



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:18 PM GMT

PDB ID : 1S3S
Title : Crystal structure of AAA ATPase p97/VCP ND1 in complex with p47 C
Authors : Dreveny, I.; Kondo, H.; Uchiyama, K.; Shaw, A.; Zhang, X.; Freemont, P.S.
Deposited on : 2004-01-14
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

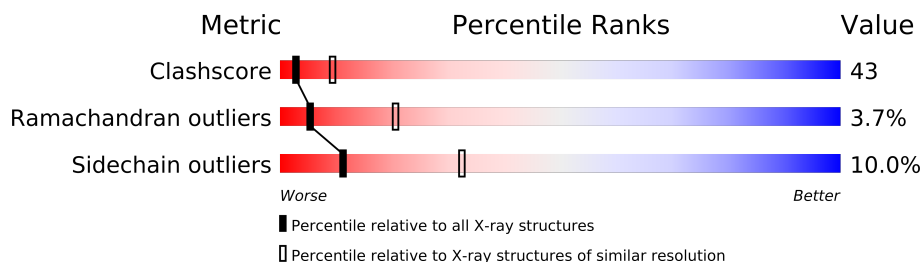
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	458	
1	B	458	
1	C	458	
1	D	458	
1	E	458	
1	F	458	
2	G	127	
2	H	127	
2	I	127	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22367 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3398	2135	601	645	17			
1	B	436	Total	C	N	O	S	0	0	0
			3390	2130	598	645	17			
1	C	437	Total	C	N	O	S	0	0	0
			3405	2139	606	642	18			
1	D	436	Total	C	N	O	S	0	0	0
			3380	2124	598	640	18			
1	E	436	Total	C	N	O	S	0	0	0
			3399	2137	603	641	18			
1	F	441	Total	C	N	O	S	0	0	0
			3432	2157	609	648	18			

- Molecule 2 is a protein called p47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	118	Total	C	N	O	S	0	0	0
			825	511	153	159	2			
2	H	107	Total	C	N	O	S	0	0	0
			758	474	140	142	2			
2	I	24	Total	C	N	O		0	0	0
			155	99	30	26				

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	10	Total	O	0	0
			10	10		
4	C	6	Total	O	0	0
			6	6		
4	D	7	Total	O	0	0
			7	7		
4	E	6	Total	O	0	0
			6	6		
4	F	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	O 2	0	0
4	H	3	Total 3	O 3	0	0
4	I	1	Total 1	O 1	0	0

