



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 AM UTC

PDB ID : 1NKT / pdb_00001nkt
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS COMPLEX WITH
ADPBS
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Consortium (TBSGC)
Deposited on : 2003-01-03
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

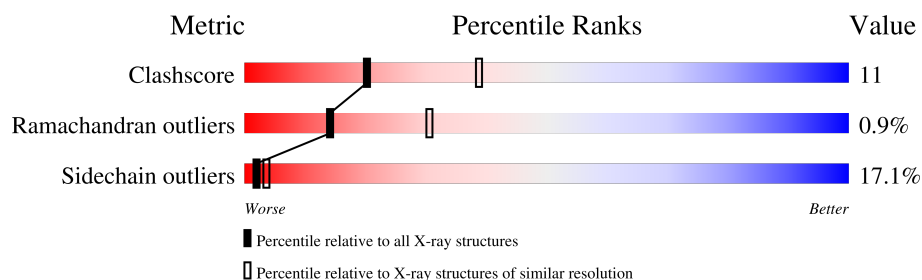
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	922	
1	B	922	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13862 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 1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	25			
1	B	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	25			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	cloning artifact	UNP P0A5Y8
A	-28	LYS	-	cloning artifact	UNP P0A5Y8
A	-27	GLU	-	cloning artifact	UNP P0A5Y8
A	-26	THR	-	cloning artifact	UNP P0A5Y8
A	-25	ALA	-	cloning artifact	UNP P0A5Y8
A	-24	ALA	-	cloning artifact	UNP P0A5Y8
A	-23	ALA	-	cloning artifact	UNP P0A5Y8
A	-22	LYS	-	cloning artifact	UNP P0A5Y8
A	-21	PHE	-	cloning artifact	UNP P0A5Y8
A	-20	GLU	-	cloning artifact	UNP P0A5Y8
A	-19	ARG	-	cloning artifact	UNP P0A5Y8
A	-18	GLN	-	cloning artifact	UNP P0A5Y8
A	-17	HIS	-	cloning artifact	UNP P0A5Y8
A	-16	MET	-	cloning artifact	UNP P0A5Y8
A	-15	ASP	-	cloning artifact	UNP P0A5Y8
A	-14	SER	-	cloning artifact	UNP P0A5Y8
A	-13	PRO	-	cloning artifact	UNP P0A5Y8
A	-12	ASP	-	cloning artifact	UNP P0A5Y8
A	-11	LEU	-	cloning artifact	UNP P0A5Y8
A	-10	GLY	-	cloning artifact	UNP P0A5Y8
A	-9	THR	-	cloning artifact	UNP P0A5Y8
A	-8	LEU	-	cloning artifact	UNP P0A5Y8
A	-7	VAL	-	cloning artifact	UNP P0A5Y8
A	-6	PRO	-	cloning artifact	UNP P0A5Y8
A	-5	ARG	-	cloning artifact	UNP P0A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP P0A5Y8
A	-3	SER	-	cloning artifact	UNP P0A5Y8
A	-2	MET	-	cloning artifact	UNP P0A5Y8
A	-1	ALA	-	cloning artifact	UNP P0A5Y8
A	0	ASP	-	cloning artifact	UNP P0A5Y8
A	1	ILE	-	cloning artifact	UNP P0A5Y8
B	-29	MET	-	cloning artifact	UNP P0A5Y8
B	-28	LYS	-	cloning artifact	UNP P0A5Y8
B	-27	GLU	-	cloning artifact	UNP P0A5Y8
B	-26	THR	-	cloning artifact	UNP P0A5Y8
B	-25	ALA	-	cloning artifact	UNP P0A5Y8
B	-24	ALA	-	cloning artifact	UNP P0A5Y8
B	-23	ALA	-	cloning artifact	UNP P0A5Y8
B	-22	LYS	-	cloning artifact	UNP P0A5Y8
B	-21	PHE	-	cloning artifact	UNP P0A5Y8
B	-20	GLU	-	cloning artifact	UNP P0A5Y8
B	-19	ARG	-	cloning artifact	UNP P0A5Y8
B	-18	GLN	-	cloning artifact	UNP P0A5Y8
B	-17	HIS	-	cloning artifact	UNP P0A5Y8
B	-16	MET	-	cloning artifact	UNP P0A5Y8
B	-15	ASP	-	cloning artifact	UNP P0A5Y8
B	-14	SER	-	cloning artifact	UNP P0A5Y8
B	-13	PRO	-	cloning artifact	UNP P0A5Y8
B	-12	ASP	-	cloning artifact	UNP P0A5Y8
B	-11	LEU	-	cloning artifact	UNP P0A5Y8
B	-10	GLY	-	cloning artifact	UNP P0A5Y8
B	-9	THR	-	cloning artifact	UNP P0A5Y8
B	-8	LEU	-	cloning artifact	UNP P0A5Y8
B	-7	VAL	-	cloning artifact	UNP P0A5Y8
B	-6	PRO	-	cloning artifact	UNP P0A5Y8
B	-5	ARG	-	cloning artifact	UNP P0A5Y8
B	-4	GLY	-	cloning artifact	UNP P0A5Y8
B	-3	SER	-	cloning artifact	UNP P0A5Y8
B	-2	MET	-	cloning artifact	UNP P0A5Y8
B	-1	ALA	-	cloning artifact	UNP P0A5Y8
B	0	ASP	-	cloning artifact	UNP P0A5Y8
B	1	ILE	-	cloning artifact	UNP P0A5Y8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

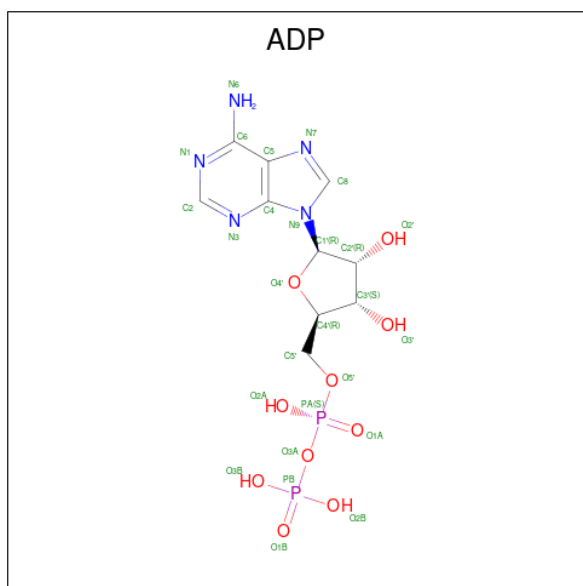
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 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	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is water.

