



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:27 AM EDT

PDB ID : 2FSI / pdb_00002fsi
Title : Complex SecA:ADP from Escherichia coli
Authors : Papanikolaou, 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

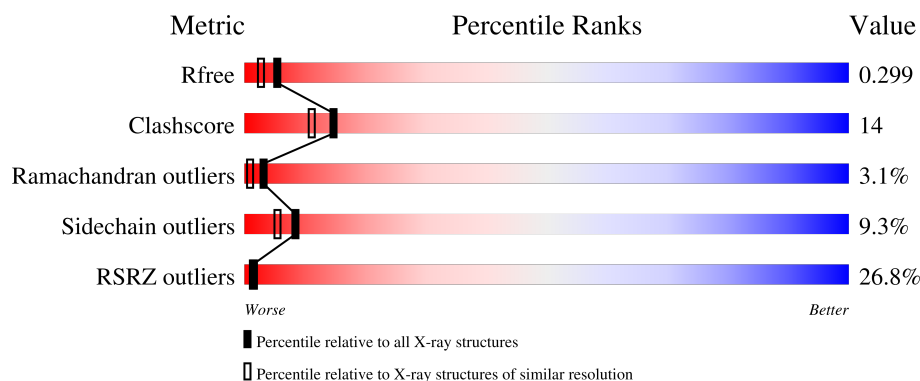
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	853	15% 57% 20% • • 19%
1	B	853	30% 47% 30% 9% • 12%

2 Entry composition [i](#)

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

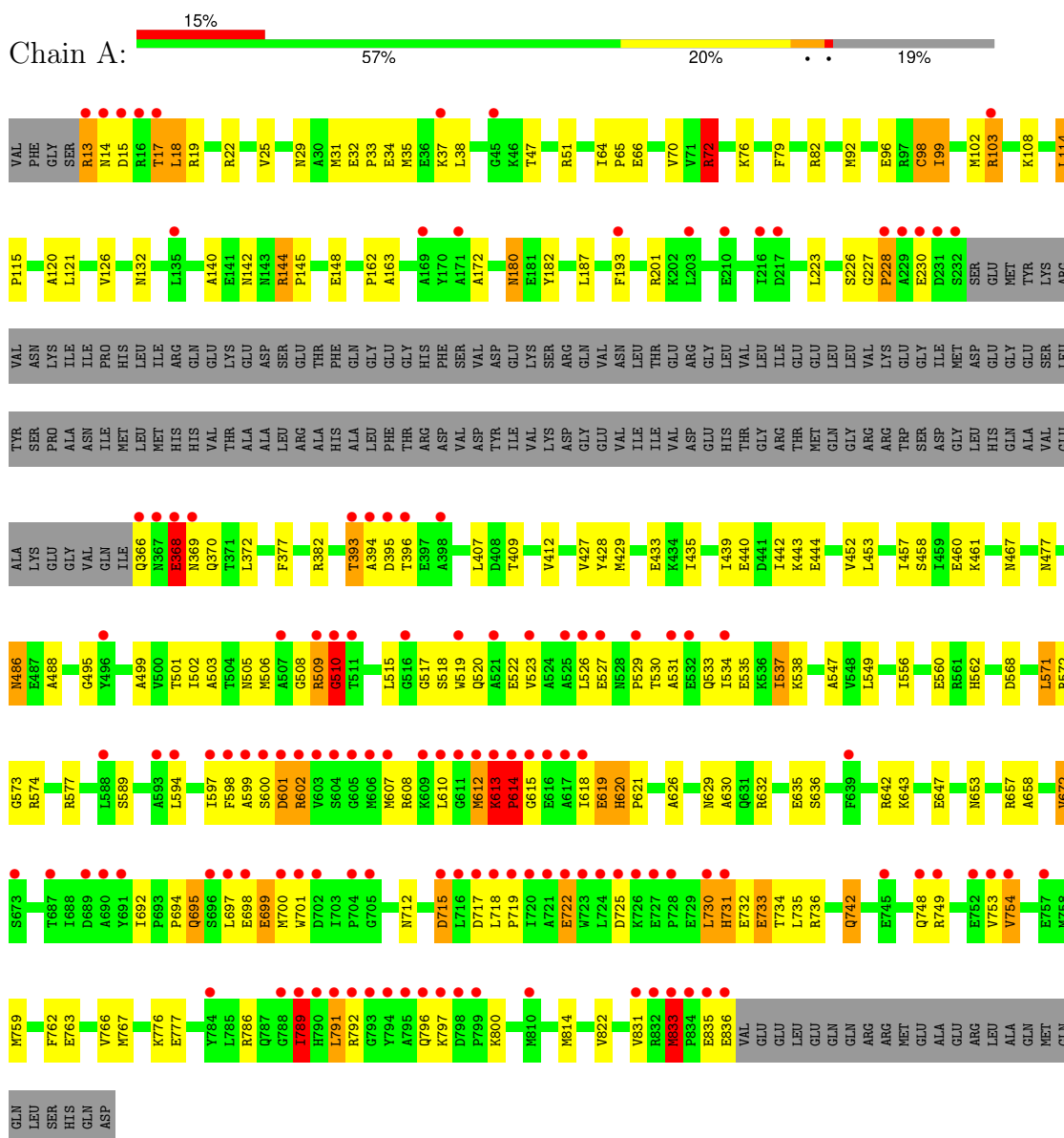


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total 179	O 179	0	0
3	B	255	Total 255	O 255	0	0

3 Residue-property plots

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 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



• Molecule 1: Preprotein translocase secA subunit



4 Data and refinement statistics

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 19.85 – 2.11	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.85-2.11) 90.8 (19.85-2.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.263 0.256 , 0.299	Depositor DCC
R_{free} test set	5666 reflections (4.55%)	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 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.60	52/5590 (0.9%)	1.33	24/7542 (0.3%)
1	B	1.88	116/6045 (1.9%)	1.54	77/8154 (0.9%)
All	All	1.75	168/11635 (1.4%)	1.44	101/15696 (0.6%)