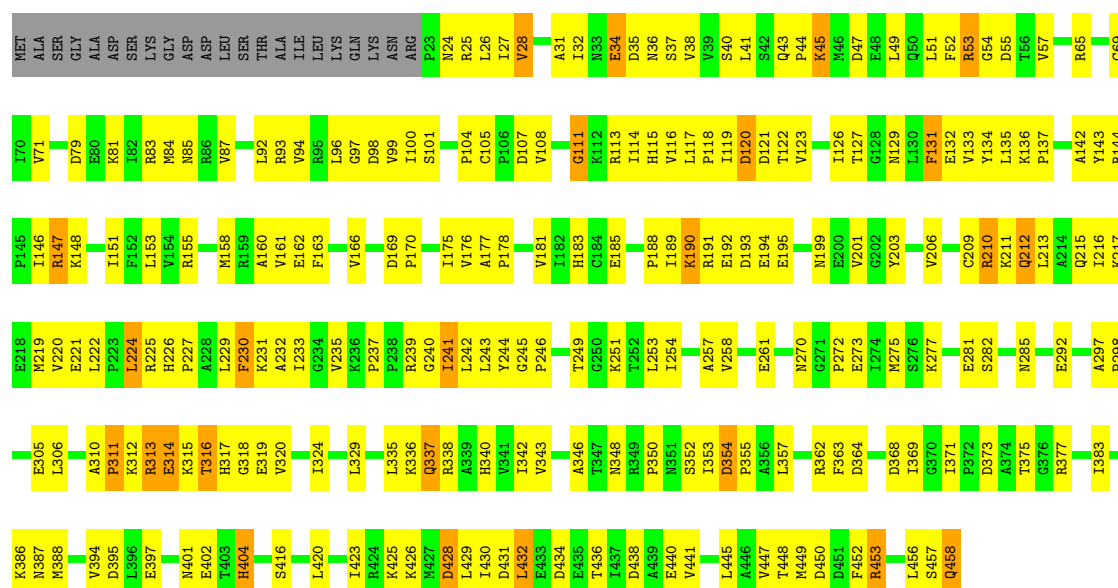
3 Residue-property plots

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

Note EDS was not executed.

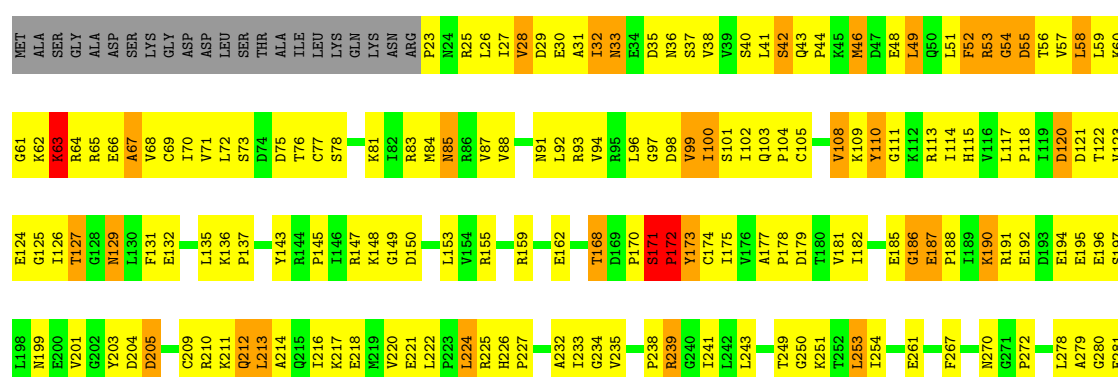
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

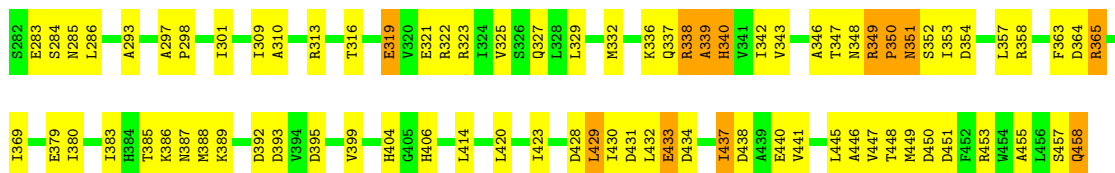
Chain A:



- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

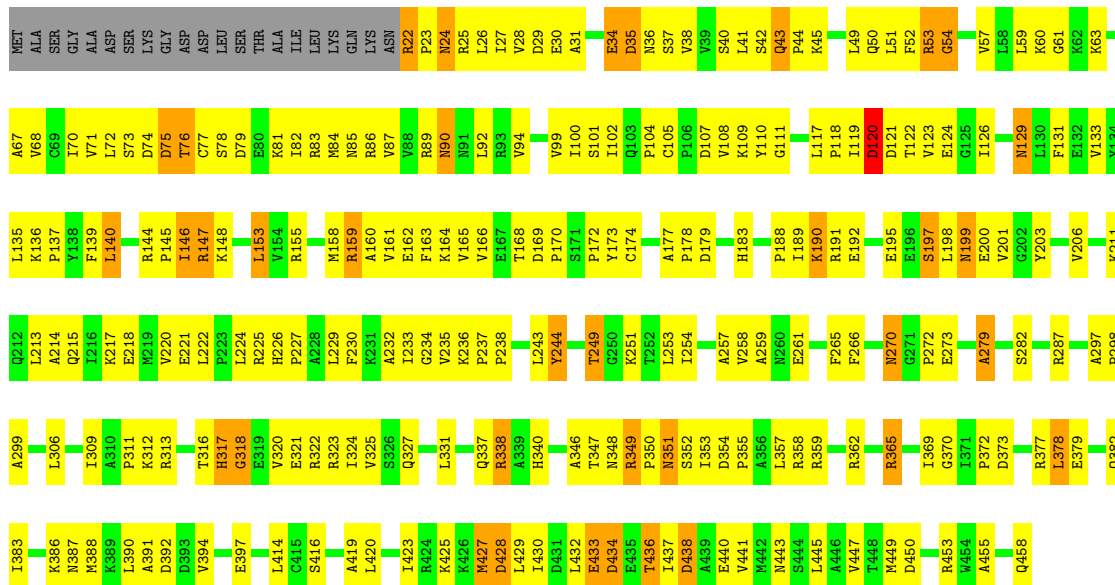
Chain B:





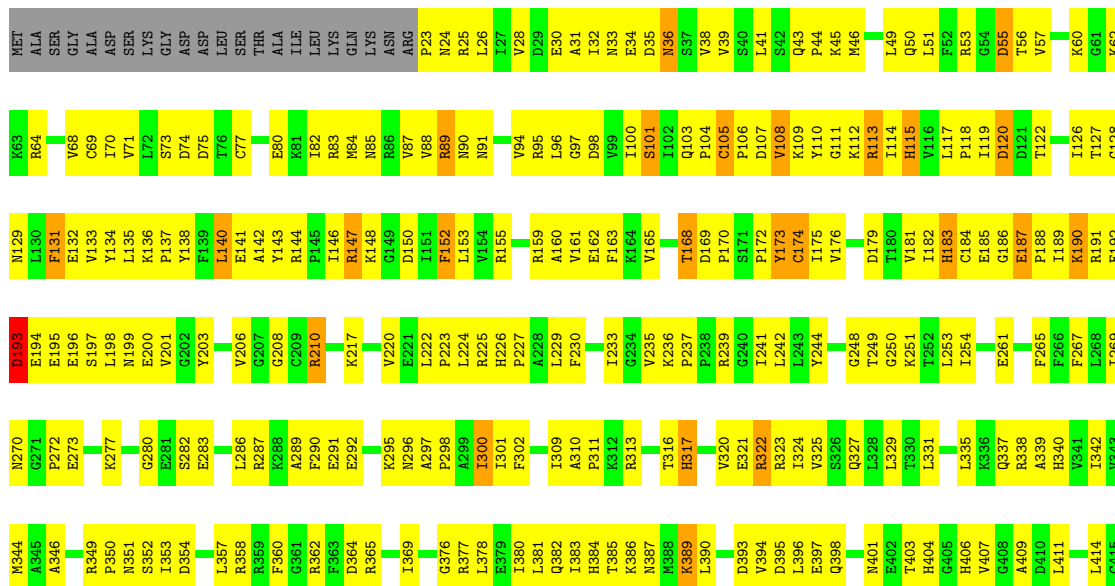
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain C:



- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

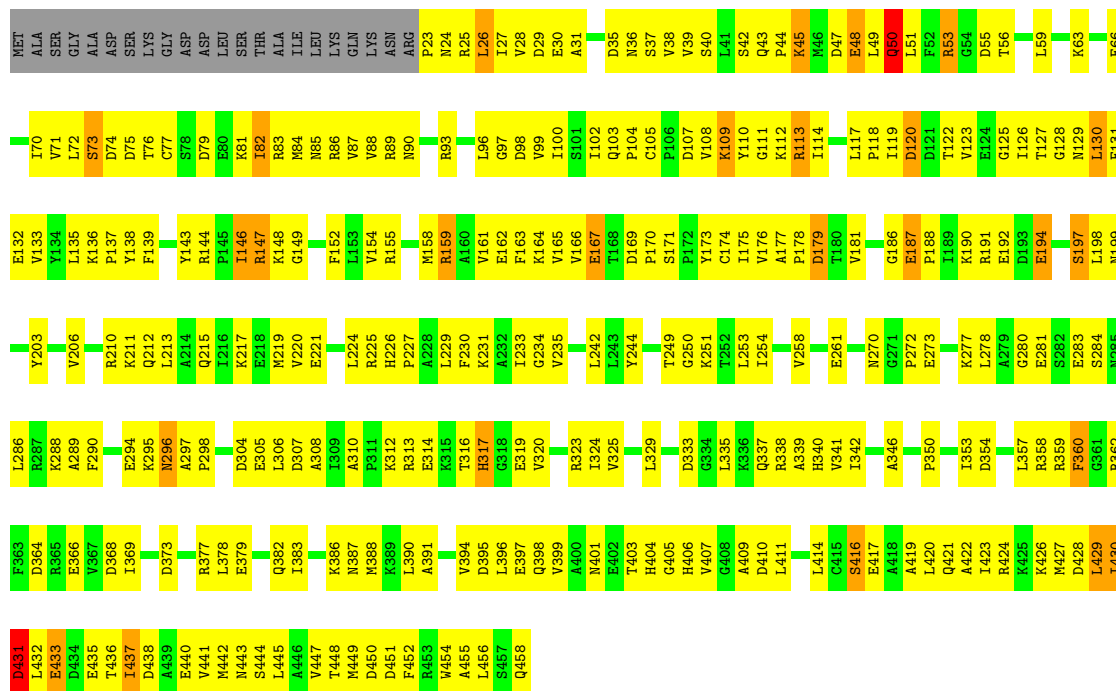
Chain D:





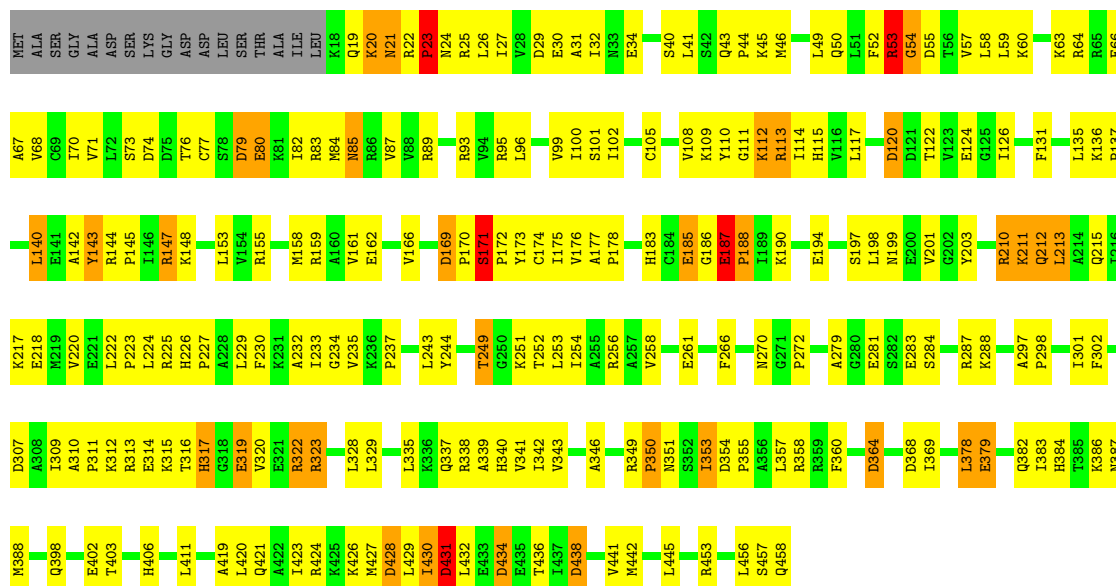
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain E:



- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain F:

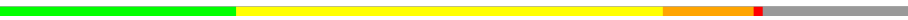


- Molecule 2: p47 protein

Chain G: 

VAL	R329	LYS	P330	PRO	A331	LYS	M332	GLY	A333	ALA	A334	PHE	T335	LYS	F253	F253	T254	G255	A264	P265	N279	K282	A283	S286	I287	L288	P294	T295	T296	N297	I298	Q299	I300	R301	L302	A303	D304	G305	G306	R307	L308	V309	Q310	K311	F312	N313	H314	S315	H316	R317	I318	S319	D320	I321	R322	L323	F324	I325	V326	D327	A328
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• Molecule 2: p47 protein

Chain H: 

VAL	LYS	PRO	GLY	ALA	PHE	LYS	ALA	PHE	THR	GLY	G257	A264	P265	GLN	VAL	LEU	ASN	THR	SER	P273	Q276	N279	I287	L288	I289	N290	E293	P294	T295	T296	N297	I298	I300	R301	L302	A303	D304	G305	G306	R307	L308	V309	Q310	K311	F312	N313	H314	S315	R317
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• Molecule 2: p47 protein

Chain I: 

VAL	LYS	PRO	GLN	LYS	ALA	PHE	LYS	ALA	PHE	THR	GLY	GLY	GLN	LYS	LEU	GLY	SER	THR	ALA	PRO	GLN	VAL	LEU	ASN	THR	SER	THR	VAL	PRO	ALA	GLN	A277	E280	A281	K282	A283	I287	LEU	ILE	ASN	GLN	THR	ALA	GLU	LYS	PRO	THR	THR	ALA	ASN	ILE	GLN	ILE	ASN	ALA	VAL	ILE	VAL	GLN	ARG
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	157.72Å 157.72Å 243.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 2.90	Depositor
% Data completeness (in resolution range)	96.3 (39.70-2.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22367	wwPDB-VP
Average B, all atoms (Å ²)	72.0	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: 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	0.43	0/3450	0.70	0/4662
1	B	0.43	0/3443	0.75	4/4656 (0.1%)
1	C	0.39	0/3458	0.64	0/4674
1	D	0.39	0/3433	0.67	0/4642
1	E	0.38	0/3452	0.65	2/4664 (0.0%)
1	F	0.46	0/3485	0.73	1/4709 (0.0%)
2	G	0.48	0/833	1.02	6/1135 (0.5%)
2	H	0.51	0/764	1.29	6/1037 (0.6%)
2	I	0.41	0/154	0.63	0/208
All	All	0.42	0/22472	0.73	19/30387 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	343	PHE	C-N-CD	-23.85	68.14	120.60
1	B	171	SER	C-N-CD	-16.94	83.33	120.60
2	G	343	PHE	C-N-CD	-14.94	87.73	120.60
2	H	343	PHE	C-N-CA	13.68	179.44	122.00
1	B	172	PRO	CA-N-CD	-7.27	101.32	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3398	0	3447	231	0
1	B	3390	0	3421	280	0
1	C	3405	0	3452	310	1
1	D	3380	0	3406	353	0
1	E	3399	0	3453	334	0
1	F	3432	0	3477	251	0
2	G	825	0	768	99	1
2	H	758	0	720	118	0
2	I	155	0	132	5	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
4	A	14	0	0	3	0
4	B	10	0	0	0	0
4	C	6	0	0	0	0
4	D	7	0	0	4	0
4	E	6	0	0	0	0
4	F	14	0	0	1	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	0	0
All	All	22367	0	22348	1924	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 1924 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:365:ARG:HG2	1:C:365:ARG:HH11	1.03	1.19
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.02	1.14
1:D:322:ARG:HH11	1:D:322:ARG:HG3	1.14	1.13
2:G:283:ALA:HB1	2:G:324:PHE:CE1	1.84	1.12
1:D:283:GLU:OE2	1:D:327:GLN:HB2	1.48	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:183:HIS:CE1	2:G:255:GLY:O[1.445]	2.17	0.03