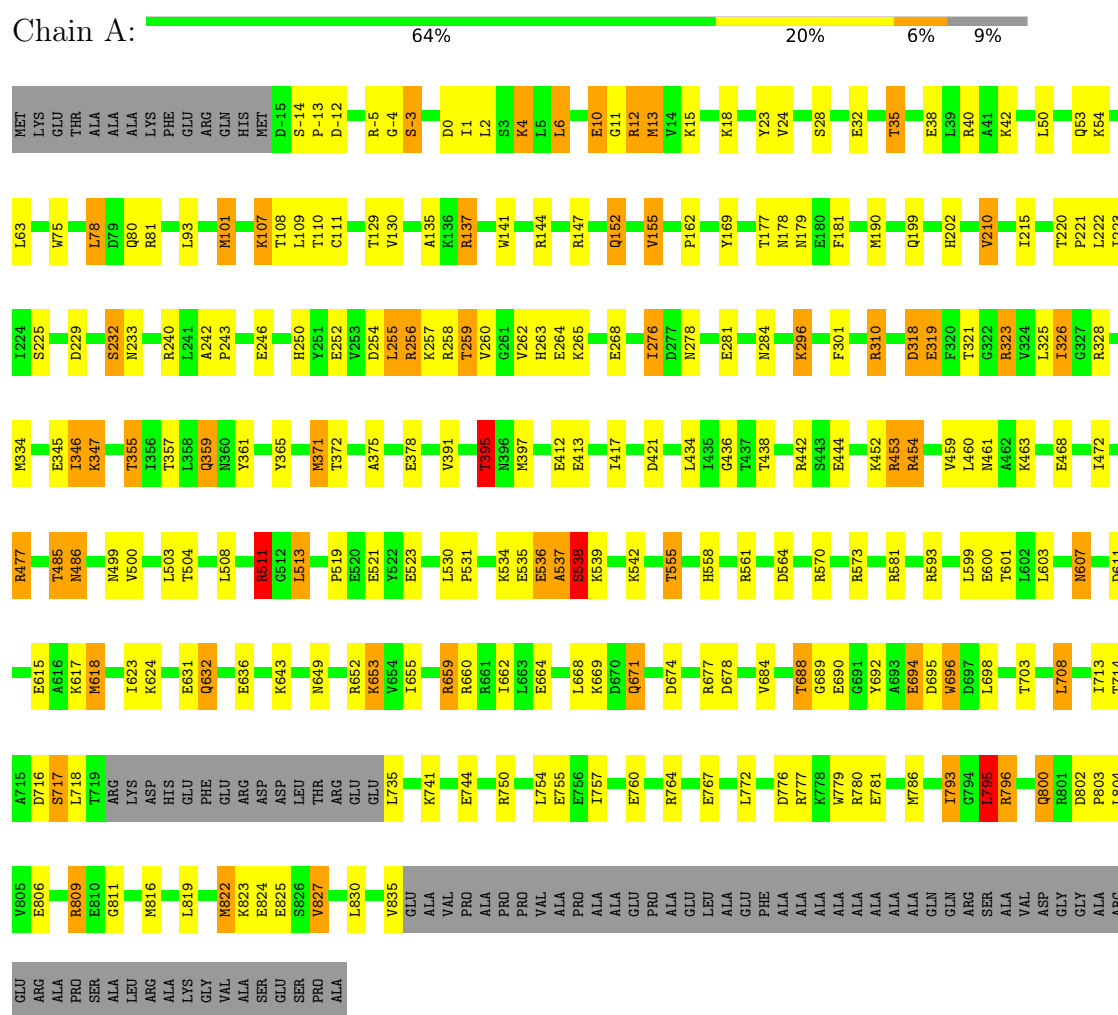
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	246	Total O 246 246	0	0
4	B	300	Total O 300 300	0	0

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. 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.

Note EDS was not executed.

- Molecule 1: Preprotein translocase secA 1 subunit





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	206.05 Å 206.05 Å 292.86 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (95.35-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.213 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.84	6/6734 (0.1%)	1.10	12/9102 (0.1%)
1	B	0.85	5/6734 (0.1%)	1.07	11/9102 (0.1%)
All	All	0.84	11/13468 (0.1%)	1.09	23/18204 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	816	MET	SD-CE	-9.62	1.55	1.79
1	A	511	ARG	C-N	8.60	1.45	1.33
1	A	513	LEU	CB-CG	7.66	1.68	1.53
1	A	816	MET	SD-CE	-7.57	1.60	1.79
1	B	511	ARG	NE-CZ	7.16	1.41	1.33
1	B	101	MET	SD-CE	-6.56	1.63	1.79
1	A	101	MET	SD-CE	-5.99	1.64	1.79
1	A	618	MET	SD-CE	5.75	1.94	1.79
1	B	417	ILE	CA-CB	5.72	1.62	1.54
1	A	326	ILE	CA-CB	5.30	1.60	1.54
1	B	399	MET	SD-CE	5.07	1.92	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	VAL	CB-CA-C	-9.66	99.39	112.04
1	B	486	ASN	CA-C-N	-8.18	105.92	121.54
1	B	486	ASN	C-N-CA	-8.18	105.92	121.54
1	B	210	VAL	CB-CA-C	-7.43	102.30	112.04
1	B	155	VAL	CB-CA-C	-7.22	99.37	110.50
1	A	155	VAL	CB-CA-C	-6.94	100.13	110.82
1	A	486	ASN	CA-C-N	-6.93	109.77	122.31
1	A	486	ASN	C-N-CA	-6.93	109.77	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	N-CA-C	6.86	121.56	111.34
1	A	395	THR	N-CA-CB	-6.03	101.50	110.17
1	A	137	ARG	N-CA-CB	5.93	118.94	110.16
1	A	454	ARG	N-CA-C	5.86	119.74	112.24
1	A	210	VAL	N-CA-CB	5.75	117.66	110.47
1	A	538	SER	N-CA-C	5.65	122.83	110.80
1	B	110	THR	CA-C-N	5.57	128.51	120.38
1	B	110	THR	C-N-CA	5.57	128.51	120.38
1	B	692	TYR	N-CA-C	5.38	122.26	110.80
1	A	607	ASN	N-CA-C	5.36	119.10	112.24
1	B	709	TYR	N-CA-C	5.28	114.38	108.25
1	A	135	ALA	N-CA-C	-5.17	105.56	111.14
1	B	395	THR	N-CA-CB	-5.09	102.38	110.06
1	A	504	THR	N-CA-C	-5.06	105.67	111.14
1	B	455	ILE	N-CA-C	5.01	112.51	107.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	6630	0	6581	148	0
1	B	6630	0	6581	158	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	246	0	0	35	0
4	B	300	0	0	42	0
All	All	13862	0	13186	300	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 11.

