



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:04 AM GMT

PDB ID : 3KO1
Title : Crystal structure of thermosome from *Acidianus tengchongensis* strain S5
Authors : Huo, Y.; Zhang, K.; Hu, Z.; Wang, L.; Zhai, Y.; Zhou, Q.; Lander, G.; He, Y.;
Zhu, J.; Xu, W.; Dong, Z.; Sun, F.
Deposited on : 2009-11-12
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

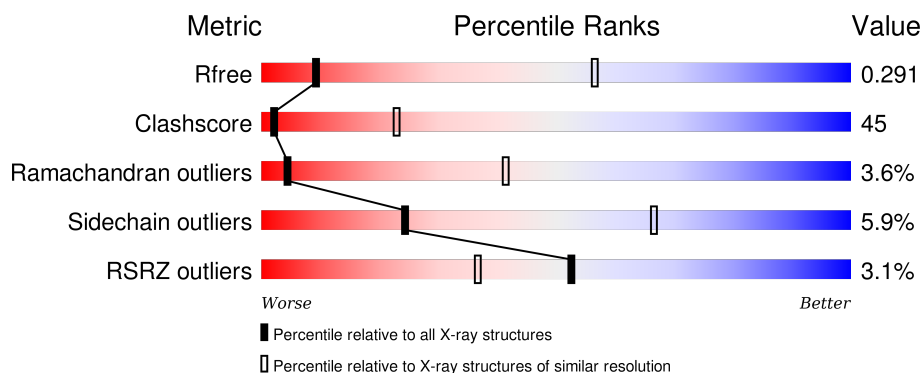
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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. 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	553	
1	B	553	
1	C	553	
1	D	553	
1	E	553	

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Mol	Chain	Length	Quality of chain
1	F	553	
1	G	553	
1	H	553	
1	I	553	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	800	-	-	-	X
2	ADP	G	800	-	-	-	X
2	ADP	H	800	-	-	-	X
2	ADP	I	800	-	-	-	X

2 Entry composition

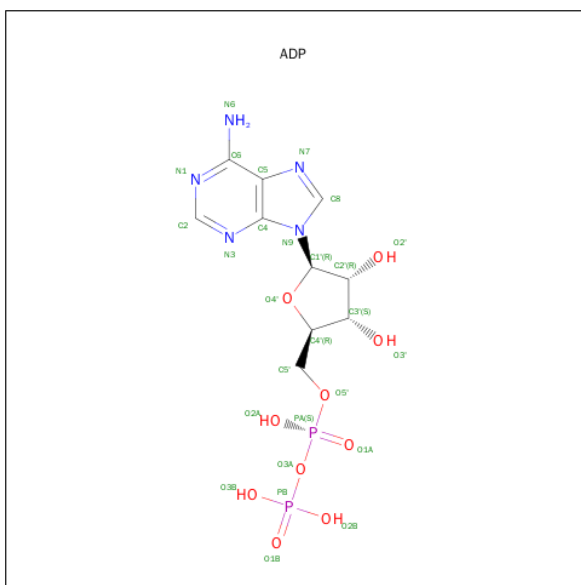
There are 2 unique types of molecules in this entry. The entry contains 34884 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chaperonin.

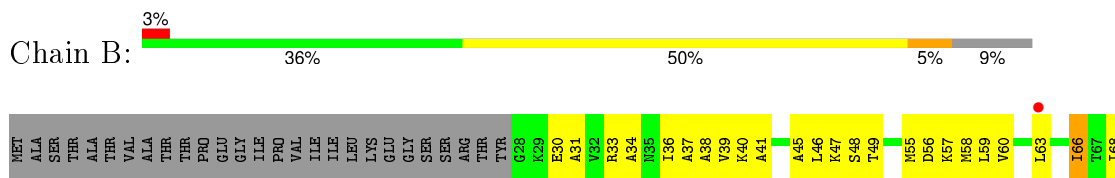
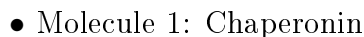
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	B	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	C	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	D	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	E	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	F	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	G	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	H	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	I	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			