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	434/458 (95%)	379 (87%)	43 (10%)	12 (3%)	8	29
1	B	434/458 (95%)	362 (83%)	51 (12%)	21 (5%)	4	12
1	C	435/458 (95%)	374 (86%)	50 (12%)	11 (2%)	9	32
1	D	434/458 (95%)	372 (86%)	50 (12%)	12 (3%)	8	29
1	E	434/458 (95%)	365 (84%)	57 (13%)	12 (3%)	8	29
1	F	439/458 (96%)	378 (86%)	43 (10%)	18 (4%)	4	17
2	G	116/127 (91%)	94 (81%)	13 (11%)	9 (8%)	1	3
2	H	103/127 (81%)	82 (80%)	13 (13%)	8 (8%)	1	3
2	I	20/127 (16%)	18 (90%)	1 (5%)	1 (5%)	3	11
All	All	2849/3129 (91%)	2424 (85%)	321 (11%)	104 (4%)	5	20

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	120	ASP
1	A	230	PHE
1	A	314	GLU
1	A	316	THR

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	369/390 (95%)	340 (92%)	29 (8%)	18	46
1	B	367/390 (94%)	325 (89%)	42 (11%)	8	24
1	C	369/390 (95%)	329 (89%)	40 (11%)	9	27
1	D	364/390 (93%)	330 (91%)	34 (9%)	13	37
1	E	369/390 (95%)	334 (90%)	35 (10%)	12	35
1	F	371/390 (95%)	335 (90%)	36 (10%)	12	35
2	G	75/105 (71%)	66 (88%)	9 (12%)	7	21
2	H	68/105 (65%)	59 (87%)	9 (13%)	6	16
2	I	10/105 (10%)	7 (70%)	3 (30%)	0	1
All	All	2362/2655 (89%)	2125 (90%)	237 (10%)	11	32

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	438	ASP
1	D	190	LYS
2	G	310	GLN
1	C	458	GLN
1	D	113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	387	ASN
1	D	285	ASN
2	G	313	ASN
1	C	443	ASN
1	D	36	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	$\# Z > 2$
3	ADP	A	800	-	29,29,29	1.56	6 (20%)	45,45,45	2.30	6 (13%)
3	ADP	B	801	-	29,29,29	1.79	8 (27%)	45,45,45	2.33	5 (11%)
3	ADP	C	802	-	29,29,29	1.62	3 (10%)	45,45,45	2.30	6 (13%)
3	ADP	D	803	-	29,29,29	1.59	5 (17%)	45,45,45	2.28	6 (13%)
3	ADP	E	804	-	29,29,29	1.62	4 (13%)	45,45,45	2.28	8 (17%)
3	ADP	F	805	-	29,29,29	1.74	9 (31%)	45,45,45	2.30	5 (11%)

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	A	800	-	-	0/16/32/32	0/1/3/3
3	ADP	B	801	-	-	0/16/32/32	0/1/3/3
3	ADP	C	802	-	-	0/16/32/32	0/1/3/3
3	ADP	D	803	-	-	0/16/32/32	0/1/3/3
3	ADP	E	804	-	-	0/16/32/32	0/1/3/3
3	ADP	F	805	-	-	0/16/32/32	0/1/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	ADP	C4-N9	-5.15	1.30	1.37
3	E	804	ADP	C4-N9	-5.10	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ADP	C4-N9	-4.92	1.30	1.37
3	D	803	ADP	C4-N9	-4.46	1.31	1.37
3	F	805	ADP	C4-N9	-4.42	1.31	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ADP	N3-C2-N1	-12.92	117.91	128.71
3	A	800	ADP	N3-C2-N1	-12.52	118.25	128.71
3	F	805	ADP	N3-C2-N1	-12.49	118.27	128.71
3	C	802	ADP	N3-C2-N1	-12.44	118.31	128.71
3	D	803	ADP	N3-C2-N1	-12.31	118.42	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.