All (300) 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:101:MET:HE1	1:B:110:THR:HG21	1.26	1.09
1:A:11:GLY:HA2	4:A:1387:HOH:O	1.53	1.08
1:A:809:ARG:HH11	1:A:809:ARG:HB3	1.26	1.00
1:A:107:LYS:HD3	4:A:1370:HOH:O	1.62	0.98
1:A:107:LYS:CD	4:A:1370:HOH:O	2.14	0.95
1:A:660:ARG:HG2	4:A:1349:HOH:O	1.66	0.93
1:B:147:ARG:HD2	4:B:1211:HOH:O	1.66	0.93
1:A:359:GLN:H	1:A:359:GLN:HE21	1.15	0.91
1:A:35:THR:HG22	1:A:38:GLU:H	1.32	0.91
1:A:809:ARG:HH11	1:A:809:ARG:CB	1.85	0.89
1:A:777:ARG:NH2	1:A:825:GLU:OE1	2.06	0.88
1:B:454:ARG:HG3	1:B:454:ARG:O	1.72	0.88
1:B:660:ARG:HG3	4:B:1355:HOH:O	1.74	0.87
1:A:461:ASN:HA	1:A:485:THR:HG23	1.56	0.86
1:A:534:LYS:O	1:A:538:SER:HB3	1.75	0.86
1:B:233:ASN:H	1:B:233:ASN:HD22	1.20	0.85
1:A:101:MET:HE1	1:A:110:THR:HG21	1.56	0.85
1:A:806:GLU:HG2	4:A:1502:HOH:O	1.75	0.85
1:B:6:LEU:HD12	4:B:1433:HOH:O	1.77	0.85
1:B:666:GLU:HG3	4:B:1491:HOH:O	1.75	0.84
1:B:611:ASP:HB3	4:B:1296:HOH:O	1.77	0.84
1:B:359:GLN:H	1:B:359:GLN:HE21	1.20	0.83
1:B:346:ILE:HB	4:B:1180:HOH:O	1.80	0.81
1:A:395:THR:CG2	1:A:397:MET:O	2.28	0.81
1:A:643:LYS:HD3	1:A:804:LEU:HD22	1.62	0.80
1:B:780:ARG:HD3	4:B:1519:HOH:O	1.80	0.79
1:B:785:GLU:OE1	4:B:1414:HOH:O	2.00	0.79
1:B:809:ARG:HD3	4:B:1131:HOH:O	1.81	0.79
1:A:511:ARG:NH1	4:A:1210:HOH:O	2.15	0.79
1:B:329:ARG:HD3	4:B:1414:HOH:O	1.81	0.78
1:B:395:THR:HG23	1:B:397:MET:O	1.83	0.77
1:B:461:ASN:HA	1:B:485:THR:HG23	1.65	0.77
1:B:511:ARG:NH2	1:B:529:GLU:OE2	2.18	0.77
1:B:246:GLU:H	1:B:250:HIS:HD2	1.30	0.77
1:B:785:GLU:HG3	4:B:1092:HOH:O	1.85	0.76
1:B:660:ARG:CG	4:B:1355:HOH:O	2.32	0.75
1:A:436:GLY:O	1:A:555:THR:HB	1.86	0.75
1:B:129:THR:HB	4:B:1212:HOH:O	1.87	0.75
1:A:678:ASP:OD1	1:A:823:LYS:HE3	1.87	0.75
1:B:-5:ARG:HD2	4:B:1489:HOH:O	1.87	0.73
1:B:558:HIS:HD2	1:B:564:ASP:OD2	1.73	0.71
1:B:501:ASP:HB3	4:B:1229:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ARG:CG	4:A:1349:HOH:O	2.33	0.70
1:B:192:HIS:HD2	4:B:1510:HOH:O	1.74	0.69
1:B:454:ARG:HH11	1:B:454:ARG:HB2	1.57	0.69
1:A:80:GLN:HE21	1:A:109:LEU:HD22	1.57	0.69
1:B:698:LEU:HD11	4:B:1295:HOH:O	1.93	0.69
1:B:649:ASN:HD22	1:B:652:ARG:HH21	1.41	0.68
1:B:228:ALA:HB3	4:B:1292:HOH:O	1.94	0.68
1:A:809:ARG:CB	1:A:809:ARG:NH1	2.56	0.67
1:B:246:GLU:H	1:B:250:HIS:CD2	2.11	0.67
1:B:258:ARG:HH11	1:B:258:ARG:HB2	1.58	0.67
1:B:144:ARG:HD2	1:B:523:GLU:OE2	1.95	0.67
1:A:2:LEU:HB3	1:A:13:MET:HE3	1.75	0.66
1:A:643:LYS:HE2	4:A:1464:HOH:O	1.95	0.66
1:B:674:ASP:OD1	1:B:677:ARG:NH1	2.22	0.66
1:B:346:ILE:HG22	4:B:1494:HOH:O	1.96	0.66
1:A:276:ILE:HG13	1:A:281:GLU:OE2	1.96	0.65
1:B:372:THR:CG2	1:B:375:ALA:HB2	2.27	0.65
1:A:809:ARG:NE	4:A:1149:HOH:O	2.30	0.65
1:B:436:GLY:O	1:B:555:THR:HB	1.96	0.65
1:B:233:ASN:H	1:B:233:ASN:ND2	1.95	0.64
1:B:357:THR:HB	1:B:359:GLN:NE2	2.13	0.64
1:B:735:LEU:N	4:B:1166:HOH:O	2.30	0.64
1:B:719:THR:O	1:B:719:THR:HG22	1.97	0.63
1:A:581:ARG:HD2	4:A:1298:HOH:O	1.98	0.63
1:A:809:ARG:HD3	4:A:1149:HOH:O	1.98	0.63
1:A:255:LEU:HD12	1:A:256:ARG:HD2	1.81	0.63
1:B:191:ALA:O	1:B:659:ARG:NH2	2.32	0.63
1:B:276:ILE:HG13	1:B:281:GLU:OE2	1.98	0.63
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.63	0.62
1:A:107:LYS:O	1:A:371:MET:HE1	1.99	0.62
1:B:649:ASN:HD22	1:B:652:ARG:NH2	1.97	0.62
1:A:246:GLU:H	1:A:250:HIS:CD2	2.18	0.61
1:A:395:THR:HG22	1:A:397:MET:O	1.98	0.61