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



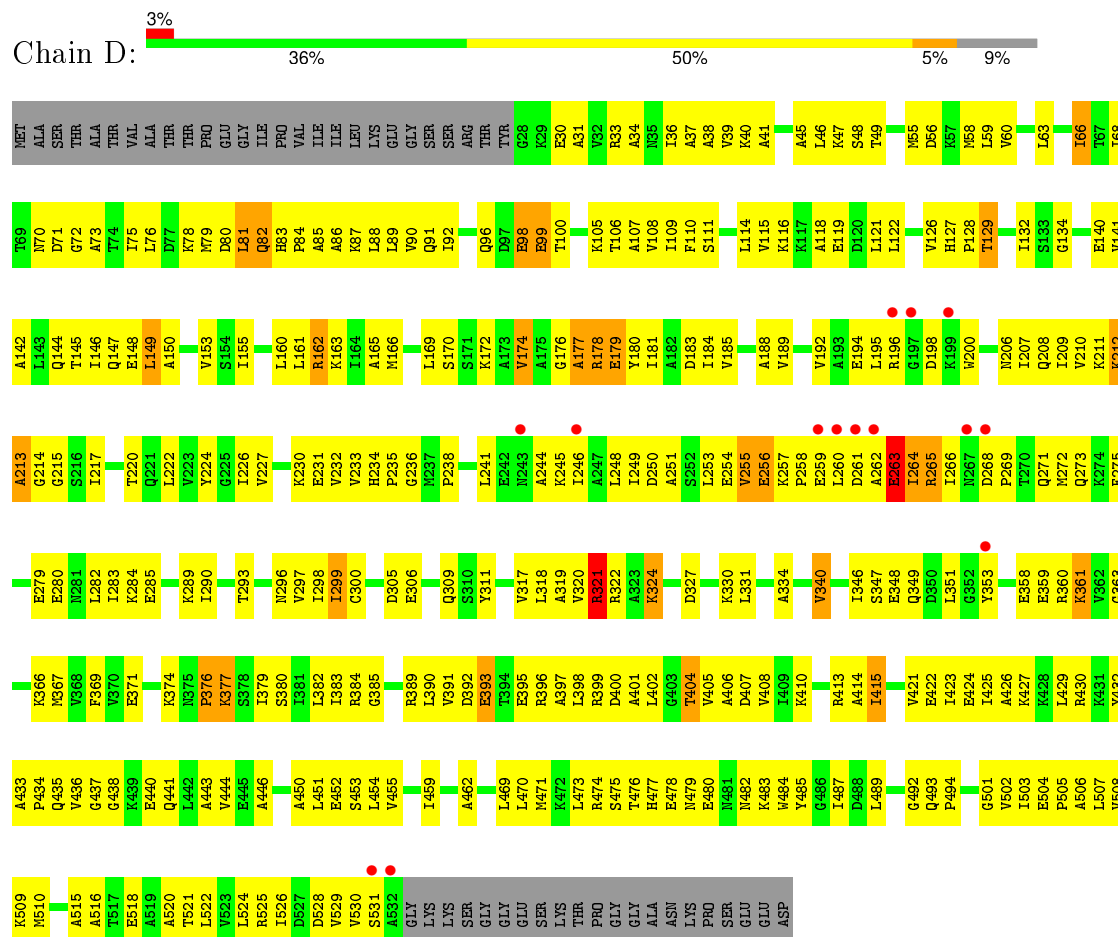
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	7	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	7	0