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 (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	LEU	C-O	15.24	1.45	1.23
1	A	698	GLU	C-O	12.71	1.40	1.24
1	B	126	VAL	C-O	-11.82	1.11	1.24
1	B	801	GLN	N-CA	11.67	1.61	1.46
1	B	73	GLU	N-CA	10.47	1.59	1.46
1	B	122	THR	C-O	-9.45	1.11	1.24
1	B	23	LYS	CE-NZ	9.35	1.77	1.49
1	A	163	ALA	C-O	-9.04	1.16	1.24
1	A	439	ILE	CA-CB	8.99	1.66	1.54
1	B	25	VAL	C-O	-8.78	1.13	1.24
1	A	626	ALA	CA-CB	-8.65	1.39	1.53
1	B	163	ALA	CA-CB	8.58	1.65	1.53
1	A	699	GLU	CD-OE1	8.31	1.41	1.25
1	A	501	THR	C-O	-8.28	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	518	SER	CA-C	8.28	1.63	1.53
1	A	658	ALA	C-O	-8.21	1.14	1.24
1	B	419	ILE	CA-CB	8.21	1.64	1.54
1	B	37	LYS	N-CA	7.73	1.56	1.46
1	B	394	ALA	CA-CB	7.55	1.66	1.53
1	B	43	LEU	C-O	7.50	1.32	1.24
1	B	150	LEU	CA-C	-7.39	1.42	1.52
1	B	404	ILE	CA-CB	-7.38	1.44	1.54
1	A	517	GLY	C-O	-7.37	1.17	1.23
1	B	631	GLN	C-O	-7.36	1.15	1.24
1	B	394	ALA	CA-C	7.32	1.62	1.52
1	B	24	VAL	CA-CB	-7.27	1.45	1.54
1	A	393	THR	CA-CB	7.22	1.66	1.53
1	B	475	LYS	CA-C	-7.17	1.43	1.52
1	A	699	GLU	CD-OE2	7.17	1.39	1.25
1	B	174	ILE	CA-CB	-7.16	1.45	1.54
1	B	158	LEU	CA-C	-7.07	1.45	1.52
1	B	393	THR	CA-CB	7.04	1.65	1.53
1	B	22	ARG	C-O	-7.00	1.16	1.24
1	B	584	SER	CA-C	6.96	1.60	1.52
1	B	393	THR	N-CA	6.95	1.55	1.46
1	B	71	VAL	CB-CG2	6.95	1.75	1.52
1	B	69	ALA	N-CA	6.93	1.54	1.46
1	B	207	LEU	CA-C	-6.90	1.44	1.53
1	B	391	THR	C-O	-6.76	1.15	1.23
1	B	116	ALA	CA-C	-6.64	1.44	1.52
1	A	140	ALA	C-O	-6.63	1.16	1.24
1	B	476	HIS	C-O	-6.63	1.17	1.24
1	B	404	ILE	CA-C	6.61	1.63	1.52
1	A	442	ILE	CA-C	-6.58	1.44	1.52
1	A	126	VAL	C-O	-6.58	1.17	1.24
1	A	79	PHE	CA-C	-6.57	1.44	1.52
1	B	73	GLU	C-O	-6.56	1.16	1.24
1	B	187	LEU	N-CA	-6.55	1.38	1.46
1	B	101	GLU	CA-C	6.48	1.61	1.52
1	B	80	GLY	C-O	-6.47	1.14	1.24
1	B	137	GLN	N-CA	-6.46	1.38	1.46
1	A	172	ALA	CA-CB	-6.45	1.43	1.53
1	B	43	LEU	N-CA	6.45	1.54	1.46
1	B	196	GLU	C-O	-6.40	1.15	1.24
1	A	144	ARG	C-O	-6.34	1.18	1.24
1	A	443	LYS	C-O	-6.30	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	ARG	N-CA	6.29	1.57	1.45
1	B	208	VAL	CA-CB	-6.27	1.46	1.54
1	B	86	VAL	N-CA	6.26	1.54	1.46
1	B	126	VAL	CA-C	-6.24	1.45	1.52
1	B	191	MET	C-O	-6.24	1.15	1.24
1	B	394	ALA	N-CA	6.23	1.54	1.46
1	B	588	LEU	C-O	-6.22	1.16	1.23
1	A	789	ILE	CA-CB	6.19	1.62	1.54
1	B	178	THR	N-CA	6.14	1.53	1.45
1	A	792	ARG	CA-C	6.14	1.57	1.52
1	B	654	ASP	CG-OD1	6.13	1.36	1.25
1	B	41	GLU	C-O	-6.08	1.17	1.24
1	A	182	TYR	C-O	6.07	1.31	1.24
1	A	382	ARG	CA-C	6.01	1.60	1.52
1	B	71	VAL	CA-CB	-5.98	1.47	1.54
1	B	103	ARG	CG-CD	5.97	1.70	1.52
1	A	452	VAL	C-O	-5.95	1.18	1.24
1	B	124	LYS	C-O	-5.95	1.16	1.24
1	B	29	ASN	N-CA	5.93	1.53	1.46
1	A	694	PRO	CA-C	5.92	1.59	1.52
1	B	144	ARG	C-O	-5.92	1.18	1.24
1	B	801	GLN	CA-C	-5.91	1.44	1.52
1	B	128	VAL	CA-CB	-5.90	1.46	1.54
1	B	169	ALA	CA-CB	-5.89	1.44	1.53
1	A	537	ILE	CA-CB	5.89	1.61	1.54
1	B	183	GLY	C-O	5.86	1.30	1.23
1	B	210	GLU	CG-CD	5.85	1.66	1.52
1	B	46	LYS	CB-CG	-5.85	1.34	1.52
1	B	634	VAL	CA-C	5.83	1.60	1.52
1	B	214	ILE	CA-C	5.83	1.60	1.52
1	A	99	ILE	CA-CB	5.82	1.61	1.54
1	B	523	VAL	CA-C	5.82	1.60	1.52
1	B	115	PRO	CG-CD	5.81	1.70	1.50
1	A	822	VAL	CA-CB	-5.79	1.47	1.54
1	B	76	LYS	C-O	-5.74	1.17	1.24
1	B	35	MET	CA-CB	-5.71	1.44	1.53
1	A	822	VAL	C-O	-5.70	1.17	1.24
1	B	400	GLU	C-O	5.67	1.30	1.24
1	B	636	SER	N-CA	-5.66	1.39	1.46
1	A	180	ASN	C-O	-5.66	1.17	1.24
1	B	114	LEU	N-CA	-5.65	1.42	1.46
1	B	664	ASN	C-O	5.63	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	ARG	CB-CG	-5.63	1.35	1.52
1	B	572	ARG	CB-CG	-5.62	1.35	1.52
1	B	831	VAL	CA-CB	5.61	1.61	1.54
1	A	477	ASN	C-O	-5.61	1.17	1.23
1	A	499	ALA	N-CA	-5.59	1.39	1.46
1	A	98	CYS	CB-SG	-5.57	1.62	1.81
1	A	792	ARG	N-CA	5.57	1.51	1.46
1	B	465	VAL	CA-CB	5.56	1.61	1.54
1	B	28	ILE	CA-CB	-5.56	1.48	1.54
1	A	630	ALA	CA-C	5.56	1.59	1.52
1	B	476	HIS	N-CA	-5.55	1.39	1.46
1	B	521	ALA	CA-C	-5.54	1.46	1.52
1	B	452	VAL	CA-CB	-5.53	1.47	1.54
1	B	789	ILE	CA-CB	5.53	1.61	1.54
1	B	32	GLU	C-O	-5.51	1.17	1.24
1	B	616	GLU	CA-C	5.50	1.60	1.52
1	B	438	ILE	CA-CB	-5.50	1.48	1.54
1	B	419	ILE	C-O	-5.49	1.16	1.24
1	A	187	LEU	C-O	-5.49	1.17	1.24
1	A	653	ASN	C-O	-5.47	1.17	1.24
1	B	484	HIS	C-O	-5.47	1.17	1.24
1	B	377	PHE	CA-C	-5.46	1.45	1.52
1	B	471	LYS	C-O	-5.44	1.17	1.24
1	B	29	ASN	C-O	5.43	1.30	1.24
1	A	488	ALA	CA-C	5.42	1.59	1.52
1	B	64	ILE	C-O	-5.41	1.19	1.24
1	B	179	ASN	C-O	5.38	1.30	1.24
1	B	48	ALA	C-O	-5.37	1.17	1.24
1	B	121	LEU	CA-C	-5.34	1.45	1.52
1	A	547	ALA	C-O	-5.34	1.17	1.24
1	A	503	ALA	CA-CB	-5.33	1.40	1.54
1	B	44	LYS	C-O	-5.33	1.17	1.24
1	B	766	VAL	CA-CB	-5.33	1.47	1.54
1	A	193	PHE	C-O	-5.30	1.16	1.24
1	A	495	GLY	C-O	-5.30	1.19	1.24
1	B	85	ASP	C-O	-5.29	1.18	1.24
1	B	392	GLY	N-CA	5.27	1.51	1.45
1	B	385	GLU	CD-OE2	5.26	1.35	1.25
1	B	111	THR	CA-C	5.25	1.59	1.52
1	A	162	PRO	C-O	-5.24	1.17	1.23
1	B	161	MET	N-CA	-5.20	1.39	1.45
1	A	114	LEU	N-CA	5.19	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	578	GLN	CB-CG	5.19	1.68	1.52
1	A	433	GLU	C-O	-5.18	1.18	1.24
1	A	515	LEU	C-O	-5.18	1.17	1.23
1	A	393	THR	N-CA	5.17	1.52	1.46
