



wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 06:08 AM GMT

PDB ID : 3H4P
Title : Proteasome 20S core particle from Methanocaldococcus jannaschii
Authors : Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on : 2009-04-20
Resolution : 4.10 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>

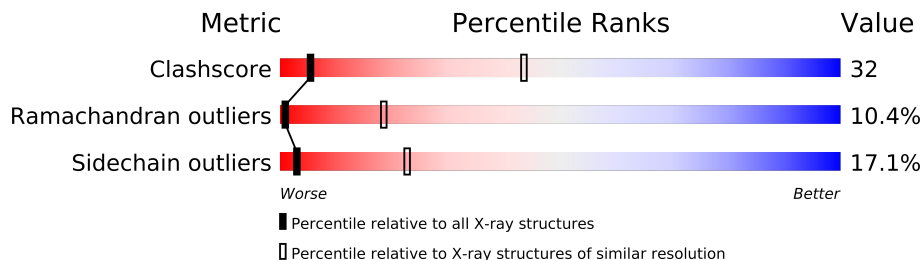
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
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 4.10 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	1248 (4.70-3.50)
Ramachandran outliers	78287	1183 (4.70-3.50)
Sidechain outliers	78261	1168 (4.70-3.50)











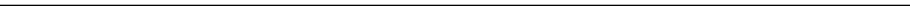
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	
1	C	264	
1	D	264	
1	E	264	
1	F	264	
1	G	264	
1	H	264	
1	I	264	
1	J	264	
1	K	264	
1	L	264	
1	M	264	
1	N	264	
2	a	219	
2	b	219	
2	c	219	

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Mol	Chain	Length	Quality of chain
2	d	219	
2	e	219	
2	f	219	
2	g	219	
2	h	219	
2	i	219	
2	j	219	
2	k	219	
2	l	219	
2	m	219	
2	n	219	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46648 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	B	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	C	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	D	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	E	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	F	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	G	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	H	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	I	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	J	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	K	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	L	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	M	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	N	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q60177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q60177
A	0	HIS	-	EXPRESSION TAG	UNP Q60177
B	-2	GLY	-	EXPRESSION TAG	UNP Q60177
B	-1	SER	-	EXPRESSION TAG	UNP Q60177
B	0	HIS	-	EXPRESSION TAG	UNP Q60177
C	-2	GLY	-	EXPRESSION TAG	UNP Q60177
C	-1	SER	-	EXPRESSION TAG	UNP Q60177
C	0	HIS	-	EXPRESSION TAG	UNP Q60177
D	-2	GLY	-	EXPRESSION TAG	UNP Q60177
D	-1	SER	-	EXPRESSION TAG	UNP Q60177
D	0	HIS	-	EXPRESSION TAG	UNP Q60177
E	-2	GLY	-	EXPRESSION TAG	UNP Q60177
E	-1	SER	-	EXPRESSION TAG	UNP Q60177
E	0	HIS	-	EXPRESSION TAG	UNP Q60177
F	-2	GLY	-	EXPRESSION TAG	UNP Q60177
F	-1	SER	-	EXPRESSION TAG	UNP Q60177
F	0	HIS	-	EXPRESSION TAG	UNP Q60177
G	-2	GLY	-	EXPRESSION TAG	UNP Q60177
G	-1	SER	-	EXPRESSION TAG	UNP Q60177
G	0	HIS	-	EXPRESSION TAG	UNP Q60177
H	-2	GLY	-	EXPRESSION TAG	UNP Q60177
H	-1	SER	-	EXPRESSION TAG	UNP Q60177
H	0	HIS	-	EXPRESSION TAG	UNP Q60177
I	-2	GLY	-	EXPRESSION TAG	UNP Q60177
I	-1	SER	-	EXPRESSION TAG	UNP Q60177
I	0	HIS	-	EXPRESSION TAG	UNP Q60177
J	-2	GLY	-	EXPRESSION TAG	UNP Q60177
J	-1	SER	-	EXPRESSION TAG	UNP Q60177
J	0	HIS	-	EXPRESSION TAG	UNP Q60177
K	-2	GLY	-	EXPRESSION TAG	UNP Q60177
K	-1	SER	-	EXPRESSION TAG	UNP Q60177
K	0	HIS	-	EXPRESSION TAG	UNP Q60177
L	-2	GLY	-	EXPRESSION TAG	UNP Q60177
L	-1	SER	-	EXPRESSION TAG	UNP Q60177
L	0	HIS	-	EXPRESSION TAG	UNP Q60177
M	-2	GLY	-	EXPRESSION TAG	UNP Q60177
M	-1	SER	-	EXPRESSION TAG	UNP Q60177
M	0	HIS	-	EXPRESSION TAG	UNP Q60177
N	-2	GLY	-	EXPRESSION TAG	UNP Q60177
N	-1	SER	-	EXPRESSION TAG	UNP Q60177
N	0	HIS	-	EXPRESSION TAG	UNP Q60177