1:A:819:LEU:HD23	1:A:822:MET:HE1	1.81	0.61
1:A:12:ARG:HH11	1:A:12:ARG:CG	2.14	0.61
1:B:534:LYS:O	1:B:538:SER:HB3	2.00	0.61
1:A:246:GLU:H	1:A:250:HIS:HD2	1.49	0.61
1:A:144:ARG:HD2	1:A:523:GLU:OE2	2.01	0.60
1:A:421:ASP:OD1	1:A:453:ARG:NH2	2.34	0.60
1:B:347:LYS:HD3	4:B:1526:HOH:O	2.00	0.60
1:A:223:ILE:HG12	1:A:355:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ALA:O	1:B:601:THR:HG23	2.01	0.60
1:B:777:ARG:NH2	1:B:825:GLU:OE1	2.35	0.60
1:A:780:ARG:HD2	4:A:1506:HOH:O	2.02	0.59
1:B:659:ARG:NH1	1:B:776:ASP:OD1	2.33	0.59
1:A:147:ARG:HD2	4:A:1371:HOH:O	2.01	0.59
1:B:350:ASN:HB3	4:B:1254:HOH:O	2.03	0.58
1:B:101:MET:O	1:B:107:LYS:HE2	2.02	0.58
1:B:2:LEU:HD13	1:B:13:MET:HE3	1.84	0.58
1:A:611:ASP:HB3	4:A:1498:HOH:O	2.04	0.58
1:B:798:MET:HG2	1:B:800:GLN:HB2	1.86	0.58
1:B:804:LEU:O	1:B:808:GLN:HG3	2.03	0.58
1:A:93:LEU:HD11	1:A:371:MET:HE3	1.86	0.58
1:A:684:VAL:O	1:A:688:THR:HB	2.03	0.57
1:B:395:THR:CG2	1:B:397:MET:O	2.52	0.57
1:B:493:ASP:OD2	1:B:573:ARG:NH1	2.35	0.57
1:A:780:ARG:CD	4:A:1506:HOH:O	2.53	0.57
1:A:535:GLU:O	1:A:537:ALA:O	2.23	0.57
1:A:346:ILE:HG13	4:A:1430:HOH:O	2.04	0.57
1:A:129:THR:HB	4:A:1383:HOH:O	2.05	0.56
1:B:677:ARG:O	1:B:681:THR:OG1	2.24	0.56
1:B:788:TYR:HB3	4:B:1334:HOH:O	2.06	0.56
1:B:372:THR:HG21	1:B:375:ALA:HB2	1.88	0.55
1:B:558:HIS:HE1	4:B:1456:HOH:O	1.89	0.55
1:A:809:ARG:CD	4:A:1149:HOH:O	2.51	0.55
1:A:310:ARG:HA	1:A:310:ARG:HE	1.72	0.55
1:B:219:ARG:HD2	4:B:1259:HOH:O	2.06	0.55
1:B:223:ILE:HG12	1:B:355:THR:HG23	1.88	0.55
1:B:461:ASN:OD1	1:B:485:THR:HG21	2.06	0.55
1:B:454:ARG:HH11	1:B:454:ARG:CB	2.19	0.55
1:A:795:LEU:HA	1:B:618:MET:HE3	1.87	0.55
1:A:323:ARG:HE	1:B:615:GLU:HB2	1.72	0.55
1:A:764:ARG:HA	1:A:767:GLU:OE1	2.07	0.55
1:B:-3:SER:HB3	4:B:1375:HOH:O	2.05	0.55
1:B:381:GLU:OE2	1:B:638:ARG:HD2	2.08	0.54
1:A:346:ILE:HB	4:A:1430:HOH:O	2.06	0.54
1:A:357:THR:HB	1:A:359:GLN:NE2	2.22	0.54
1:A:107:LYS:CE	4:A:1370:HOH:O	2.54	0.54
1:A:793:ILE:HD12	1:A:796:ARG:CZ	2.37	0.54
1:B:680:ILE:O	1:B:684:VAL:HG23	2.08	0.54
1:A:793:ILE:HD12	1:A:796:ARG:NH1	2.23	0.53
1:B:129:THR:CB	4:B:1212:HOH:O	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:OD1	1:B:485:THR:CG2	2.56	0.53
1:B:303:ARG:O	1:B:304:ASP:HB2	2.09	0.53
1:A:561:ARG:O	1:A:564:ASP:HB2	2.09	0.53
1:B:536:GLU:C	1:B:537:ALA:O	2.49	0.53
1:B:671:GLN:H	1:B:671:GLN:HE21	1.58	0.52
1:B:798:MET:HG3	1:B:799:ALA:N	2.24	0.52
1:B:714:THR:O	1:B:717:SER:HB2	2.10	0.52
1:A:325:LEU:HD22	1:A:328:ARG:HH21	1.75	0.52
1:B:600:GLU:HG3	1:B:601:THR:N	2.24	0.52
1:B:63:LEU:HB3	1:B:64:PRO:HD3	1.92	0.52
1:B:767:GLU:HA	1:B:830:LEU:HD21	1.92	0.52
1:A:767:GLU:HA	1:A:830:LEU:HD21	1.92	0.52
1:B:649:ASN:O	1:B:653:LYS:HG2	2.10	0.52
1:A:461:ASN:OD1	1:A:485:THR:HG21	2.10	0.51
1:B:671:GLN:H	1:B:671:GLN:NE2	2.09	0.51
1:A:461:ASN:OD1	1:A:485:THR:CG2	2.58	0.51
1:B:687:ALA:HB3	1:B:701:LEU:HD13	1.91	0.51
1:A:107:LYS:HE3	4:A:1370:HOH:O	2.10	0.51
1:A:177:THR:HG23	4:A:1361:HOH:O	2.10	0.51
1:A:674:ASP:OD1	1:A:677:ARG:NH1	2.40	0.51
1:B:558:HIS:CD2	1:B:564:ASP:OD2	2.59	0.51
1:B:478:ARG:HD3	1:B:543:GLU:HB3	1.93	0.51
1:B:529:GLU:HA	1:B:532:ILE:HD12	1.93	0.51
1:B:780:ARG:HG2	4:B:1405:HOH:O	2.10	0.50
1:A:372:THR:HG21	1:A:375:ALA:HB2	1.94	0.50
1:B:801:ARG:NH1	1:B:806:GLU:HG3	2.25	0.50
1:A:558:HIS:HD2	1:A:564:ASP:OD2	1.94	0.50
4:A:1299:HOH:O	1:B:310:ARG:HD3	2.10	0.50