1	B	800	LYS	C-O	-5.17	1.17	1.23
1	A	791	LEU	CA-C	5.17	1.57	1.52
1	A	571	LEU	C-O	-5.15	1.18	1.24
1	B	96	GLU	CD-OE1	5.14	1.35	1.25
1	A	612	MET	CA-C	5.11	1.59	1.52
1	B	149	PHE	C-O	-5.11	1.17	1.24
1	B	680	ARG	C-O	5.10	1.30	1.24
1	B	668	ASP	CA-CB	-5.10	1.45	1.53
1	B	384	TYR	CA-CB	-5.10	1.44	1.53
1	B	767	MET	N-CA	-5.09	1.40	1.46
1	B	49	GLU	CA-C	5.08	1.59	1.52
1	B	76	LYS	CE-NZ	5.08	1.64	1.49
1	B	88	LEU	CG-CD2	-5.07	1.35	1.52
1	B	169	ALA	N-CA	5.07	1.52	1.46
1	B	200	GLN	N-CA	5.06	1.51	1.45
1	B	543	VAL	CA-CB	-5.06	1.48	1.54
1	A	201	ARG	CZ-NH2	-5.06	1.26	1.33
1	B	56	LYS	CD-CE	5.05	1.67	1.52
1	A	695	GLN	C-O	5.04	1.31	1.23
1	B	204	HIS	CA-CB	5.04	1.61	1.53
1	B	184	PHE	CA-C	5.04	1.59	1.52
1	B	656	ARG	CB-CG	5.03	1.67	1.52
1	B	68	PHE	CD2-CE2	5.02	1.53	1.38
1	B	395	ASP	CA-C	5.00	1.59	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	613	LYS	CA-C-N	10.68	133.19	119.84
1	B	613	LYS	C-N-CA	10.68	133.19	119.84
1	A	620	HIS	CA-C-N	9.91	132.23	119.84
1	A	620	HIS	C-N-CA	9.91	132.23	119.84
1	A	613	LYS	CA-C-N	9.50	131.72	119.84
1	A	613	LYS	C-N-CA	9.50	131.72	119.84
1	A	412	VAL	CA-C-N	8.98	129.01	119.76
1	A	412	VAL	C-N-CA	8.98	129.01	119.76
1	B	792	ARG	N-CA-C	-8.63	101.36	112.23
1	B	367	ASN	CA-CB-CG	-8.38	104.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	ASN	CA-C-N	8.15	128.64	119.92
1	B	528	ASN	C-N-CA	8.15	128.64	119.92
1	B	800	LYS	N-CA-C	-8.13	99.57	110.55
1	A	517	GLY	N-CA-C	-8.10	103.27	111.85
1	B	764	LYS	N-CA-C	-7.78	102.74	111.07
1	B	654	ASP	N-CA-C	-7.65	102.28	111.69
1	B	801	GLN	N-CA-CB	7.62	123.36	110.49
1	B	412	VAL	CA-C-N	-7.41	113.10	120.21
1	B	412	VAL	C-N-CA	-7.41	113.10	120.21
1	A	672	VAL	N-CA-CB	-7.23	102.95	112.36
1	B	381	PHE	N-CA-C	7.13	119.91	111.71
1	B	367	ASN	CB-CA-C	7.06	123.51	110.10
1	B	800	LYS	CA-C-N	-7.03	108.11	121.54
1	B	800	LYS	C-N-CA	-7.03	108.11	121.54
1	B	800	LYS	O-C-N	-6.92	114.96	122.85
1	B	803	TYR	CA-C-O	-6.91	113.51	120.90
1	B	657	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	821	GLU	CB-CA-C	-6.76	99.35	110.85
1	B	683	VAL	N-CA-C	-6.57	104.08	110.72
1	B	183	GLY	N-CA-C	6.54	120.81	112.83
1	B	119	ASN	N-CA-C	6.44	120.85	113.19
1	B	720	ILE	CB-CA-C	-6.44	103.45	112.14
1	B	723	TRP	CA-CB-CG	6.31	125.59	113.60
1	B	793	GLY	N-CA-C	6.31	118.45	110.38
1	B	367	ASN	N-CA-CB	-6.28	99.83	110.50
1	B	668	ASP	N-CA-C	6.24	120.58	113.15
1	B	805	ARG	CB-CA-C	-6.23	99.30	110.70
1	B	730	LEU	N-CA-C	6.19	117.71	110.97
1	A	72	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	567	ILE	N-CA-C	6.12	116.28	110.53
1	B	798	ASP	CA-C-N	6.11	127.47	119.84
1	B	798	ASP	C-N-CA	6.11	127.47	119.84
1	B	661	SER	O-C-N	6.04	128.30	122.07
1	A	833	MET	N-CA-C	-6.03	100.86	109.24
1	B	377	PHE	N-CA-C	6.02	118.61	111.33
1	B	23	LYS	CD-CE-NZ	6.00	131.09	111.90
1	A	657	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	568	ASP	N-CA-C	-5.96	104.86	111.36
1	B	786	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	439	ILE	N-CA-C	-5.92	104.74	110.72
1	B	97	ARG	N-CA-C	-5.88	100.03	109.39
1	B	661	SER	CA-C-N	5.86	128.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	661	SER	C-N-CA	5.86	128.13	120.28
1	B	51	ARG	N-CA-C	5.80	118.38	111.71
1	B	230	GLU	N-CA-C	5.79	117.77	109.14
1	B	798	ASP	N-CA-C	5.78	122.59	109.81
1	B	794	TYR	N-CA-C	5.75	123.05	110.80
1	B	801	GLN	CB-CA-C	-5.74	99.00	110.42
1	B	367	ASN	N-CA-C	5.65	126.83	111.00
1	B	168	GLU	CB-CA-C	-5.65	102.01	110.88
1	B	751	GLU	N-CA-C	5.65	117.24	111.14
1	B	518	SER	N-CA-C	5.64	118.72	107.62
1	B	661	SER	CA-C-O	-5.62	114.92	120.82
1	A	18	LEU	N-CA-C	5.61	117.40	111.28
1	A	121	LEU	N-CA-C	5.61	117.84	111.11
1	B	394	ALA	N-CA-C	5.58	122.68	110.80
1	B	200	GLN	N-CA-C	-5.57	102.22	110.46
1	B	73	GLU	N-CA-C	-5.55	104.87	111.69
1	B	833	MET	CA-C-N	5.50	126.72	119.84
1	B	833	MET	C-N-CA	5.50	126.72	119.84
1	A	614	PRO	N-CA-C	5.50	123.80	112.47
1	B	677	ASN	N-CA-C	-5.49	105.30	111.28
1	A	467	ASN	N-CA-C	5.47	117.95	111.33
1	B	82	ARG	CB-CG-CD	-5.44	98.78	111.30
1	A	712	ASN	N-CA-C	5.42	118.10	111.82
1	B	64	ILE	O-C-N	5.38	123.86	120.42
1	B	86	VAL	N-CA-C	5.33	117.72	111.05
1	A	549	LEU	N-CA-C	5.32	117.08	111.28
1	B	167	ARG	CD-NE-CZ	5.32	131.85	124.40
1	B	43	LEU	CA-C-O	5.29	126.16	120.55
1	B	672	VAL	N-CA-CB	-5.28	105.25	112.28
1	B	105	GLY	N-CA-C	-5.24	107.88	115.27
1	B	547	ALA	N-CA-C	5.19	117.68	111.71
1	B	801	GLN	CA-CB-CG	5.18	124.47	114.10
1	A	672	VAL	CB-CA-C	5.17	116.62	110.93
1	A	777	GLU	CB-CA-C	-5.16	102.78	110.88
1	B	144	ARG	NE-CZ-NH1	-5.12	116.39	121.50
1	B	102	MET	CG-SD-CE	-5.10	89.68	100.90
1	B	415	ASN	N-CA-C	-5.08	105.74	111.28
1	B	173	ASP	N-CA-C	5.07	117.20	111.11
1	B	803	TYR	N-CA-CB	5.07	117.49	109.94
1	B	646	LEU	N-CA-C	-5.06	106.36	112.54
1	B	194	SER	CA-C-N	5.06	124.66	119.05
1	B	194	SER	C-N-CA	5.06	124.66	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LYS	CB-CG-CD	5.04	122.90	111.30
1	B	293	ASP	N-CA-C	5.04	121.54	110.80
1	B	103	ARG	CB-CG-CD	5.04	122.89	111.30
1	A	486	ASN	N-CA-C	-5.03	105.79	111.28
1	A	120	ALA	CA-C-N	5.02	127.32	120.54
1	A	120	ALA	C-N-CA	5.02	127.32	120.54
1	B	93	VAL	N-CA-C	5.01	115.62	110.36