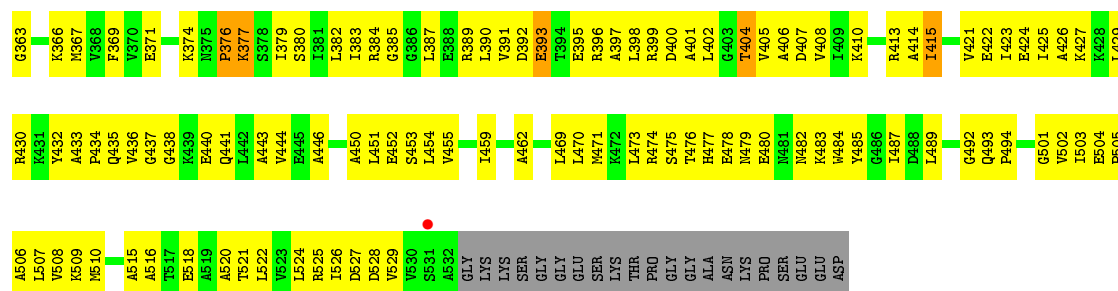
- Molecule 1: Chaperonin



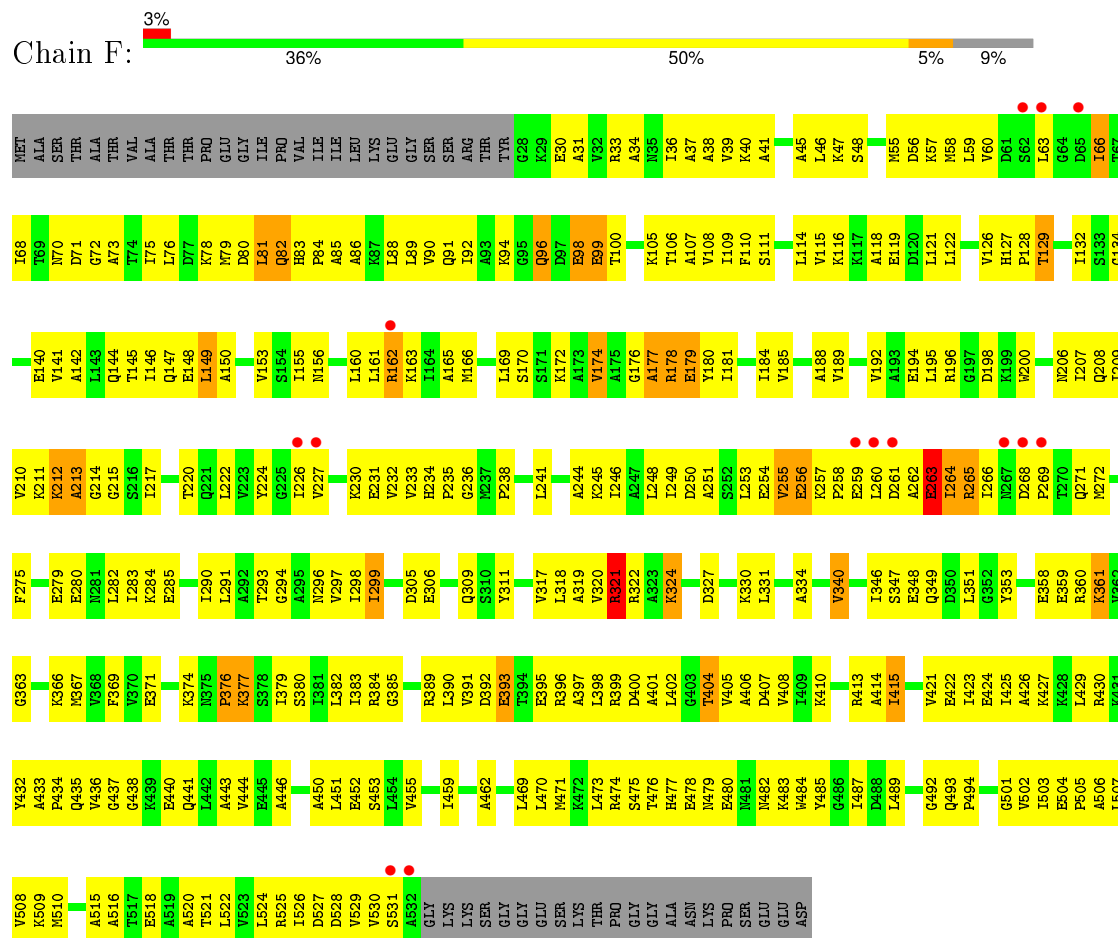


● Molecule 1: Chaperonin

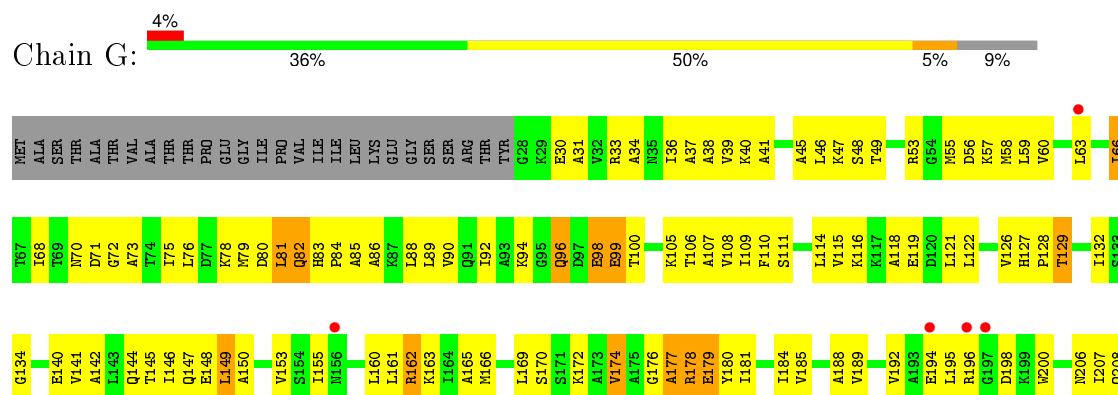


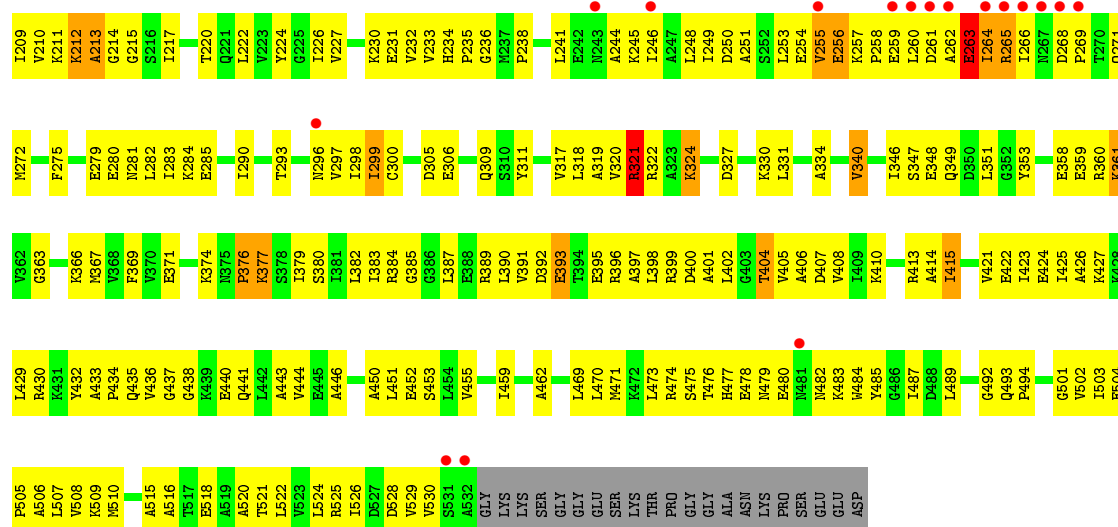


• Molecule 1: Chaperonin

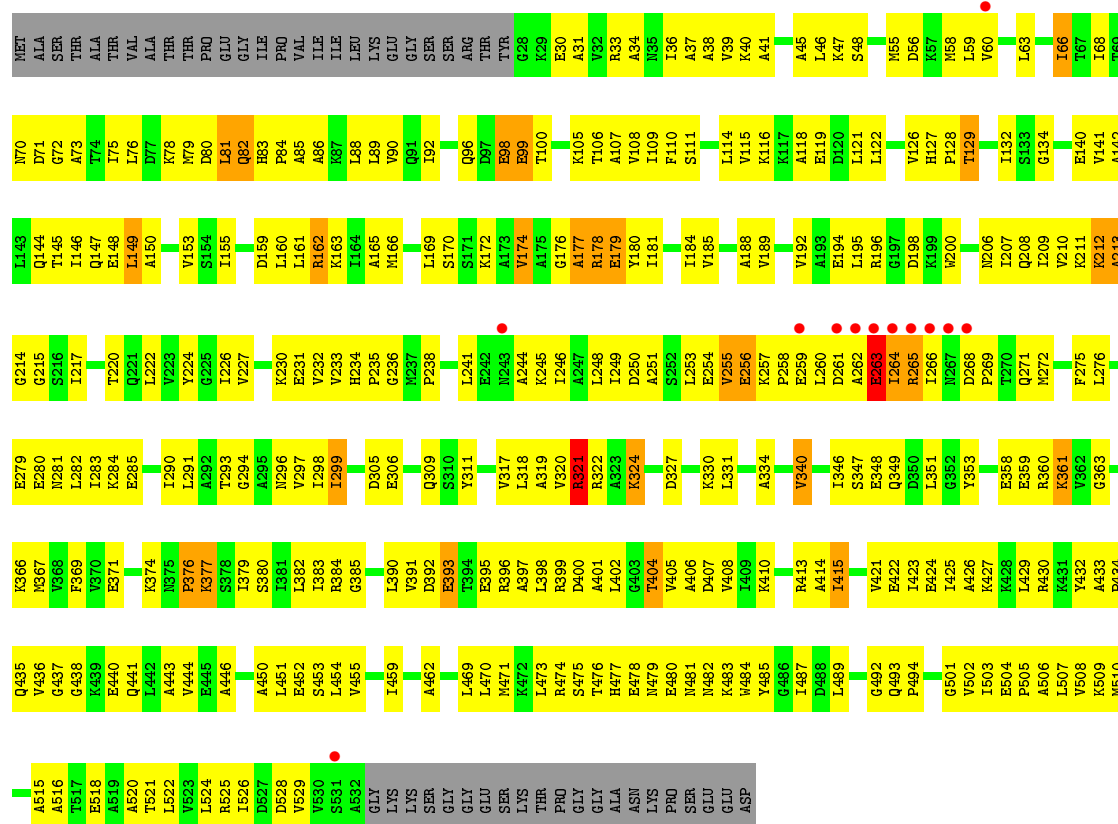


• Molecule 1: Chaperonin





• Molecule 1: Chaperonin



• Molecule 1: Chaperonin



A515	A516	T517	E518	A519	A520	T521	L522	V523	L524	R525	I526	D527	D528	V529	V530	S531	A532	GLY	LYS	LYS	SER	GLY	GLY	GLU	SER	LYS	THR	PRO	GLY	GLY	ALA	ASN	LYS	PRO	SER	GLU	GLU	ASP		
V436	G437	G438	K439	E440	Q441	L442	A443	V444	E445	A446	A450	L451	E452	S453	L454	V455	L459	I459	A462	L469	L470	K472	R473	R474	S475	T476	H477	E478	M479	E480	M481	K482	K483	M484	Y485	G486	I487	D488	L489	