1:B:242:ALA:HB3	1:B:243:PRO:HD3	1.94	0.50
1:A:301:PHE:CE1	1:A:334:MET:HE2	2.47	0.50
1:A:708:LEU:HD12	1:A:827:VAL:HG22	1.94	0.50
1:A:35:THR:HG22	1:A:38:GLU:N	2.14	0.50
1:B:107:LYS:HE3	3:B:901:ADP:O1B	2.12	0.50
1:B:639:LYS:O	1:B:643:LYS:HG3	2.12	0.50
1:B:796:ARG:HD2	4:B:1250:HOH:O	2.12	0.50
1:A:607:ASN:ND2	1:B:788:TYR:OH	2.35	0.49
1:A:372:THR:CG2	1:A:375:ALA:HB2	2.42	0.49
1:A:649:ASN:HD22	1:A:652:ARG:HH21	1.59	0.49
1:A:536:GLU:C	1:A:537:ALA:O	2.55	0.49
1:A:671:GLN:CD	1:A:671:GLN:H	2.21	0.49
1:A:162:PRO:HD2	4:A:1413:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:THR:HB	1:A:717:SER:H	1.78	0.49
1:B:19:LYS:HD3	4:B:1468:HOH:O	2.12	0.49
1:A:793:ILE:HD11	1:A:806:GLU:HB3	1.94	0.49
1:B:276:ILE:HG13	1:B:281:GLU:CD	2.37	0.49
1:B:801:ARG:HH11	1:B:806:GLU:HG3	1.77	0.48
1:A:35:THR:HG23	4:A:1182:HOH:O	2.12	0.48
1:A:242:ALA:N	1:A:243:PRO:HD2	2.29	0.48
1:A:310:ARG:HG2	1:B:612:VAL:HG22	1.94	0.48
1:A:359:GLN:H	1:A:359:GLN:NE2	1.97	0.48
1:B:632:GLN:HA	1:B:632:GLN:NE2	2.28	0.48
1:B:118:ASN:HD21	1:B:367:LYS:NZ	2.12	0.48
1:B:687:ALA:CB	1:B:701:LEU:HD13	2.43	0.48
1:B:80:GLN:HE21	1:B:109:LEU:HD22	1.79	0.48
1:B:139:SER:O	1:B:143:GLY:HA3	2.14	0.48
1:B:649:ASN:ND2	1:B:652:ARG:HH21	2.08	0.48
1:B:681:THR:O	1:B:685:ASP:HB2	2.13	0.48
1:A:649:ASN:O	1:A:653:LYS:HG2	2.14	0.48
1:A:713:ILE:HD12	1:A:718:LEU:HD11	1.96	0.48
1:A:558:HIS:HE1	4:A:1421:HOH:O	1.97	0.47
1:A:819:LEU:CD2	1:A:822:MET:HE1	2.45	0.47
1:B:112:VAL:HG13	1:B:146:HIS:CE1	2.50	0.47
1:B:254:ASP:OD2	1:B:257:LYS:HB2	2.14	0.47
1:A:537:ALA:O	1:A:539:LYS:N	2.46	0.47
1:B:438:THR:HG23	1:B:438:THR:O	2.15	0.47
1:A:6:LEU:HD21	1:A:391:VAL:HG22	1.96	0.47
1:A:80:GLN:NE2	1:A:109:LEU:HD22	2.27	0.47
1:B:681:THR:HG23	1:B:736:LEU:HD21	1.96	0.47
1:A:35:THR:HB	1:A:38:GLU:OE1	2.14	0.47
1:A:347:LYS:HD2	4:A:1095:HOH:O	2.15	0.47
1:A:668:LEU:HD22	1:A:671:GLN:HG3	1.96	0.47
1:B:178:ASN:OD1	1:B:358:LEU:HD21	2.15	0.47
1:A:786:MET:HE1	1:A:811:GLY:HA3	1.97	0.47
1:B:12:ARG:HG2	4:B:1469:HOH:O	2.13	0.47
1:A:659:ARG:HD2	1:A:776:ASP:OD1	2.15	0.46
1:B:24:VAL:HG22	1:B:64:PRO:HA	1.97	0.46
1:B:147:ARG:CD	4:B:1211:HOH:O	2.42	0.46
1:B:78:LEU:HB3	1:B:80:GLN:HG2	1.97	0.46
1:A:141:TRP:O	1:A:144:ARG:HG3	2.15	0.46
1:A:662:ILE:HG21	1:A:772:LEU:HB2	1.97	0.46
1:A:10:GLU:OE1	1:A:10:GLU:HA	2.15	0.46
1:A:809:ARG:NH1	1:A:809:ARG:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LEU:HB3	1:B:531:PRO:HD3	1.98	0.46
1:A:477:ARG:HD2	4:A:1290:HOH:O	2.15	0.46
1:A:615:GLU:HG2	4:B:1226:HOH:O	2.14	0.46
1:A:75:TRP:HB2	1:A:81:ARG:HB2	1.98	0.46
1:A:310:ARG:HG2	1:B:612:VAL:CG2	2.46	0.46
1:B:413:GLU:HA	4:B:1331:HOH:O	2.16	0.46
1:A:152:GLN:HE21	1:A:152:GLN:HB3	1.57	0.45
1:A:318:ASP:OD2	1:A:318:ASP:C	2.59	0.45
1:A:178:ASN:ND2	4:A:1153:HOH:O	2.44	0.45
1:A:395:THR:HG21	1:A:397:MET:O	2.12	0.45
1:A:15:LYS:HD3	4:A:1310:HOH:O	2.16	0.45
1:B:670:ASP:HB2	1:B:671:GLN:NE2	2.32	0.45
1:B:220:THR:HA	1:B:221:PRO:HD3	1.86	0.45
1:A:-14:SER:HB3	1:A:-13:PRO:HD2	1.99	0.45
1:B:661:ARG:HD2	1:B:668:LEU:HD21	1.97	0.45
1:B:39:LEU:HD23	1:B:148:PHE:HE1	1.83	0.44
1:B:672:ALA:HA	1:B:675:MET:HE2	1.98	0.44
1:B:735:LEU:CA	4:B:1166:HOH:O	2.65	0.44
1:B:137:ARG:HD3	4:B:1222:HOH:O	2.17	0.44
1:A:35:THR:HB	1:A:38:GLU:HB2	1.99	0.44
1:A:42:LYS:HD2	1:A:42:LYS:HA	1.76	0.44
1:B:671:GLN:NE2	1:B:671:GLN:N	2.65	0.44
1:B:740:LEU:HD12	4:B:1241:HOH:O	2.17	0.44