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	115	0
1	B	5948	0	5946	214	0
2	A	27	0	12	0	0
2	B	27	0	12	3	0
3	A	179	0	0	11	0
3	B	255	0	0	34	0
All	All	11936	0	11451	320	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 14.

All (320) 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	1.38	1.20
1:A:538:LYS:NZ	1:B:528:ASN:HD22	1.48	1.10
1:B:17:THR:HG22	1:B:21:MET:HE2	1.26	1.09
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:81:MET:HE2	2:B:901:ADP:C4	2.01	0.95
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:302:ALA:HA	1:B:810:MET:HE3	1.56	0.86
1:B:800:LYS:O	1:B:801:GLN:HB2	1.75	0.86
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: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:A:753:VAL:HG21	1:A:833:MET:HE2	1.65	0.78
1:B:17:THR:HG22	1:B:21:MET:CE	2.09	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:B:316:ALA:O	1:B:317:HIS:CG	2.40	0.75
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:A:395:ASP:CG	1:A:396:THR:N	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:LYS:HE3	3:B:1135:HOH:O	1.93	0.68
1:A:699:GLU:OE2	1:A:700:MET:HE1	1.94	0.67
1:B:395:ASP:CA	3:B:1109:HOH:O	2.41	0.67
1:A:508:GLY:C	1:A:510:GLY:H	2.02	0.67
1:A:395:ASP:CG	1:A:396:THR:H	2.04	0.66
1:B:782:MET:HE1	1:B:810:MET:SD	2.36	0.66
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:A:520:GLN:CD	3:A:1029:HOH:O	2.39	0.65
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:81:MET:HE1	2:B:901:ADP:O2'	1.97	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:B:198:ARG:HH21	1:B:664:ASN:HD22	1.47	0.62
1:B:307:MET:HE3	1:B:311:THR:CG2	2.30	0.61
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: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:A:715:ASP:CG	1:A:715:ASP:O	2.45	0.60
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.83	0.60
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:A:538:LYS:HZ3	1:B:528:ASN:HD22	0.68	0.59
1:B:657:ARG:HD3	3:B:1144:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:233:SER:O	1:B:234:GLU:HB2	2.04	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:B:307:MET:HE3	1:B:311:THR:HG22	1.86	0.57
1:A:510:GLY:CA	1:A:574:ARG:NH1	2.68	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:282:ILE:HD13	1:B:286:LEU:HD13	1.87	0.56
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:590:MET:HE1	1:B:604:SER:O	2.05	0.55
1:B:738:ARG:O	1:B:742:GLN:HG2	2.06	0.55
1:B:81:MET:HE2	2:B:901:ADP:N3	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:O	1:A:619:GLU:CB	2.55	0.55
1:B:759:MET:HE1	1:B:762:PHE:CD2	2.40	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:771:LEU:C	1:B:771:LEU:HD23	2.32	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:B:712:ASN:C	1:B:828:LYS:HZ1	2.16	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:B:102:MET:HE1	1:B:111:THR:HG21	1.91	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:A:460:GLU:CD	1:A:460:GLU:H	2.16	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: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
1:A:368:GLU:CD	1:A:368:GLU:N	2.70	0.50
1:B:228:PRO:O	1:B:230:GLU:CB	2.59	0.50
1:B:713:ASP:C	1:B:828:LYS:NZ	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:102:MET:HE3	1:A:108:LYS:HG2	1.95	0.48
1:B:105:GLY:O	1:B:578:GLN:NE2	2.43	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:518:SER:C	3:B:1001:HOH:O	2.54	0.48
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.46	0.48
1:A:427:VAL:HG12	1:A:612:MET:HE2	1.95	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:B:735:LEU:C	1:B:735:LEU:HD12	2.38	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:759:MET:HE1	1:B:762:PHE:HD2	1.78	0.47
1:A:33:PRO:O	1:A:34:GLU:C	2.57	0.47
1:B:14:ASN:ND2	1:B:411:VAL:H	2.12	0.47
1:A:47:THR:O	1:A:51:ARG:HG3	2.14	0.47
1:B:461:LYS:O	1:B:465:VAL:HG12	2.15	0.47
1:B:759:MET:HA	1:B:759:MET:HE3	1.96	0.47
1:B:598:PHE:C	1:B:600:SER:H	2.15	0.47
1:B:757:GLU:O	1:B:761:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LYS:NZ	1:B:241:LYS:HD2	2.30	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:B:534:ILE:O	1:B:535:GLU:C	2.57	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: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: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:598:PHE:C	1:A:600:SER:N	2.75	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:A:833:MET:HE2	1:A:833:MET:HA	1.98	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: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:747:TYR:OH	1:B:763:GLU:OE2	2.31	0.45
1:A:831:VAL:HG12	1:A:833:MET:HE3	1.99	0.44
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
1:B:404:ILE:O	1:B:404:ILE:HG22	2.18	0.44
1:A:31:MET:HE1	1:A:66:GLU:HG2	2.00	0.44
1:B:60:LEU:O	1:B:63:LEU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:O	1:B:83:HIS:C	2.61	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:697:LEU:HD12	1:B:697:LEU:H	1.82	0.44
1:B:697:LEU:C	1:B:699:GLU:H	2.26	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:A:598:PHE:C	1:A:600:SER:H	2.26	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: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:713:ASP:C	1:B:828:LYS:HZ3	2.27	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:14:ASN:CG	1:A:15:ASP:H	2.27	0.42
1:A:601:ASP:O	1:A:602:ARG:C	2.63	0.42
1:A:719:PRO:HB2	1:A:722:GLU:HB2	2.01	0.42
1:B:286:LEU:HA	1:B:292:MET:HE1	1.99	0.42
1:B:788:GLY:O	1:B:792:ARG:CG	2.67	0.42
1:A:508:GLY:C	1:A:510:GLY:N	2.72	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:538:LYS:HZ2	1:B:528:ASN:ND2	2.10	0.42
1:B:12:SER:HB2	1:B:15:ASP:CG	2.44	0.42
1:A:814:MET:HE2	1:A:814:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:717:ASP:C	1:A:718:LEU:HD23	2.45	0.42
1:A:228:PRO:O	1:A:230:GLU:HG3	2.20	0.42
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:788:GLY:HA3	3:B:1137:HOH:O	2.14	0.41
1:A:13:ARG:C	1:A:17:THR:HG23	2.45	0.41
1:B:607:MET:HE2	1:B:610:LEU:HB2	2.03	0.41
1:A:25:VAL:HG23	1:A:92:MET:HE1	2.03	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:64:ILE:O	1:A:65:PRO:C	2.61	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