M367	V368	F369	V370	E371	K374	R375	P376	K377	S378	I379	S380	I381	L382	I383	R384	G385	L390	V391	D392	E393	T394	E395	R396	A397	L398	R399	D400	A401	L402	G403	T404	V405	A406	D407	V408	I409	K410	R413	A414	I415
V436	G437	G438	K439	E440	Q441	L442	A443	V444	E445	A446	A450	L451	E452	S453	L454	V455	L459	I459	A462	L469	L470	K472	R473	R474	S475	T476	H477	E478	M479	E480	M481	K482	K483	M484	Y485	G486	I487	D488	L489	
M367	V368	F369	V370	E371	K374	R375	P376	K377	S378	I379	S380	I381	L382	I383	R384	G385	L390	V391	D392	E393	T394	E395	R396	A397	L398	R399	D400	A401	L402	G403	T404	V405	A406	D407	V408	I409	K410	R413	A414	I415
V436	G437	G438	K439	E440	Q441	L442	A443	V444	E445	A446	A450	L451	E452	S453	L454	V455	L459	I459	A462	L469	L470	K472	R473	R474	S475	T476	H477	E478	M479	E480	M481	K482	K483	M484	Y485	G486	I487	D488	L489	
M367	V368	F369	V370	E371	K374	R375	P376	K377	S378	I379	S380	I381	L382	I383	R384	G385	L390	V391	D392	E393	T394	E395	R396	A397	L398	R399	D400	A401	L402	G403	T404	V405	A406	D407	V408	I409	K410	R413	A414	I415
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V436	G437	G438	K439	E440	Q441	L442	A443	V444	E445	A446	A450	L451	E452	S453	L454	V455	L459	I459	A462	L469	L470	K472	R473	R474	S475	T476	H477	E478	M479	E480										

