	Chain	Res	Type
1	B	800	LYS
1	B	831	VAL
1	B	833	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	484	HIS
1	A	486	ASN
1	A	533	GLN
1	A	542	GLN
1	A	629	ASN
1	A	662	GLN
1	A	742	GLN
1	A	761	HIS
1	B	14	ASN
1	B	180	ASN
1	B	240	ASN
1	B	303	ASN
1	B	308	HIS
1	B	317	HIS
1	B	369	ASN
1	B	484	HIS
1	B	486	ASN
1	B	520	GLN
1	B	528	ASN
1	B	545	HIS
1	B	629	ASN
1	B	638	ASN
1	B	664	ASN
1	B	731	HIS
1	B	742	GLN
1	B	761	HIS
1	B	769	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	ADP	B	901	-	24,29,29	1.54	3 (12%)	29,45,45	1.75	6 (20%)
2	ADP	A	900	-	24,29,29	1.38	3 (12%)	29,45,45	1.58	5 (17%)

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	ADP	B	901	-	-	3/12/32/32	0/3/3/3
2	ADP	A	900	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ADP	O4'-C1'	4.90	1.47	1.41
2	A	900	ADP	O4'-C1'	3.74	1.46	1.41
2	A	900	ADP	C2-N3	2.94	1.36	1.32
2	A	900	ADP	C2'-C1'	-2.77	1.49	1.53
2	B	901	ADP	PA-O1A	-2.74	1.41	1.50
2	B	901	ADP	C5-C4	2.68	1.48	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	ADP	N3-C2-N1	-4.19	122.13	128.68
2	A	900	ADP	O4'-C1'-C2'	-4.15	100.86	106.93
2	B	901	ADP	N6-C6-N1	3.95	126.77	118.57
2	B	901	ADP	C5-C6-N6	-3.80	114.58	120.35
2	B	901	ADP	O3B-PB-O2B	3.39	120.58	107.64
2	B	901	ADP	N3-C2-N1	-3.25	123.60	128.68
2	A	900	ADP	C5-C6-N6	-2.84	116.03	120.35
2	B	901	ADP	PA-O3A-PB	-2.80	123.22	132.83
2	A	900	ADP	N6-C6-N1	2.35	123.46	118.57
2	B	901	ADP	O2B-PB-O1B	-2.11	102.42	110.68
2	A	900	ADP	O3B-PB-O1B	-2.10	102.45	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	ADP	PA-O3A-PB-O3B
2	B	901	ADP	PA-O3A-PB-O3B
2	A	900	ADP	PA-O3A-PB-O1B
2	B	901	ADP	PA-O3A-PB-O1B
2	B	901	ADP	PA-O3A-PB-O2B

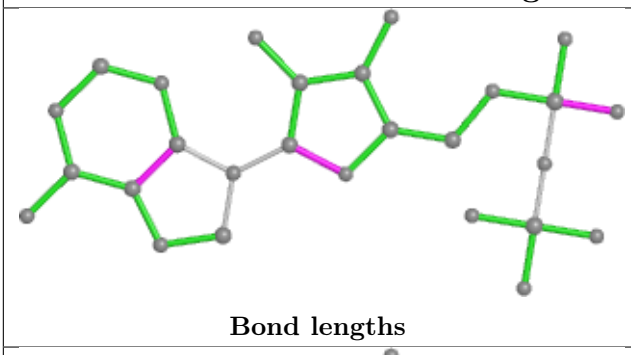
There are no ring outliers.

1 monomer is involved in 4 short contacts:

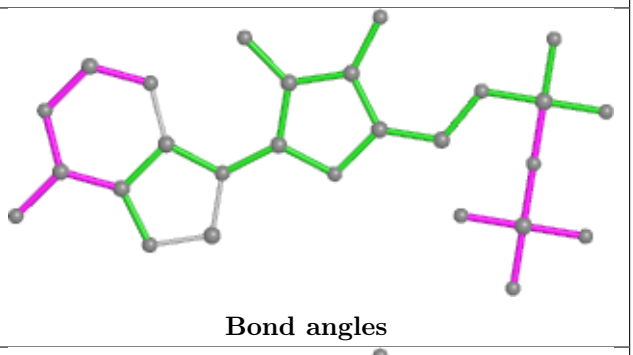
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ADP	4	0

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.