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	687/853 (80%)	639 (93%)	36 (5%)	12 (2%)	7	3
1	B	742/853 (87%)	657 (88%)	53 (7%)	32 (4%)	2	0
All	All	1429/1706 (84%)	1296 (91%)	89 (6%)	44 (3%)	3	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

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Mol	Chain	Res	Type
1	A	789	ILE
1	B	287	VAL
1	B	835	GLU
1	A	228	PRO
1	A	510	GLY
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%)	545 (93%)	41 (7%)	14	11
1	B	635/728 (87%)	562 (88%)	73 (12%)	5	3
All	All	1221/1456 (84%)	1107 (91%)	114 (9%)	8	5

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	17	THR
1	A	37	LYS
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

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Mol	Chain	Res	Type
1	A	369	ASN
1	A	393	THR
1	A	409	THR
1	A	435	ILE
1	A	502	ILE
1	A	506	MET
1	A	523	VAL
1	A	527	GLU
1	A	537	ILE
1	A	607	MET
1	A	610	LEU
1	A	635	GLU
1	A	636	SER
1	A	672	VAL
1	A	695	GLN
1	A	715	ASP
1	A	722	GLU
1	A	725	ASP
1	A	730	LEU
1	A	731	HIS
1	A	733	GLU
1	A	735	LEU
1	A	742	GLN
1	A	748	GLN
1	A	749	ARG
1	A	754	VAL
1	A	791	LEU
1	A	796	GLN
1	A	797	LYS
1	A	800	LYS
1	A	833	MET
1	B	38	LEU
1	B	49	GLU
1	B	102	MET
1	B	103	ARG
1	B	108	LYS
1	B	148	GLU
1	B	196	GLU
1	B	210	GLU
1	B	225	ILE
1	B	226	SER
1	B	237	LYS

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Mol	Chain	Res	Type
1	B	241	LYS
1	B	242	ILE
1	B	281	LEU
1	B	282	ILE
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	294	GLU
1	B	306	LEU
1	B	310	VAL
1	B	368	GLU
1	B	393	THR
1	B	409	THR
1	B	416	ARG
1	B	439	ILE
1	B	440	GLU
1	B	457	ILE
1	B	509	ARG
1	B	518	SER
1	B	520	GLN
1	B	523	VAL
1	B	526	LEU
1	B	527	GLU
1	B	530	THR
1	B	535	GLU
1	B	536	LYS
1	B	537	ILE
1	B	606	MET
1	B	607	MET
1	B	609	LYS
1	B	612	MET
1	B	614	PRO
1	B	632	ARG
1	B	643	LYS
1	B	657	ARG
1	B	679	ILE
1	B	697	LEU
1	B	703	ILE
1	B	707	GLN
1	B	711	LYS
1	B	718	LEU
1	B	722	GLU

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Mol	Chain	Res	Type
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	744	ILE
1	B	745	GLU
1	B	760	ARG
1	B	769	GLN
1	B	779	LEU
1	B	789	ILE
1	B	796	GLN
1	B	800	LYS
1	B	831	VAL
1	B	833	MET
1	B	835	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	180	ASN
1	A	436	GLN
1	A	484	HIS
1	A	486	ASN
1	A	533	GLN
1	A	578	GLN
1	A	629	ASN
1	A	662	GLN
1	A	707	GLN
1	A	731	HIS
1	A	742	GLN
1	A	761	HIS
1	B	14	ASN
1	B	180	ASN
1	B	249	GLN
1	B	303	ASN
1	B	308	HIS

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Mol	Chain	Res	Type
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	761	HIS
1	B	769	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	900	-	28,29,29	1.50	5 (17%)	43,45,45	2.26	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	901	-	28,29,29	1.79	5 (17%)	43,45,45	2.10	11 (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	ADP	A	900	-	-	2/16/32/32	0/3/3/3
2	ADP	B	901	-	-	3/16/32/32	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	ADP	PA-O3A	5.00	1.64	1.59
2	B	901	ADP	C5-C4	5.00	1.48	1.39
2	A	900	ADP	C5-C4	3.61	1.45	1.39
2	A	900	ADP	PA-O3A	3.22	1.63	1.59
2	B	901	ADP	C8-N7	2.86	1.37	1.31
2	B	901	ADP	PA-O1A	-2.78	1.41	1.50
2	A	900	ADP	C5-N7	-2.77	1.34	1.39
2	A	900	ADP	C8-N7	2.72	1.36	1.31
2	B	901	ADP	O4'-C1'	2.56	1.47	1.42
2	A	900	ADP	C5-C6	2.16	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ADP	C5-C4-N3	-7.82	115.95	126.72
2	A	900	ADP	N3-C4-N9	6.25	137.79	127.17
2	B	901	ADP	C5-C4-N3	-5.62	118.97	126.72
2	B	901	ADP	N3-C4-N9	5.32	136.22	127.17
2	A	900	ADP	C2-N3-C4	4.83	123.63	111.83
2	A	900	ADP	N3-C2-N1	-4.26	122.13	128.58
2	B	901	ADP	N6-C6-N1	3.77	126.77	118.38
2	B	901	ADP	O2A-PA-O3A	3.68	117.22	107.27
2	B	901	ADP	C5-C6-N6	-3.52	114.58	123.29
2	B	901	ADP	C2-N3-C4	3.44	120.24	111.83
2	B	901	ADP	O3B-PB-O2B	3.41	120.58	107.80
2	B	901	ADP	N3-C2-N1	-3.29	123.60	128.58
2	A	900	ADP	C5-C6-N6	-2.93	116.03	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	C4-N9-C8	2.79	108.67	105.74
2	A	900	ADP	C5-N7-C8	2.71	107.71	103.45
2	A	900	ADP	O4'-C1'-C2'	-2.69	100.86	106.62
2	A	900	ADP	N9-C8-N7	-2.57	110.29	113.94
2	A	900	ADP	N6-C6-N1	2.28	123.46	118.38
2	A	900	ADP	C4-C5-N7	-2.23	108.03	110.58
2	B	901	ADP	O2B-PB-O1B	-2.16	102.42	110.83
2	A	900	ADP	O3B-PB-O1B	-2.15	102.45	110.83
2	B	901	ADP	O2'-C2'-C1'	2.03	117.10	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