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	b	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	c	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	d	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	e	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	f	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	g	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	h	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	i	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	j	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	k	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	l	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	m	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	n	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	6	MET	-	EXPRESSION TAG	UNP Q58634
b	6	MET	-	EXPRESSION TAG	UNP Q58634
c	6	MET	-	EXPRESSION TAG	UNP Q58634
d	6	MET	-	EXPRESSION TAG	UNP Q58634
e	6	MET	-	EXPRESSION TAG	UNP Q58634
f	6	MET	-	EXPRESSION TAG	UNP Q58634
g	6	MET	-	EXPRESSION TAG	UNP Q58634
h	6	MET	-	EXPRESSION TAG	UNP Q58634
i	6	MET	-	EXPRESSION TAG	UNP Q58634
j	6	MET	-	EXPRESSION TAG	UNP Q58634
k	6	MET	-	EXPRESSION TAG	UNP Q58634
l	6	MET	-	EXPRESSION TAG	UNP Q58634

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Chain	Residue	Modelled	Actual	Comment	Reference
m	6	MET	-	EXPRESSION TAG	UNP Q58634
n	6	MET	-	EXPRESSION TAG	UNP Q58634

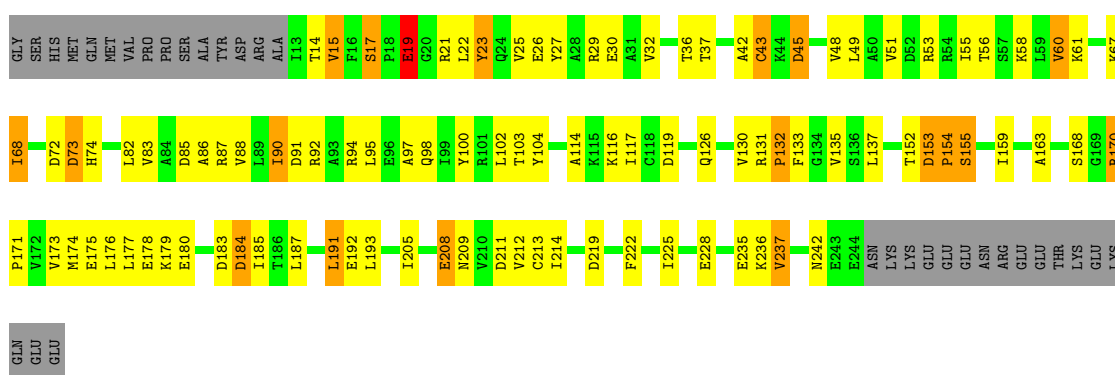
3 Residue-property plots

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 failed to run properly.

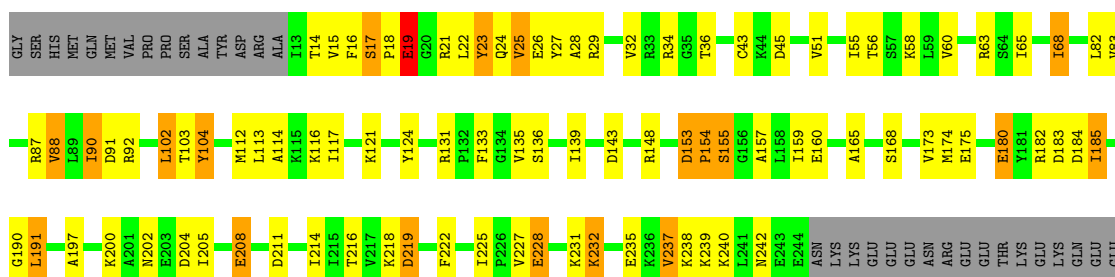
- Molecule 1: Proteasome subunit alpha

Chain A:



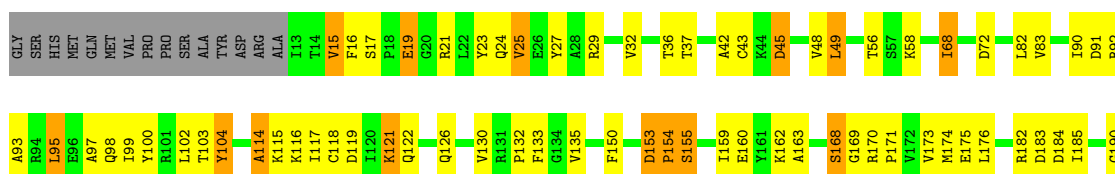
- Molecule 1: Proteasome subunit alpha

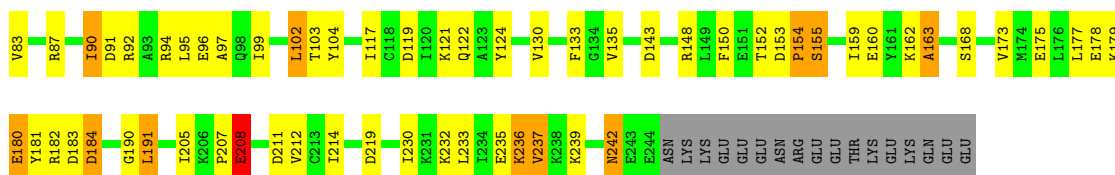
Chain B:



- Molecule 1: Proteasome subunit alpha

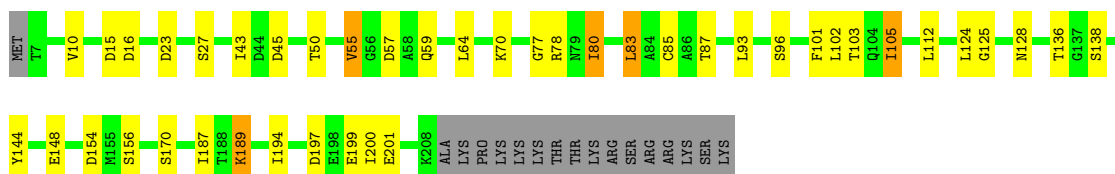
Chain C:





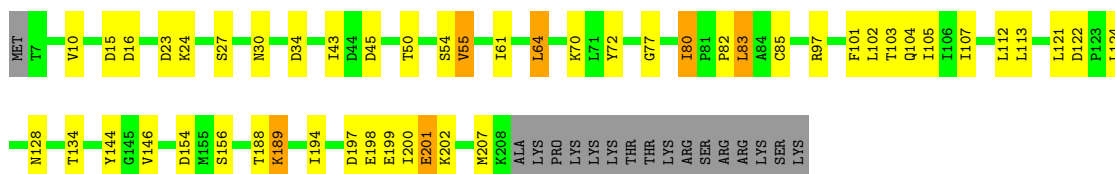
• Molecule 2: Proteasome subunit beta

Chain a:



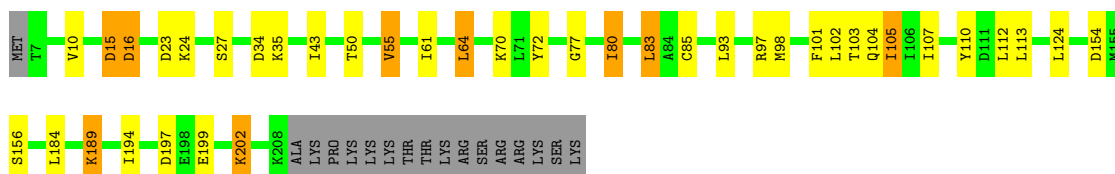
• Molecule 2: Proteasome subunit beta

Chain b:



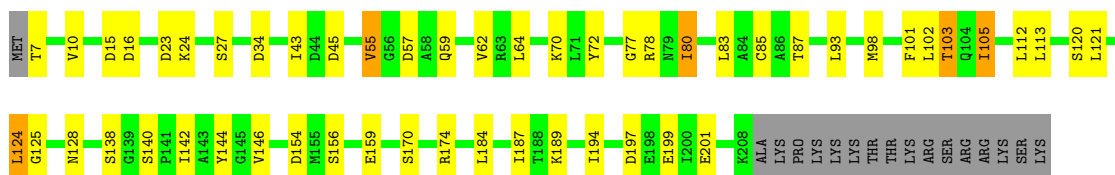
• Molecule 2: Proteasome subunit beta

Chain c:



• Molecule 2: Proteasome subunit beta

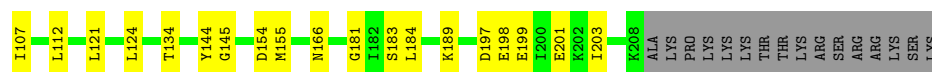
Chain d:



• Molecule 2: Proteasome subunit beta

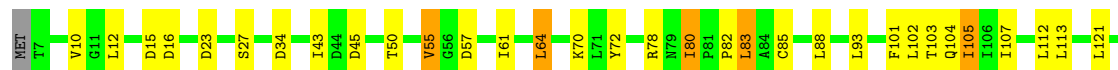
Chain e:





- Molecule 2: Proteasome subunit beta

Chain f:



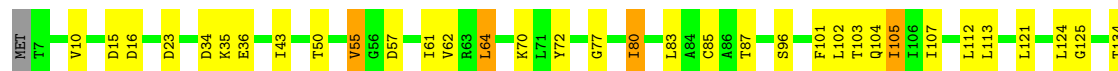
- Molecule 2: Proteasome subunit beta

Chain g:



- Molecule 2: Proteasome subunit beta

Chain h:



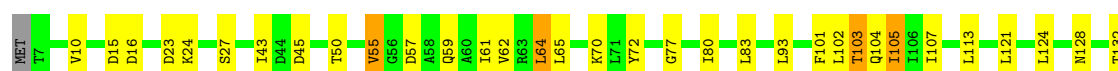
- Molecule 2: Proteasome subunit beta

Chain i:



- Molecule 2: Proteasome subunit beta

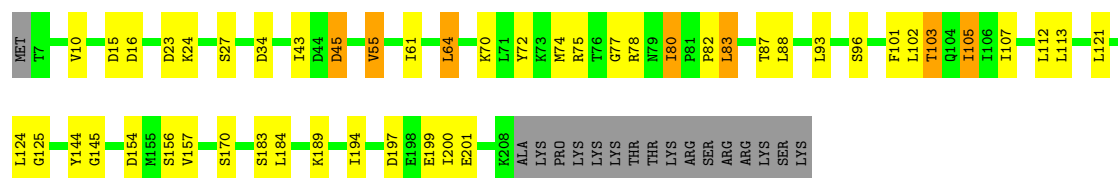
Chain j:



- Molecule 2: Proteasome subunit beta

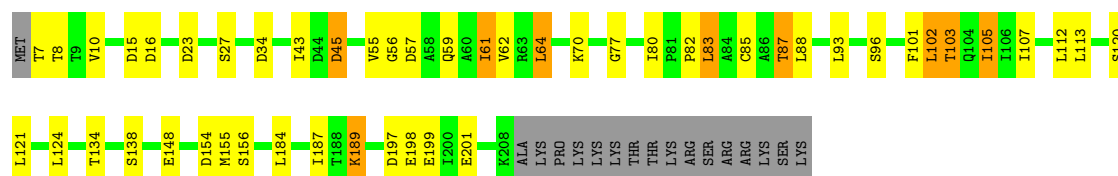


Chain k: 



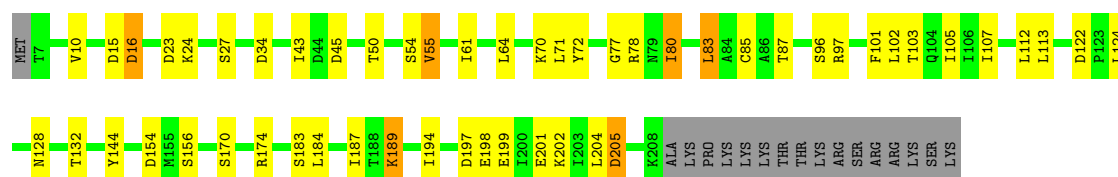
- Molecule 2: Proteasome subunit beta

Chain l: 



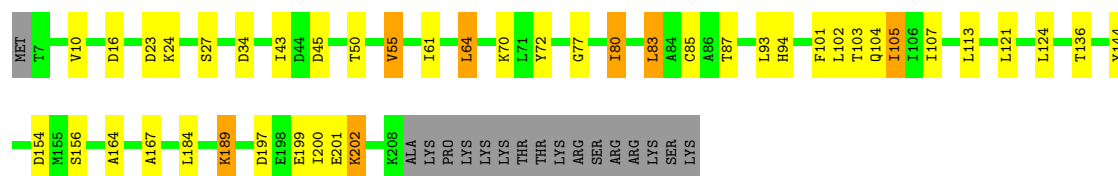
- Molecule 2: Proteasome subunit beta

Chain m: 