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.67Å 283.04Å 160.75Å 90.00° 133.90° 90.00°	Depositor
Resolution (Å)	48.39 – 3.70 48.39 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.39-3.70) 99.5 (48.39-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.277 , 0.283 0.286 , 0.291	Depositor DCC
R_{free} test set	3825 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.6	EDS
Estimated twinning fraction	0.080 for h+2*k,-h-l 0.099 for -h-2*k,-k,l 0.089 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 76142 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34884	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/3886	0.67	3/5245 (0.1%)
1	B	0.46	0/3886	0.67	3/5245 (0.1%)
1	C	0.46	0/3886	0.67	3/5245 (0.1%)
1	D	0.46	0/3886	0.67	3/5245 (0.1%)
1	E	0.46	0/3886	0.67	3/5245 (0.1%)
1	F	0.46	0/3886	0.67	3/5245 (0.1%)
1	G	0.46	0/3886	0.67	3/5245 (0.1%)
1	H	0.46	0/3886	0.67	3/5245 (0.1%)
1	I	0.46	0/3886	0.67	3/5245 (0.1%)
All	All	0.46	0/34974	0.67	27/47205 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	257	LYS	C-N-CD	-7.18	104.80	120.60
1	B	257	LYS	C-N-CD	-7.18	104.81	120.60
1	F	257	LYS	C-N-CD	-7.18	104.81	120.60
1	H	257	LYS	C-N-CD	-7.17	104.81	120.60
1	A	257	LYS	C-N-CD	-7.17	104.83	120.60

There are no chirality outliers.

There are no planarity outliers.

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	3849	0	3995	360	2
1	B	3849	0	3995	358	11
1	C	3849	0	3995	346	5
1	D	3849	0	3995	363	6
1	E	3849	0	3995	378	12
1	F	3849	0	3995	389	1
1	G	3849	0	3995	374	2
1	H	3849	0	3995	348	11
1	I	3849	0	3995	351	3
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	1	0
2	I	27	0	12	1	0
All	All	34884	0	36063	3175	28

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 45.

The worst 5 of 3175 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:D:260:LEU:HD12	1:D:261:ASP:N	1.43	1.34
1:A:260:LEU:HD12	1:A:261:ASP:N	1.43	1.33
1:G:260:LEU:HD12	1:G:261:ASP:N	1.43	1.32
1:E:260:LEU:HD12	1:E:261:ASP:N	1.43	1.32
1:H:260:LEU:HD12	1:H:261:ASP:N	1.43	1.32

The worst 5 of 28 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:MET:CE	1:B:275:PHE:CD1[2_656]	1.14	1.06
1:E:273:GLN:NE2	1:H:276:LEU:CD1[2_656]	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLN:NE2	1:H:478:GLU:O[1_556]	1.36	0.84
1:B:264:ILE:O	1:B:266:ILE:O[2_656]	1.37	0.83
1:D:183:ASP:OD2	1:H:159:ASP:OD1[1_556]	1.39	0.81

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	B	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	C	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	D	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	E	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	F	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	G	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	H	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	I	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
All	All	4527/4977 (91%)	3568 (79%)	797 (18%)	162 (4%)	4	41

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	99	GLU
1	A	213	ALA
1	A	321	ARG
1	B	96	GLN

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	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	B	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	C	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	D	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	E	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	F	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	G	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	H	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	I	410/447 (92%)	386 (94%)	24 (6%)	24	66
All	All	3690/4023 (92%)	3474 (94%)	216 (6%)	24	66