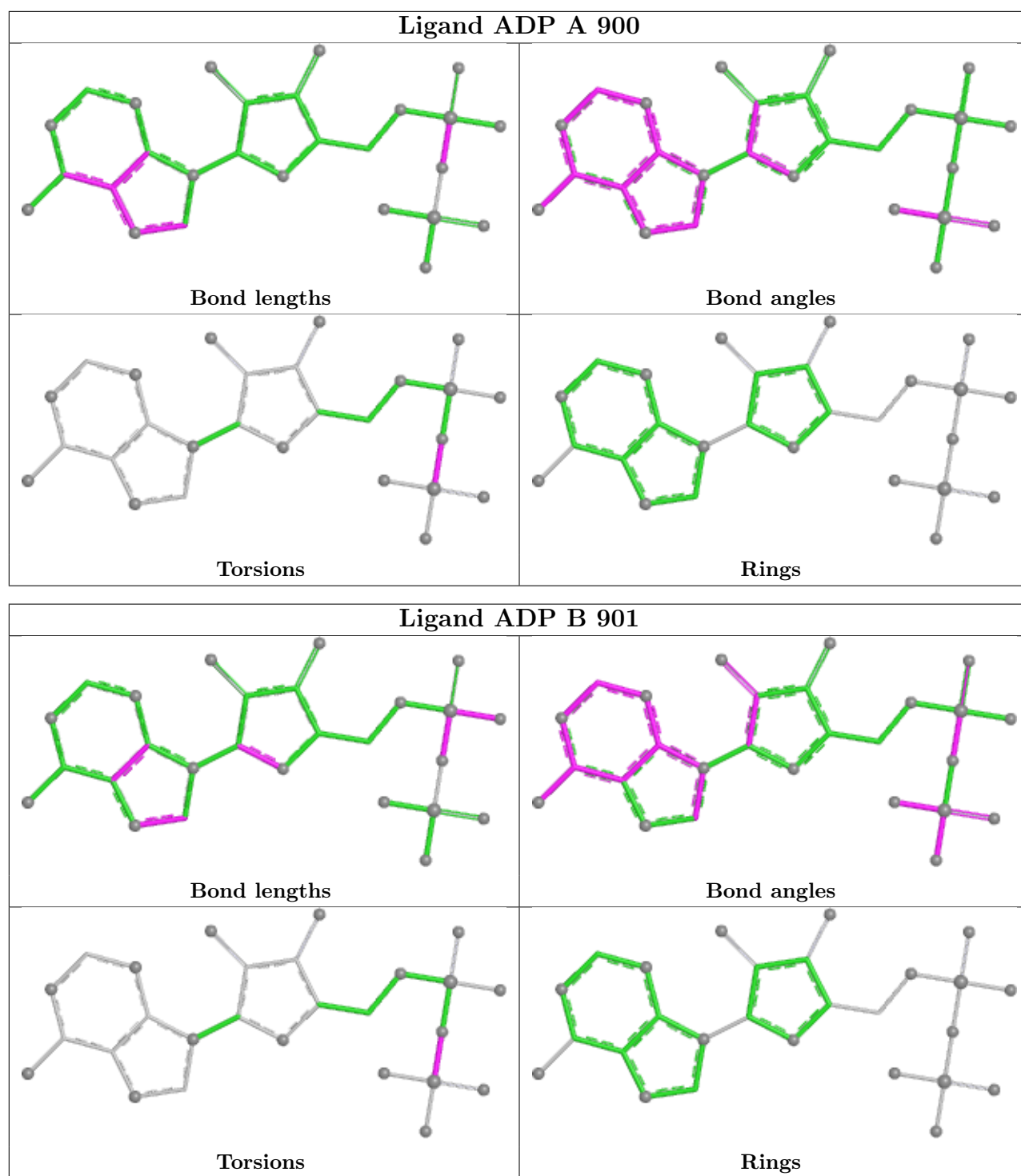
Mol	Chain	Res	Type	Atoms
2	A	900	ADP	PA-O3A-PB-O3B
2	B	901	ADP	PA-O3A-PB-O3B
2	A	900	ADP	PA-O3A-PB-O1B
2	B	901	ADP	PA-O3A-PB-O1B
2	B	901	ADP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ADP	3	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 than 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.