1:A:0:ASP:O	1:A:1:ILE:C	2.59	0.44
1:A:169:TYR:CZ	1:A:199:GLN:HG2	2.53	0.44
1:A:-5:ARG:O	1:A:-3:SER:N	2.51	0.44
1:B:477:ARG:HD3	1:B:540:GLU:HG2	1.98	0.44
1:A:780:ARG:NE	4:A:1506:HOH:O	2.51	0.44
1:B:165:ARG:HD3	1:B:184:ASP:OD1	2.17	0.43
1:A:202:HIS:O	1:A:365:TYR:HA	2.18	0.43
1:A:260:VAL:HG23	1:A:296:LYS:HG2	2.00	0.43
1:A:655:ILE:HG13	1:A:779:TRP:CE3	2.53	0.43
1:B:4:LYS:HE3	1:B:4:LYS:HA	1.99	0.43
1:B:67:PHE:CD1	1:B:113:LEU:HB3	2.53	0.43
1:A:220:THR:HA	1:A:221:PRO:HD3	1.87	0.43
1:B:222:LEU:O	1:B:355:THR:CG2	2.66	0.43
1:A:714:THR:HG22	1:A:716:ASP:H	1.83	0.43
1:A:780:ARG:HD3	4:A:1490:HOH:O	2.19	0.43
1:A:181:PHE:HB3	1:A:361:TYR:OH	2.17	0.43
1:A:4:LYS:HA	4:A:1418:HOH:O	2.18	0.43
1:A:328:ARG:HH12	1:A:796:ARG:HE	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD22	1:A:468:GLU:HG2	1.99	0.43
1:B:284:ASN:HA	4:B:1524:HOH:O	2.19	0.43
1:A:78:LEU:HB3	1:A:80:GLN:HG2	2.00	0.43
1:A:802:ASP:HA	1:A:803:PRO:HD3	1.86	0.43
1:B:81:ARG:O	1:B:82:PRO:C	2.61	0.43
1:B:608:LEU:HA	1:B:609:PRO:HD3	1.93	0.43
1:B:143:GLY:HA2	1:B:153:VAL:HG21	2.01	0.43
1:B:537:ALA:O	1:B:538:SER:HB3	2.19	0.43
1:B:693:ALA:O	1:B:694:GLU:C	2.62	0.43
1:A:63:LEU:HD23	1:A:63:LEU:C	2.44	0.43
1:A:110:THR:HB	1:A:371:MET:HE1	2.01	0.43
1:B:179:ASN:HB2	4:B:1081:HOH:O	2.19	0.43
1:B:254:ASP:HB3	1:B:259:THR:HG22	2.01	0.43
1:B:612:VAL:HA	1:B:613:PRO:HD3	1.94	0.43
1:B:50:LEU:HD11	1:B:59:LEU:CD2	2.49	0.42
1:B:472:ILE:HG21	1:B:492:THR:HB	2.00	0.42
1:B:469:ALA:O	1:B:470:THR:C	2.62	0.42
1:A:328:ARG:HH12	1:A:796:ARG:NE	2.16	0.42
1:A:278:ASN:O	1:A:281:GLU:HG2	2.19	0.42
1:B:246:GLU:HB3	1:B:249:VAL:HB	2.01	0.42
1:A:519:PRO:HD2	4:A:1410:HOH:O	2.18	0.42
1:A:23:TYR:O	1:A:24:VAL:C	2.63	0.42
1:A:649:ASN:HD22	1:A:652:ARG:NH2	2.17	0.42
1:B:463:LYS:HA	1:B:463:LYS:HD2	1.86	0.42
1:B:646:GLU:HA	1:B:646:GLU:OE1	2.19	0.42
1:A:108:THR:O	1:A:111:CYS:HB3	2.19	0.42
1:A:232:SER:HB3	1:A:346:ILE:HD12	2.02	0.42
1:A:819:LEU:HD23	1:A:822:MET:CE	2.47	0.41
1:B:759:GLY:O	1:B:760:GLU:C	2.62	0.41
1:B:216:ASP:O	1:B:219:ARG:HG3	2.20	0.41
1:A:690:GLU:C	1:A:692:TYR:H	2.28	0.41
1:B:303:ARG:HD2	1:B:342:GLU:OE1	2.20	0.41
1:B:694:GLU:O	1:B:696:TRP:N	2.53	0.41
1:A:499:ASN:O	1:A:503:LEU:HD12	2.20	0.41
1:A:513:LEU:CD2	1:A:521:GLU:HB3	2.51	0.41
1:A:632:GLN:O	1:A:636:GLU:HG2	2.20	0.41
1:B:55:ASN:HB3	4:B:1271:HOH:O	2.21	0.41
1:B:78:LEU:O	1:B:79:ASP:HB2	2.19	0.41
1:B:107:LYS:HG2	1:B:371:MET:HE2	2.03	0.41
1:B:605:ARG:HE	1:B:605:ARG:HB2	1.80	0.41
1:B:755:GLU:O	1:B:759:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.70	0.41
1:B:6:LEU:C	1:B:8:LEU:N	2.79	0.41
1:A:694:GLU:O	1:A:696:TRP:N	2.54	0.41
1:B:-15:ASP:HB3	4:B:1068:HOH:O	2.21	0.41
1:A:254:ASP:HB2	1:A:259:THR:HG22	2.03	0.40
1:A:615:GLU:HG3	1:B:323:ARG:HG3	2.03	0.40
1:B:660:ARG:HG2	4:B:1355:HOH:O	2.09	0.40
1:A:229:ASP:HB3	4:A:1506:HOH:O	2.21	0.40
1:B:818:MET:O	1:B:822:MET:HG3	2.21	0.40
1:A:412:GLU:O	1:A:413:GLU:C	2.64	0.40
1:A:530:LEU:HB3	1:A:531:PRO:HD3	2.03	0.40
1:A:250:HIS:O	1:A:263:HIS:HB2	2.21	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	832/922 (90%)	781 (94%)	41 (5%)	10 (1%)	10	23
1	B	832/922 (90%)	784 (94%)	43 (5%)	5 (1%)	21	42
All	All	1664/1844 (90%)	1565 (94%)	84 (5%)	15 (1%)	14	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	486	ASN
1	A	538	SER
1	A	689	GLY
1	A	695	ASP
1	B	695	ASP