- Molecule 2: Proteasome subunit beta

Chain n: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.72Å 219.54Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 4.10	Depositor
% Data completeness (in resolution range)	99.8 (49.98-4.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.254 , 0.325	Depositor
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.499	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	9 of 53849 reflections (0.017%)	Xtriage
Total number of atoms	46648	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.49	0/1832	0.66	0/2468
1	B	0.47	0/1832	0.67	0/2468
1	C	0.50	0/1832	0.69	0/2468
1	D	0.57	1/1832 (0.1%)	0.76	2/2468 (0.1%)
1	E	0.48	0/1832	0.69	1/2468 (0.0%)
1	F	0.57	0/1832	0.72	1/2468 (0.0%)
1	G	0.55	0/1832	0.73	0/2468
1	H	0.50	0/1832	0.69	1/2468 (0.0%)
1	I	0.49	0/1832	0.70	1/2468 (0.0%)
1	J	0.53	0/1832	0.69	0/2468
1	K	0.51	0/1832	0.69	0/2468
1	L	0.53	0/1832	0.70	0/2468
1	M	0.48	0/1832	0.67	0/2468
1	N	0.47	0/1832	0.65	0/2468
2	a	0.52	0/1536	0.72	0/2070
2	b	0.52	0/1536	0.74	1/2070 (0.0%)
2	c	0.51	0/1536	0.74	2/2070 (0.1%)
2	d	0.53	0/1536	0.77	1/2070 (0.0%)
2	e	0.55	0/1536	0.77	4/2070 (0.2%)
2	f	0.60	0/1536	0.80	1/2070 (0.0%)
2	g	0.58	0/1536	0.79	1/2070 (0.0%)
2	h	0.53	0/1536	0.75	1/2070 (0.0%)
2	i	0.57	0/1536	0.79	2/2070 (0.1%)
2	j	0.61	0/1536	0.84	1/2070 (0.0%)
2	k	0.59	0/1536	0.79	1/2070 (0.0%)
2	l	0.54	0/1536	0.79	3/2070 (0.1%)
2	m	0.51	0/1536	0.75	1/2070 (0.0%)
2	n	0.50	0/1536	0.74	1/2070 (0.0%)
All	All	0.53	1/47152 (0.0%)	0.73	26/63532 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ASP	CB-CG	5.38	1.63	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	64	LEU	CA-CB-CG	7.58	132.73	115.30
2	e	64	LEU	CA-CB-CG	7.57	132.70	115.30
2	d	64	LEU	CA-CB-CG	7.28	132.04	115.30
2	l	64	LEU	CA-CB-CG	6.86	131.09	115.30
2	n	64	LEU	CA-CB-CG	6.73	130.77	115.30

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	1813	0	0	60	0
1	B	1813	0	0	55	2
1	C	1813	0	0	47	0
1	D	1813	0	0	73	0
1	E	1813	0	0	77	1
1	F	1813	0	0	55	1
1	G	1813	0	0	65	0
1	H	1813	0	0	61	0
1	I	1813	0	0	65	1
1	J	1813	0	0	59	0
1	K	1813	0	0	68	0
1	L	1813	0	0	55	0
1	M	1813	0	0	60	2
1	N	1813	0	0	49	0
2	a	1519	0	0	0	0
2	b	1519	0	0	0	0
2	c	1519	0	0	0	2
2	d	1519	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	e	1519	0	0	0	0
2	f	1519	0	0	0	1
2	g	1519	0	0	0	0
2	h	1519	0	0	0	0
2	i	1519	0	0	0	2
2	j	1519	0	0	0	0
2	k	1519	0	0	0	0
2	l	1519	0	0	0	0
2	m	1519	0	0	0	1
2	n	1519	0	0	0	0
All	All	46648	0	0	793	7

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 32.

The worst 5 of 793 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:153:ASP:O	1:H:155:SER:N	2.06	0.89
1:G:207:PRO:O	1:G:208:GLU:CG	2.21	0.88
1:I:90:ILE:O	1:I:92:ARG:N	2.13	0.82
1:D:153:ASP:O	1:D:155:SER:N	2.12	0.82
1:I:153:ASP:O	1:I:155:SER:N	2.13	0.81