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, 95th 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 ²)	Q<0.9
1	A	691/853 (81%)	1.18	127 (18%) 3 4	30, 44, 75, 88	0
1	B	748/853 (87%)	1.80	258 (34%) 1 1	28, 46, 77, 98	0
All	All	1439/1706 (84%)	1.51	385 (26%) 1 1	28, 45, 76, 98	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	794	TYR	8.7
1	B	318	ALA	8.7
1	B	507	ALA	8.6
1	B	314	LEU	8.3
1	B	697	LEU	8.3
1	A	229	ALA	8.0
1	B	291	ILE	8.0
1	B	610	LEU	7.7
1	B	728	PRO	7.3
1	A	723	TRP	6.7
1	B	718	LEU	6.5
1	B	791	LEU	6.5
1	B	723	TRP	6.5
1	B	313	ALA	6.5
1	B	239	VAL	6.4
1	B	301	PRO	6.3
1	B	615	GLY	6.2
1	B	703	ILE	6.1
1	B	312	ALA	6.0
1	B	280	VAL	6.0
1	B	299	TYR	5.8
1	B	394	ALA	5.8
1	B	244	PRO	5.7
1	A	616	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	614	PRO	5.6
1	B	607	MET	5.6
1	B	696	SER	5.6
1	B	235	MET	5.6
1	B	603	VAL	5.5
1	B	725	ASP	5.5
1	A	604	SER	5.4
1	B	835	GLU	5.3
1	A	791	LEU	5.3
1	B	724	LEU	5.3
1	B	730	LEU	5.3
1	B	236	TYR	5.3
1	B	727	GLU	5.2
1	B	229	ALA	5.2
1	B	510	GLY	5.1
1	B	597	ILE	5.1
1	B	720	ILE	5.1
1	B	317	HIS	5.1
1	A	597	ILE	5.1
1	B	12	SER	5.1
1	B	241	LYS	5.1
1	B	793	GLY	5.0
1	B	393	THR	5.0
1	A	610	LEU	5.0
1	A	614	PRO	5.0
1	B	509	ARG	4.9
1	B	789	ILE	4.9
1	B	292	MET	4.9
1	B	245	HIS	4.8
1	B	519	TRP	4.8
1	B	281	LEU	4.8
1	B	834	PRO	4.8
1	B	684	PHE	4.8
1	B	289	GLU	4.8
1	A	602	ARG	4.8
1	B	247	ILE	4.7
1	B	704	PRO	4.7
1	B	714	PHE	4.7
1	B	290	GLY	4.7
1	B	797	LYS	4.7
1	B	243	ILE	4.7
1	B	618	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	734	THR	4.6
1	B	706	LEU	4.6
1	B	719	PRO	4.6
1	A	612	MET	4.6
1	B	294	GLU	4.6
1	B	233	SER	4.6
1	A	795	ALA	4.6
1	A	526	LEU	4.5
1	B	237	LYS	4.5
1	A	523	VAL	4.5
1	A	794	TYR	4.5
1	B	688	ILE	4.5
1	A	788	GLY	4.5
1	B	531	ALA	4.5
1	B	790	HIS	4.5
1	A	731	HIS	4.4
1	B	722	GLU	4.4
1	B	240	ASN	4.4
1	B	242	ILE	4.4
1	A	797	LYS	4.4
1	B	283	GLU	4.4
1	A	720	ILE	4.3
1	A	789	ILE	4.3
1	B	695	GLN	4.3
1	A	719	PRO	4.3
1	A	728	PRO	4.3
1	B	525	ALA	4.3
1	B	702	ASP	4.2
1	B	284	GLU	4.2
1	B	795	ALA	4.2
1	A	615	GLY	4.2
1	B	700	MET	4.2
1	B	523	VAL	4.2
1	A	697	LEU	4.1
1	B	315	ARG	4.1
1	B	611	GLY	4.1
1	B	295	GLY	4.1
1	B	248	ARG	4.1
1	B	691	TYR	4.1
1	A	14	ASN	4.0
1	B	721	ALA	4.0
1	B	707	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	508	GLY	4.0
1	B	528	ASN	4.0
1	B	833	MET	4.0
1	B	246	LEU	4.0
1	B	831	VAL	4.0
1	B	701	TRP	3.9
1	B	231	ASP	3.9
1	A	721	ALA	3.9
1	B	594	LEU	3.9
1	A	700	MET	3.9
1	A	232	SER	3.9
1	B	521	ALA	3.9
1	A	790	HIS	3.8
1	B	598	PHE	3.8
1	B	606	MET	3.8
1	A	230	GLU	3.8
1	B	617	ALA	3.8
1	B	836	GLU	3.8
1	A	599	ALA	3.7
1	B	726	LYS	3.7
1	B	310	VAL	3.7
1	B	285	LEU	3.7
1	B	735	LEU	3.7
1	B	669	VAL	3.7
1	A	519	TRP	3.6
1	A	525	ALA	3.6
1	A	834	PRO	3.6
1	A	15	ASP	3.6
1	B	103	ARG	3.6
1	B	738	ARG	3.6
1	B	287	VAL	3.5
1	B	694	PRO	3.5
1	B	249	GLN	3.5
1	B	796	GLN	3.5
1	A	784	TYR	3.5
1	B	689	ASP	3.5
1	B	602	ARG	3.5
1	B	731	HIS	3.5
1	B	752	GLU	3.5
1	A	369	ASN	3.5
1	B	282	ILE	3.5
1	A	793	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	608	ARG	3.5
1	B	605	GLY	3.4
1	B	526	LEU	3.4
1	B	832	ARG	3.4
1	B	303	ASN	3.4
1	B	11	GLY	3.4
1	B	820	TYR	3.4
1	A	603	VAL	3.4
1	B	126	VAL	3.4
1	B	293	ASP	3.4
1	B	604	SER	3.4
1	A	521	ALA	3.4
1	B	128	VAL	3.3
1	A	509	ARG	3.3
1	A	725	ASP	3.3
1	A	532	GLU	3.3
1	A	529	PRO	3.3
1	B	753	VAL	3.3
1	B	316	ALA	3.3
1	A	724	LEU	3.3
1	B	733	GLU	3.3
1	B	616	GLU	3.2
1	A	231	ASP	3.2
1	A	366	GLN	3.2
1	B	524	ALA	3.2
1	B	609	LYS	3.2
1	B	739	ILE	3.2
1	B	517	GLY	3.2
1	A	727	GLU	3.2
1	B	830	GLN	3.2
1	A	228	PRO	3.2
1	B	612	MET	3.2
1	B	174	ILE	3.1
1	A	745	GLU	3.1
1	B	311	THR	3.1
1	A	16	ARG	3.1
1	B	711	LYS	3.1
1	B	512	ASP	3.1
1	A	618	ILE	3.1
1	A	696	SER	3.1
1	A	705	GLY	3.0
1	B	369	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	593	ALA	3.0
1	A	607	MET	3.0
1	A	510	GLY	3.0
1	A	752	GLU	3.0
1	A	395	ASP	3.0
1	B	682	ASP	3.0
1	B	203	LEU	3.0
1	B	692	ILE	3.0
1	A	691	TYR	3.0
1	B	670	SER	3.0
1	A	718	LEU	3.0
1	A	511	THR	3.0
1	B	715	ASP	3.0
1	A	496	TYR	3.0
1	A	792	ARG	2.9
1	A	832	ARG	2.9
1	B	792	ARG	2.9
1	B	136	ALA	2.9
1	A	534	ILE	2.9
1	B	687	THR	2.9
1	A	598	PHE	2.9
1	B	699	GLU	2.9
1	B	93	VAL	2.9
1	B	16	ARG	2.9
1	B	205	TYR	2.9
1	A	531	ALA	2.9
1	B	158	LEU	2.9
1	B	693	PRO	2.9
1	A	836	GLU	2.9
1	B	745	GLU	2.9
1	B	297	SER	2.9
1	B	705	GLY	2.9
1	A	796	GLN	2.8
1	A	396	THR	2.8
1	B	534	ILE	2.8
1	A	37	LYS	2.8
1	A	398	ALA	2.8
1	A	507	ALA	2.8
1	B	302	ALA	2.8
1	B	288	LYS	2.8
1	B	717	ASP	2.8
1	A	394	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	729	GLU	2.8
1	B	708	GLU	2.8
1	B	690	ALA	2.8
1	B	154	VAL	2.8
1	A	798	ASP	2.7
1	A	611	GLY	2.7
1	A	716	LEU	2.7
1	B	286	LEU	2.7
1	B	511	THR	2.7
1	A	704	PRO	2.7
1	B	238	ARG	2.7
1	B	71	VAL	2.7
1	B	170	TYR	2.7
1	B	129	VAL	2.7
1	B	709	ARG	2.7
1	A	835	GLU	2.6
1	A	393	THR	2.6
1	B	747	TYR	2.6
1	A	831	VAL	2.6
1	B	530	THR	2.6
1	B	746	VAL	2.6
1	B	177	GLY	2.6
1	B	516	GLY	2.6
1	B	367	ASN	2.6
1	A	717	ASP	2.6
1	B	89	LEU	2.6
1	B	118	LEU	2.6
1	B	52	ALA	2.6
1	B	59	VAL	2.5
1	A	605	GLY	2.5
1	B	308	HIS	2.5
1	A	367	ASN	2.5
1	A	757	GLU	2.5
1	B	120	ALA	2.5
1	B	529	PRO	2.5
1	A	749	ARG	2.5
1	A	687	THR	2.5
1	B	232	SER	2.5
1	A	171	ALA	2.5
1	A	203	LEU	2.5
1	A	594	LEU	2.5
1	B	207	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	740	LEU	2.5
1	A	13	ARG	2.5
1	B	596	ARG	2.5
1	B	107	GLY	2.5
1	B	213	SER	2.4
1	B	686	ALA	2.4
1	B	156	ILE	2.4
1	B	176	TYR	2.4
1	A	17	THR	2.4
1	A	606	MET	2.4
1	B	749	ARG	2.4
1	B	710	LEU	2.4
1	B	234	GLU	2.4
1	A	715	ASP	2.4
1	B	513	ILE	2.4
1	B	676	ILE	2.4
1	B	429	MET	2.4
1	B	113	THR	2.4
1	B	685	LYS	2.4
1	A	593	ALA	2.4
1	A	730	LEU	2.4
1	B	60	LEU	2.4
1	B	114	LEU	2.4
1	B	135	LEU	2.4
1	A	210	GLU	2.4
1	B	123	GLY	2.4
1	B	742	GLN	2.4
1	A	609	LYS	2.4
1	A	613	LYS	2.4
1	B	146	LEU	2.3
1	A	45	GLY	2.3
1	B	788	GLY	2.3
1	A	601	ASP	2.3
1	B	122	THR	2.3
1	A	527	GLU	2.3
1	B	116	ALA	2.3
1	B	447	ALA	2.3
1	A	516	GLY	2.3
1	A	702	ASP	2.3
1	B	506	MET	2.3
1	A	639	PHE	2.3
1	A	698	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	722	GLU	2.3
1	B	70	VAL	2.3
1	B	799	PRO	2.3
1	B	206	ALA	2.3
1	B	741	ALA	2.3
1	A	689	ASP	2.3
1	B	124	LYS	2.3
1	A	600	SER	2.2
1	B	147	PHE	2.2
1	B	716	LEU	2.2
1	A	193	PHE	2.2
1	B	56	LYS	2.2
1	B	228	PRO	2.2
1	B	712	ASN	2.2
1	A	617	ALA	2.2
1	B	69	ALA	2.2
1	B	532	GLU	2.2
1	B	152	LEU	2.2
1	B	186	TYR	2.2
1	B	518	SER	2.2
1	A	726	LYS	2.2
1	B	214	ILE	2.2
1	B	225	ILE	2.2
1	B	101	GLU	2.2
1	B	599	ALA	2.2
1	B	159	PRO	2.1
1	B	175	THR	2.2
1	B	27	ILE	2.1
1	B	535	GLU	2.1
1	A	169	ALA	2.1
1	B	172	ALA	2.1
1	B	94	LEU	2.1
1	B	98	CYS	2.1
1	B	571	LEU	2.1
1	A	673	SER	2.1
1	B	743	SER	2.1
1	A	810	MET	2.1
1	A	701	TRP	2.1
1	B	567	ILE	2.1
1	B	754	VAL	2.1
1	A	690	ALA	2.1
1	B	757	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	ARG	2.1
1	A	753	VAL	2.1
1	A	135	LEU	2.1
1	B	54	LEU	2.1
1	B	368	GLU	2.1
1	B	736	ARG	2.1
1	A	368	GLU	2.0
1	B	674	GLU	2.0
1	A	588	LEU	2.0
1	B	110	LEU	2.0
1	A	217	ASP	2.0
1	B	601	ASP	2.0
1	B	117	TYR	2.0
1	A	216	ILE	2.0
1	B	744	ILE	2.0
1	A	754	VAL	2.0
1	A	833	MET	2.0
1	B	481	ALA	2.0
1	A	748	GLN	2.0
1	B	15	ASP	2.0
1	A	799	PRO	2.0
1	B	47	THR	2.0
1	B	130	THR	2.0
1	B	91	GLY	2.0
1	B	784	TYR	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 ⓘ