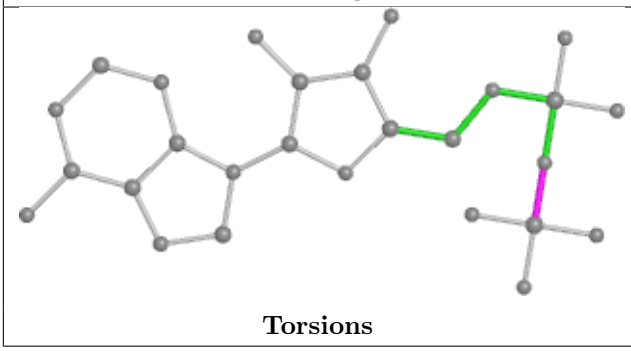
Ligand ADP B 901



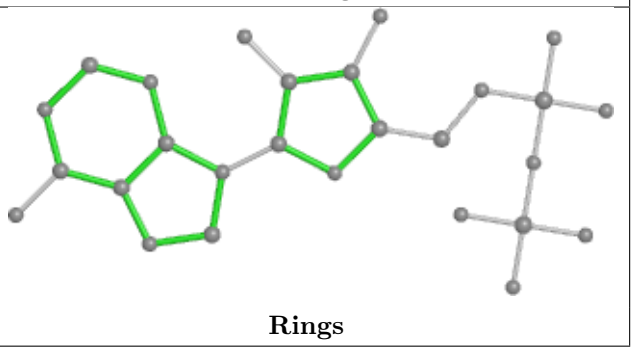
Bond lengths



Bond angles

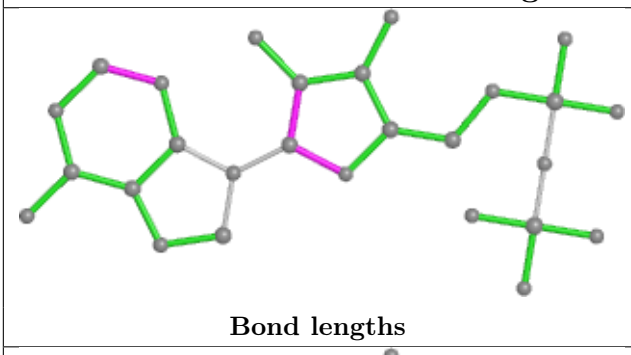


Torsions

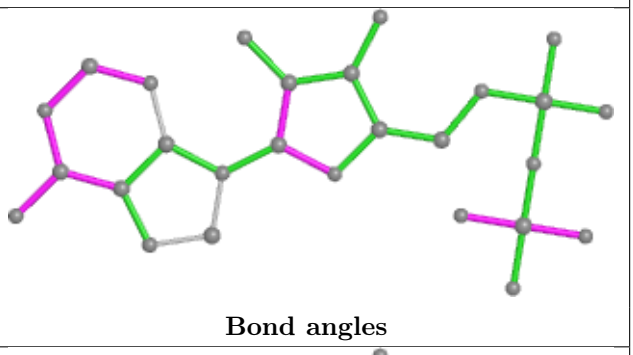


Rings

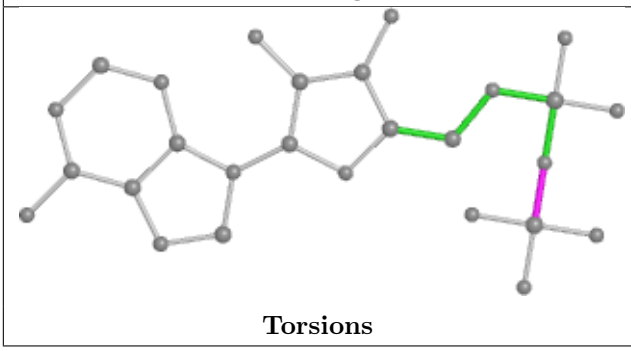