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	66	ILE
1	F	33	ARG
1	I	162	ARG
1	E	82	GLN
1	E	263	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	82	GLN
1	F	82	GLN
1	I	147	GLN
1	E	96	GLN
1	E	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	B	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.56	6 (22%)
2	ADP	C	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	D	800	-	22,29,29	1.02	1 (4%)	27,45,45	2.58	6 (22%)
2	ADP	E	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	F	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	G	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	H	800	-	22,29,29	1.02	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	I	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)

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	800	-	-	0/12/32/32	0/3/3/3
2	ADP	B	800	-	-	0/12/32/32	0/3/3/3
2	ADP	C	800	-	-	0/12/32/32	0/3/3/3
2	ADP	D	800	-	-	0/12/32/32	0/3/3/3
2	ADP	E	800	-	-	0/12/32/32	0/3/3/3
2	ADP	F	800	-	-	0/12/32/32	0/3/3/3
2	ADP	G	800	-	-	0/12/32/32	0/3/3/3
2	ADP	H	800	-	-	0/12/32/32	0/3/3/3
2	ADP	I	800	-	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	ADP	C5-C4	3.08	1.47	1.40
2	B	800	ADP	C5-C4	3.08	1.47	1.40
2	F	800	ADP	C5-C4	3.08	1.47	1.40
2	G	800	ADP	C5-C4	3.09	1.47	1.40
2	A	800	ADP	C5-C4	3.09	1.47	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	ADP	N3-C2-N1	-7.04	123.50	128.89
2	F	800	ADP	N3-C2-N1	-6.97	123.56	128.89
2	I	800	ADP	N3-C2-N1	-6.97	123.56	128.89
2	A	800	ADP	N3-C2-N1	-6.96	123.57	128.89
2	E	800	ADP	N3-C2-N1	-6.95	123.57	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	1	0
2	B	800	ADP	1	0
2	C	800	ADP	1	0
2	D	800	ADP	1	0
2	E	800	ADP	1	0
2	F	800	ADP	1	0
2	G	800	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	800	ADP	1	0
2	I	800	ADP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	505/553 (91%)	0.13	13 (2%) 59 43	64, 126, 150, 150	0
1	B	505/553 (91%)	0.11	14 (2%) 56 41	64, 126, 150, 150	0
1	C	505/553 (91%)	0.18	17 (3%) 49 34	64, 126, 150, 150	0
1	D	505/553 (91%)	0.10	14 (2%) 56 41	64, 126, 150, 150	0
1	E	505/553 (91%)	0.26	25 (4%) 32 21	64, 126, 150, 150	0
1	F	505/553 (91%)	0.18	14 (2%) 56 41	64, 126, 150, 150	0
1	G	505/553 (91%)	0.23	22 (4%) 38 25	64, 126, 150, 150	0
1	H	505/553 (91%)	0.11	12 (2%) 62 46	64, 126, 150, 150	0
1	I	505/553 (91%)	0.08	9 (1%) 71 57	64, 126, 150, 150	0
All	All	4545/4977 (91%)	0.15	140 (3%) 52 37	64, 127, 150, 150	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ASP	6.9
1	E	259	GLU	5.9
1	B	259	GLU	5.2
1	F	259	GLU	5.1
1	H	267	ASN	5.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	G	800	27/27	0.78	0.37	3.03	150,150,150,150	7
2	ADP	H	800	27/27	0.81	0.33	2.54	150,150,150,150	7
2	ADP	D	800	27/27	0.76	0.39	2.39	150,150,150,150	7
2	ADP	I	800	27/27	0.82	0.33	2.38	150,150,150,150	7
2	ADP	B	800	27/27	0.80	0.34	1.90	150,150,150,150	7
2	ADP	A	800	27/27	0.79	0.35	1.84	150,150,150,150	7
2	ADP	E	800	27/27	0.77	0.34	1.56	150,150,150,150	7
2	ADP	C	800	27/27	0.79	0.34	1.55	150,150,150,150	7
2	ADP	F	800	27/27	0.83	0.32	1.23	150,150,150,150	7

6.5 Other polymers [i](#)

There are no such residues in this entry.