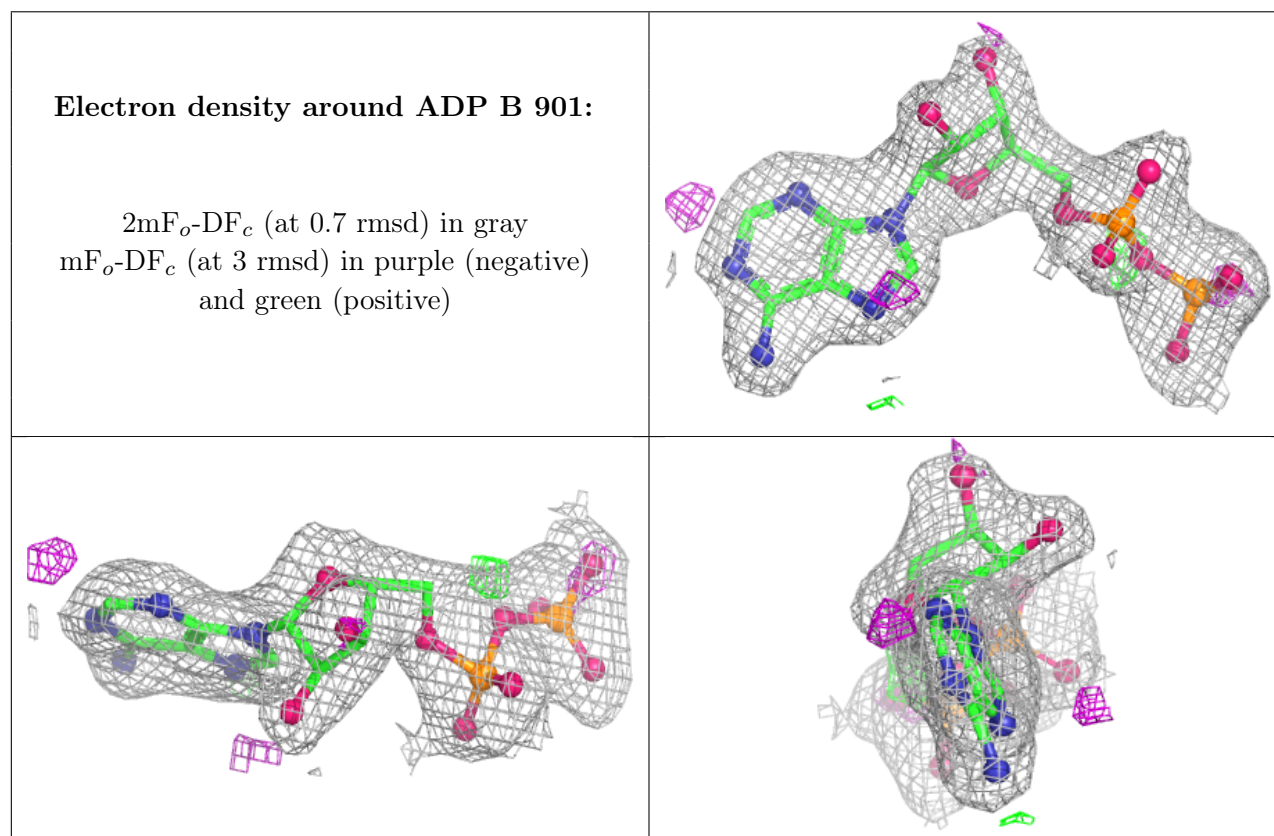
There are no oligosaccharides in this entry.

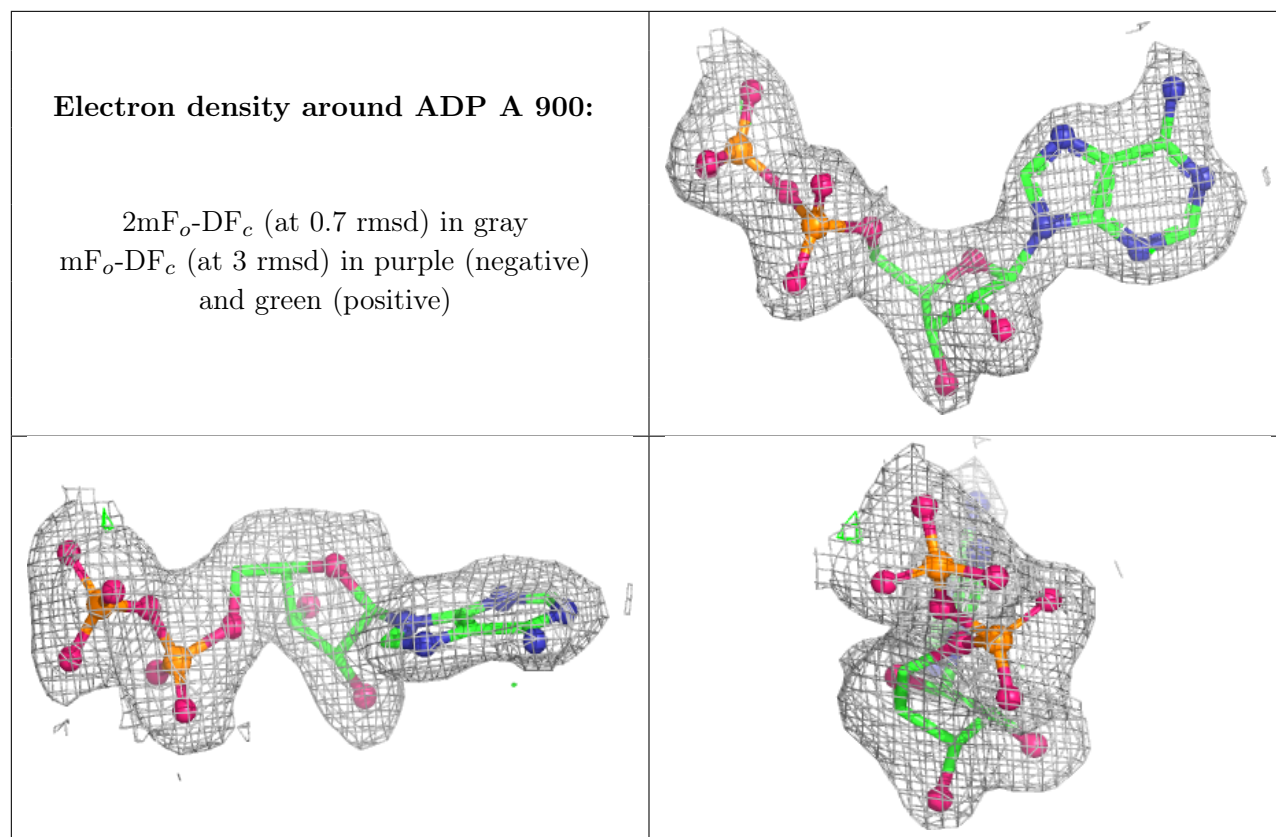
6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	901	27/27	0.94	0.08	24,34,39,42	0
2	ADP	A	900	27/27	0.95	0.09	33,46,49,50	0

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.





6.5 Other polymers ⓘ

There are no such residues in this entry.