The worst 5 of 7 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:B:232:LYS:O	2:c:110:TYR:OH[2_565]	1.88	0.32
1:I:242:ASN:O	2:m:205:ASP:OD1[4_555]	2.00	0.20
1:M:243:GLU:N	2:i:205:ASP:OD1[4_455]	2.03	0.17
1:E:180:GLU:O	1:E:182:ARG:NH2[2_665]	2.09	0.11
1:B:231:LYS:NZ	2:c:15:ASP:OD1[2_565]	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	230/264 (87%)	163 (71%)	43 (19%)	24 (10%)	1	18
1	B	230/264 (87%)	162 (70%)	46 (20%)	22 (10%)	1	21
1	C	230/264 (87%)	155 (67%)	51 (22%)	24 (10%)	1	18
1	D	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	1	17
1	E	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	1	17
1	F	230/264 (87%)	152 (66%)	53 (23%)	25 (11%)	1	17
1	G	230/264 (87%)	156 (68%)	51 (22%)	23 (10%)	1	20
1	H	230/264 (87%)	153 (66%)	49 (21%)	28 (12%)	1	14
1	I	230/264 (87%)	159 (69%)	44 (19%)	27 (12%)	1	15
1	J	230/264 (87%)	161 (70%)	45 (20%)	24 (10%)	1	18
1	K	230/264 (87%)	151 (66%)	51 (22%)	28 (12%)	1	14
1	L	230/264 (87%)	162 (70%)	39 (17%)	29 (13%)	0	13
1	M	230/264 (87%)	159 (69%)	45 (20%)	26 (11%)	1	16
1	N	230/264 (87%)	159 (69%)	48 (21%)	23 (10%)	1	20
2	a	200/219 (91%)	135 (68%)	45 (22%)	20 (10%)	1	20
2	b	200/219 (91%)	129 (64%)	53 (26%)	18 (9%)	1	24
2	c	200/219 (91%)	140 (70%)	45 (22%)	15 (8%)	2	30
2	d	200/219 (91%)	132 (66%)	46 (23%)	22 (11%)	1	17
2	e	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	24
2	f	200/219 (91%)	142 (71%)	42 (21%)	16 (8%)	1	28
2	g	200/219 (91%)	132 (66%)	43 (22%)	25 (12%)	1	14
2	h	200/219 (91%)	136 (68%)	44 (22%)	20 (10%)	1	20
2	i	200/219 (91%)	130 (65%)	46 (23%)	24 (12%)	1	14
2	j	200/219 (91%)	145 (72%)	39 (20%)	16 (8%)	1	28
2	k	200/219 (91%)	126 (63%)	50 (25%)	24 (12%)	1	14
2	l	200/219 (91%)	143 (72%)	37 (18%)	20 (10%)	1	20
2	m	200/219 (91%)	139 (70%)	43 (22%)	18 (9%)	1	24
2	n	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	24
All	All	6020/6762 (89%)	4109 (68%)	1284 (21%)	627 (10%)	1	18

5 of 627 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	43	CYS
1	A	132	PRO
1	A	155	SER
1	A	168	SER

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	195/224 (87%)	171 (88%)	24 (12%)	7	40
1	B	195/224 (87%)	167 (86%)	28 (14%)	5	32
1	C	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	D	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	E	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	F	195/224 (87%)	165 (85%)	30 (15%)	4	28
1	G	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	H	195/224 (87%)	162 (83%)	33 (17%)	3	24
1	I	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	J	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	K	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	L	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	M	195/224 (87%)	169 (87%)	26 (13%)	6	36
1	N	195/224 (87%)	170 (87%)	25 (13%)	6	38
2	a	163/179 (91%)	135 (83%)	28 (17%)	3	22
2	b	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	c	163/179 (91%)	133 (82%)	30 (18%)	2	18
2	d	163/179 (91%)	128 (78%)	35 (22%)	1	11
2	e	163/179 (91%)	129 (79%)	34 (21%)	1	13
2	f	163/179 (91%)	125 (77%)	38 (23%)	1	9
2	g	163/179 (91%)	131 (80%)	32 (20%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	i	163/179 (91%)	132 (81%)	31 (19%)	2	16
2	j	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	k	163/179 (91%)	132 (81%)	31 (19%)	2	16
2	l	163/179 (91%)	127 (78%)	36 (22%)	1	11
2	m	163/179 (91%)	124 (76%)	39 (24%)	1	8
2	n	163/179 (91%)	132 (81%)	31 (19%)	2	16
All	All	5012/5642 (89%)	4154 (83%)	858 (17%)	3	23

5 of 858 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	f	189	LYS
1	I	210	VAL
2	m	27	SER
2	g	50	THR
1	H	60	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no ligands in this entry.

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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.