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Mol	Chain	Res	Type
1	A	-4	GLY
1	A	537	ALA
1	A	760	GLU
1	A	800	GLN
1	B	319	GLU
1	A	795	LEU
1	B	689	GLY
1	B	800	GLN
1	B	230	GLY

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	697/755 (92%)	578 (83%)	119 (17%)	2	3
1	B	697/755 (92%)	577 (83%)	120 (17%)	2	3
All	All	1394/1510 (92%)	1155 (83%)	239 (17%)	2	3

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-12	ASP
1	A	-3	SER
1	A	4	LYS
1	A	6	LEU
1	A	10	GLU
1	A	12	ARG
1	A	13	MET
1	A	18	LYS
1	A	28	SER
1	A	32	GLU
1	A	35	THR
1	A	40	ARG
1	A	50	LEU
1	A	53	GLN

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Mol	Chain	Res	Type
1	A	54	LYS
1	A	78	LEU
1	A	107	LYS
1	A	130	VAL
1	A	137	ARG
1	A	152	GLN
1	A	155	VAL
1	A	179	ASN
1	A	190	MET
1	A	210	VAL
1	A	215	ILE
1	A	222	LEU
1	A	225	SER
1	A	232	SER
1	A	233	ASN
1	A	240	ARG
1	A	252	GLU
1	A	255	LEU
1	A	256	ARG
1	A	257	LYS
1	A	258	ARG
1	A	259	THR
1	A	262	VAL
1	A	264	GLU
1	A	265	LYS
1	A	268	GLU
1	A	276	ILE
1	A	284	ASN
1	A	296	LYS
1	A	310	ARG
1	A	318	ASP
1	A	319	GLU
1	A	321	THR
1	A	323	ARG
1	A	326	ILE
1	A	345	GLU
1	A	346	ILE
1	A	347	LYS
1	A	355	THR
1	A	359	GLN
1	A	371	MET
1	A	378	GLU

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Mol	Chain	Res	Type
1	A	395	THR
1	A	417	ILE
1	A	434	LEU
1	A	438	THR
1	A	442	ARG
1	A	444	GLU
1	A	452	LYS
1	A	453	ARG
1	A	454	ARG
1	A	459	VAL
1	A	463	LYS
1	A	472	ILE
1	A	477	ARG
1	A	485	THR
1	A	500	VAL
1	A	508	LEU
1	A	511	ARG
1	A	536	GLU
1	A	538	SER
1	A	542	LYS
1	A	555	THR
1	A	570	ARG
1	A	573	ARG
1	A	593	ARG
1	A	599	LEU
1	A	600	GLU
1	A	601	THR
1	A	603	LEU
1	A	617	LYS
1	A	618	MET
1	A	623	ILE
1	A	624	LYS
1	A	631	GLU
1	A	632	GLN
1	A	653	LYS
1	A	659	ARG
1	A	664	GLU
1	A	669	LYS
1	A	671	GLN
1	A	688	THR
1	A	694	GLU
1	A	696	TRP

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Mol	Chain	Res	Type
1	A	698	LEU
1	A	703	THR
1	A	708	LEU
1	A	717	SER
1	A	735	LEU
1	A	741	LYS
1	A	744	GLU
1	A	750	ARG
1	A	754	LEU
1	A	755	GLU
1	A	757	ILE
1	A	781	GLU
1	A	793	ILE
1	A	795	LEU
1	A	796	ARG
1	A	800	GLN
1	A	809	ARG
1	A	822	MET
1	A	824	GLU
1	A	827	VAL
1	A	835	VAL
1	B	-14	SER
1	B	-5	ARG
1	B	-3	SER
1	B	4	LYS
1	B	7	ARG
1	B	12	ARG
1	B	13	MET
1	B	18	LYS
1	B	33	LYS
1	B	48	ARG
1	B	50	LEU
1	B	53	GLN
1	B	54	LYS
1	B	78	LEU
1	B	130	VAL
1	B	137	ARG
1	B	152	GLN
1	B	155	VAL
1	B	179	ASN
1	B	210	VAL
1	B	222	LEU

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Mol	Chain	Res	Type
1	B	225	SER
1	B	229	ASP
1	B	233	ASN
1	B	240	ARG
1	B	247	LYS
1	B	256	ARG
1	B	258	ARG
1	B	259	THR
1	B	264	GLU
1	B	268	GLU
1	B	276	ILE
1	B	277	ASP
1	B	292	ASN
1	B	305	LYS
1	B	310	ARG
1	B	317	VAL
1	B	318	ASP
1	B	319	GLU
1	B	320	PHE
1	B	326	ILE
1	B	328	ARG
1	B	345	GLU
1	B	347	LYS
1	B	349	GLU
1	B	355	THR
1	B	359	GLN
1	B	371	MET
1	B	387	LYS
1	B	395	THR
1	B	399	MET
1	B	417	ILE
1	B	425	GLU
1	B	429	LYS
1	B	433	VAL
1	B	434	LEU
1	B	438	THR
1	B	441	GLU
1	B	444	GLU
1	B	452	LYS
1	B	454	ARG
1	B	463	LYS
1	B	472	ILE

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Mol	Chain	Res	Type
1	B	485	THR
1	B	507	ARG
1	B	510	GLU
1	B	520	GLU
1	B	535	GLU
1	B	536	GLU
1	B	539	LYS
1	B	542	LYS
1	B	555	THR
1	B	570	ARG
1	B	592	ARG
1	B	593	ARG
1	B	599	LEU
1	B	600	GLU
1	B	603	LEU
1	B	605	ARG
1	B	615	GLU
1	B	617	LYS
1	B	618	MET
1	B	624	LYS
1	B	628	THR
1	B	632	GLN
1	B	646	GLU
1	B	660	ARG
1	B	666	GLU
1	B	669	LYS
1	B	671	GLN
1	B	675	MET
1	B	680	ILE
1	B	681	THR
1	B	688	THR
1	B	690	GLU
1	B	694	GLU
1	B	698	LEU
1	B	699	ASP
1	B	703	THR
1	B	706	LYS
1	B	708	LEU
1	B	713	ILE
1	B	716	ASP
1	B	717	SER
1	B	718	LEU

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Mol	Chain	Res	Type
1	B	735	LEU
1	B	737	GLU
1	B	750	ARG
1	B	754	LEU
1	B	757	ILE
1	B	780	ARG
1	B	796	ARG
1	B	798	MET
1	B	800	GLN
1	B	810	GLU
1	B	823	LYS
1	B	824	GLU
1	B	827	VAL
1	B	833	VAL
1	B	835	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	97	ASN
1	A	118	ASN
1	A	146	HIS
1	A	152	GLN
1	A	203	HIS
1	A	233	ASN
1	A	250	HIS
1	A	293	ASN
1	A	350	ASN
1	A	359	GLN
1	A	486	ASN
1	A	558	HIS
1	A	607	ASN
1	A	627	GLN
1	A	632	GLN
1	A	649	ASN
1	A	671	GLN
1	A	800	GLN
1	B	55	ASN
1	B	80	GLN
1	B	118	ASN
1	B	146	HIS

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	192	HIS
1	B	203	HIS
1	B	233	ASN
1	B	250	HIS
1	B	293	ASN
1	B	359	GLN
1	B	558	HIS
1	B	632	GLN
1	B	649	ASN
1	B	671	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
3	ADP	B	901	2	28,29,29	1.55	5 (17%)	43,45,45	1.95	10 (23%)
3	ADP	A	900	2	28,29,29	1.34	5 (17%)	43,45,45	2.05	10 (23%)