Ligand ADP A 900



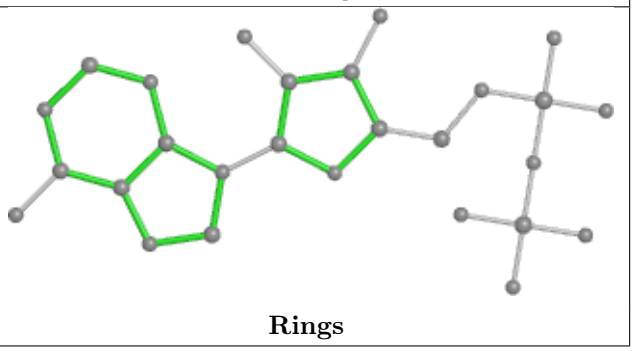
Bond lengths



Bond angles



Torsions



Rings

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.

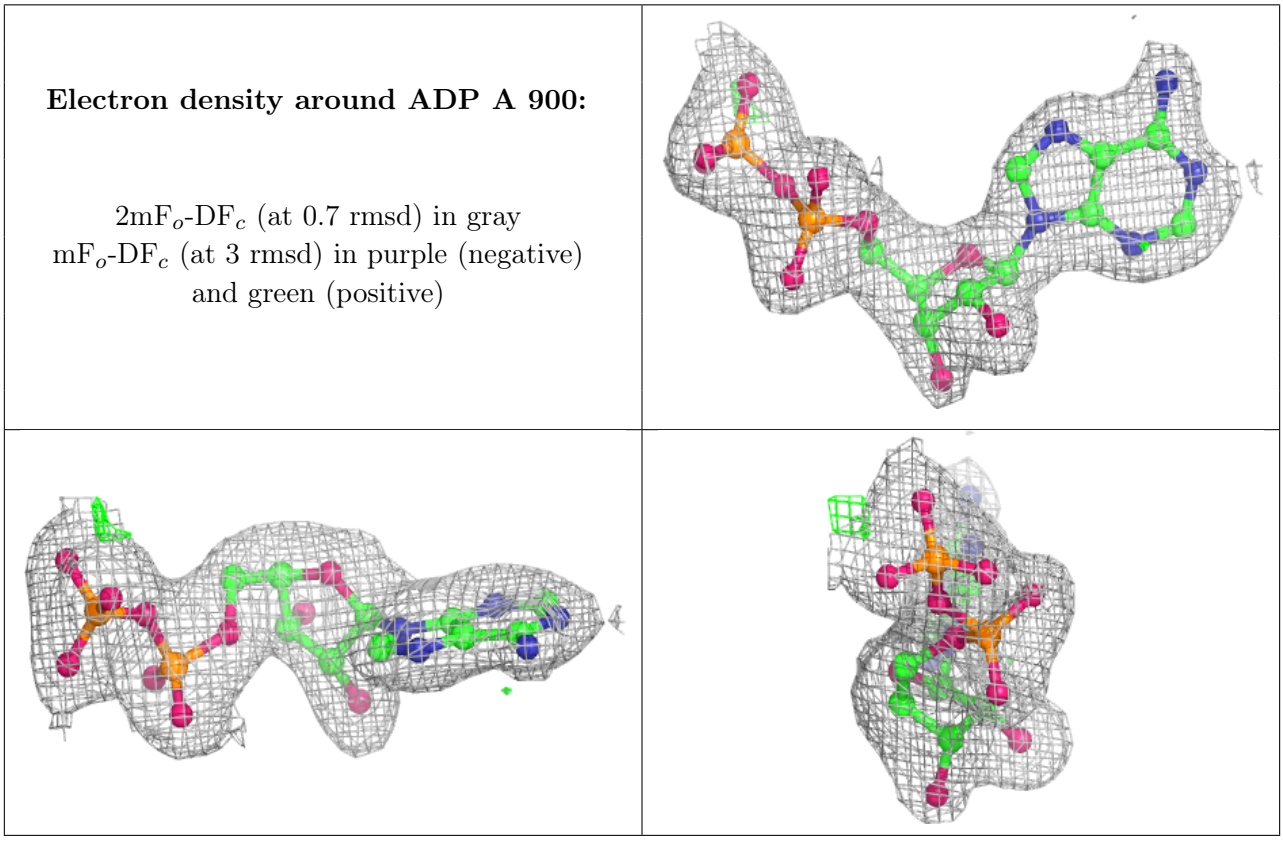
6.4 Ligands

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.

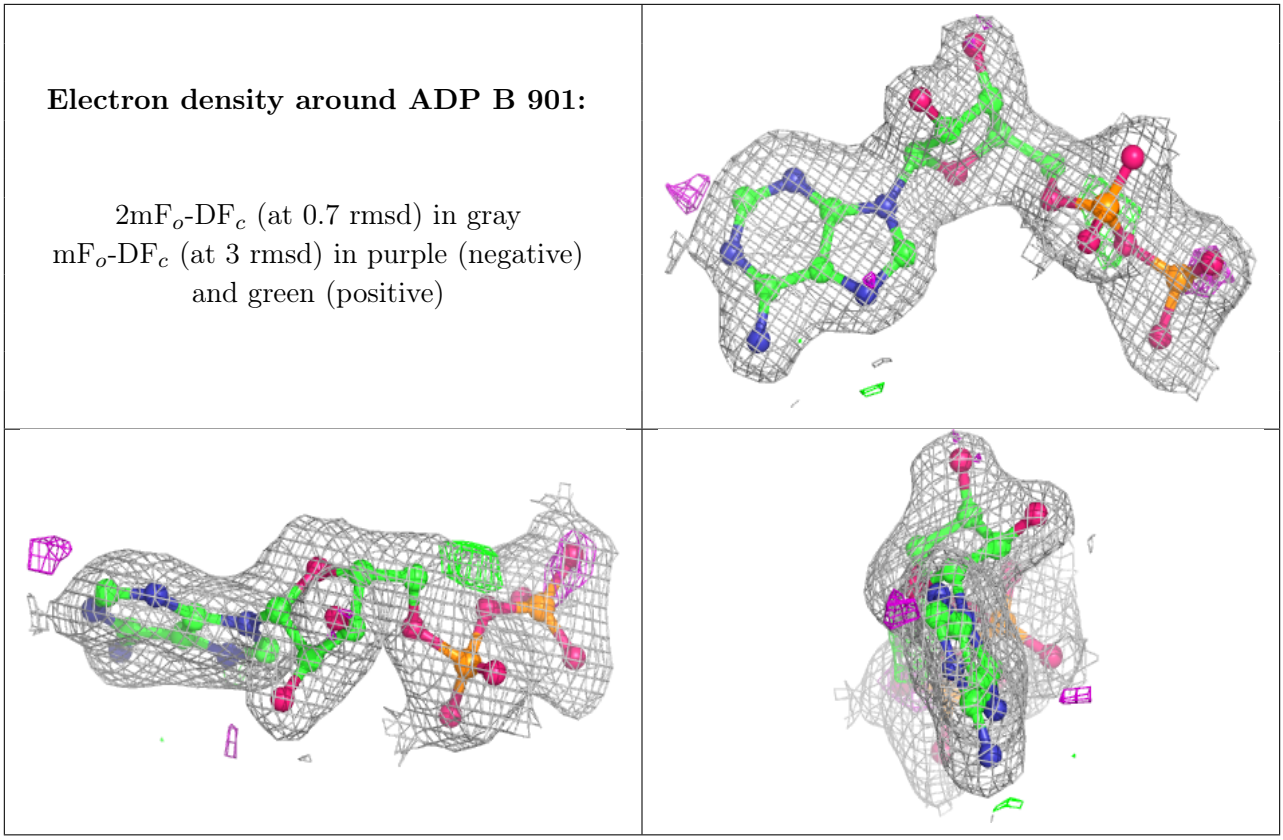
Electron density around ADP A 900:

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



Electron density around ADP 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)



6.5 Other polymers (i)

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