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
3	ADP	B	901	2	-	2/16/32/32	0/3/3/3
3	ADP	A	900	2	-	4/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ADP	PA-O3A	4.78	1.64	1.59
3	B	901	ADP	C2-N1	3.12	1.39	1.33
3	B	901	ADP	C2-N3	2.83	1.39	1.33
3	A	900	ADP	C2-N1	2.76	1.38	1.33
3	A	900	ADP	C2-N3	2.76	1.38	1.33
3	A	900	ADP	C8-N7	2.70	1.36	1.31
3	B	901	ADP	PB-O3B	2.46	1.63	1.54
3	B	901	ADP	C8-N7	2.44	1.36	1.31
3	A	900	ADP	PB-O3B	2.22	1.63	1.54
3	A	900	ADP	PA-O3A	2.07	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	ADP	N3-C2-N1	-6.70	118.44	128.58
3	B	901	ADP	N3-C2-N1	-5.62	120.07	128.58
3	A	900	ADP	C5-C4-N3	-4.79	120.12	126.72
3	B	901	ADP	C5-C4-N3	-4.35	120.72	126.72
3	A	900	ADP	C2-N3-C4	4.17	122.03	111.83
3	B	901	ADP	N9-C8-N7	-3.62	108.80	113.94
3	B	901	ADP	C5-N7-C8	3.59	109.09	103.45
3	A	900	ADP	O3A-PB-O1B	-3.51	92.56	111.04
3	B	901	ADP	O3B-PB-O3A	3.48	116.32	104.64
3	B	901	ADP	C2-N3-C4	3.48	120.34	111.83
3	B	901	ADP	O3A-PB-O1B	-3.41	93.11	111.04
3	A	900	ADP	N9-C8-N7	-3.28	109.28	113.94
3	A	900	ADP	O2A-PA-O3A	3.20	115.93	107.27
3	A	900	ADP	C5-N7-C8	3.12	108.35	103.45
3	A	900	ADP	N3-C4-N9	2.92	132.14	127.17
3	B	901	ADP	N3-C4-N9	2.80	131.94	127.17
3	B	901	ADP	C4-C5-N7	-2.55	107.67	110.58
3	B	901	ADP	O2A-PA-O3A	2.39	113.74	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	ADP	C4-C5-N7	-2.32	107.93	110.58
3	A	900	ADP	O3B-PB-O3A	2.24	112.16	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

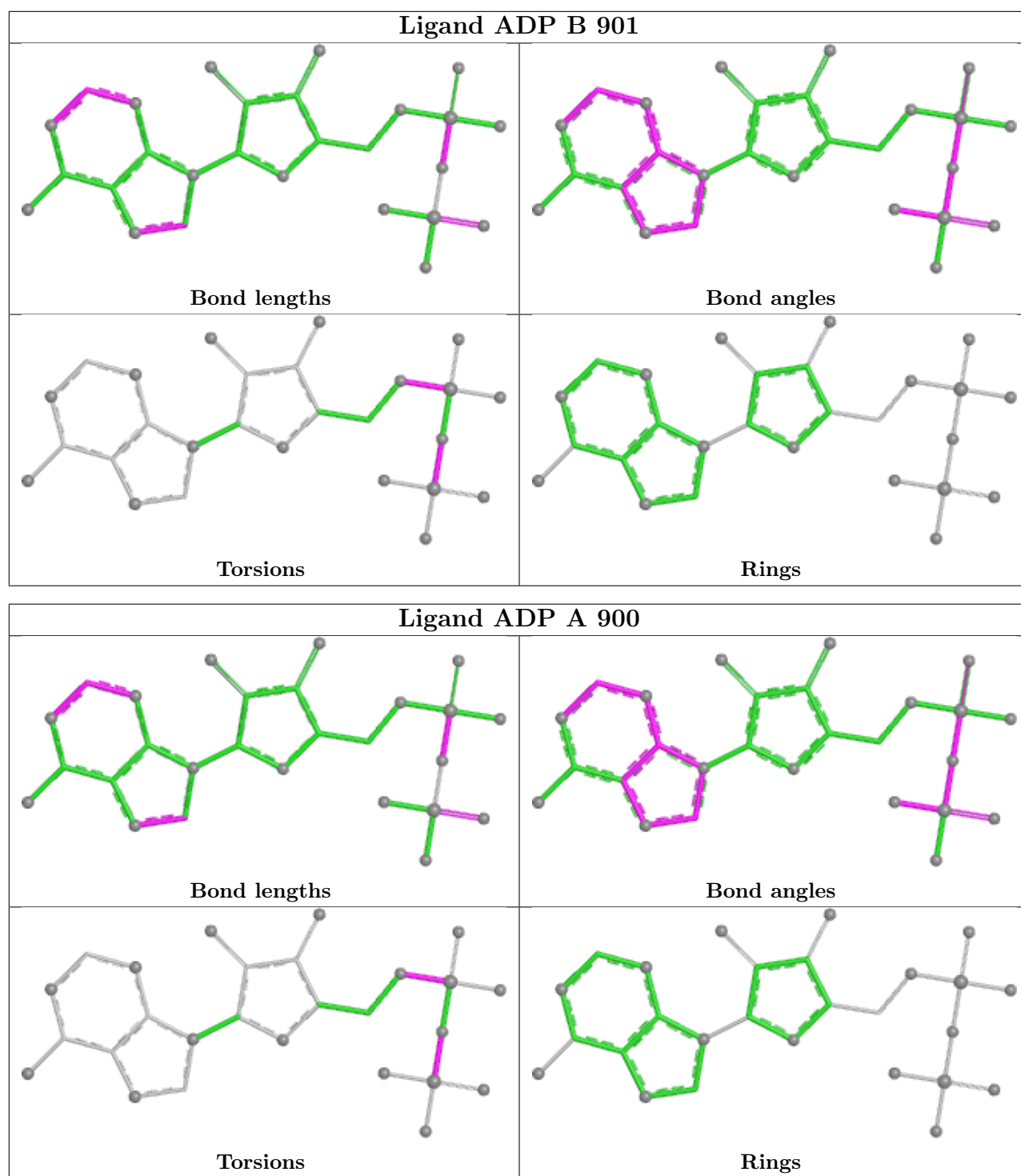
Mol	Chain	Res	Type	Atoms
3	A	900	ADP	PA-O3A-PB-O2B
3	B	901	ADP	PA-O3A-PB-O1B
3	A	900	ADP	C5'-O5'-PA-O1A
3	B	901	ADP	C5'-O5'-PA-O1A
3	A	900	ADP	PA-O3A-PB-O1B
3	A	900	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ADP	1	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.