wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:46 PM BST

PDB ID	:	2C7D
EMDB ID:	:	EMD-1181
Title	:	Fitted coordinates for GroEL-ADP7-GroES Cryo-EM complex (EMD-1181)
Authors	:	Ranson, N.A.; Clare, D.K.; Farr, G.W.; Houldershaw, D.; Horwich, A.L.; Saibil, H.R.
Deposited on	:	2005-11-22
Resolution	:	8.70 Å(reported)
Based on PDB ID	:	1AON

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

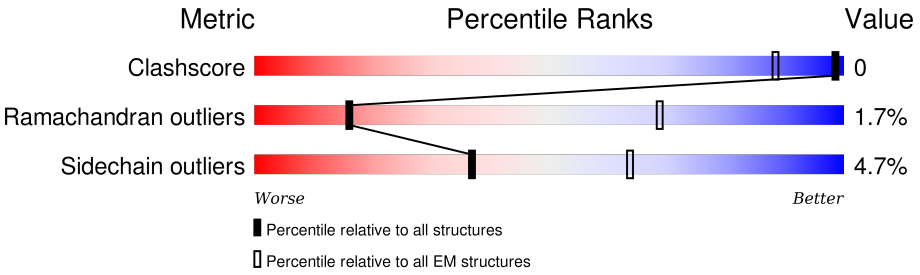
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	547	91% 5% ·
1	B	547	90% 6% ·
1	C	547	92% · ·
1	D	547	91% 5% ·
1	E	547	90% 6% ·
1	F	547	91% 5% ·
1	G	547	91% · ·
1	H	547	91% 5% ·
1	I	547	91% · ·

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Mol	Chain	Length	Quality of chain
1	J	547	91% 5%
1	K	547	90% 6%
1	L	547	90% 5%
1	M	547	91% 5%
1	N	547	90% 5%
2	O	97	82% 11%
2	P	97	82% 12%
2	Q	97	81% 13%
2	R	97	80% 14%
2	S	97	77% 18%
2	T	97	81% 13%
2	U	97	77% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57946 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	B	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	C	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	D	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	E	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	F	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	G	525	Total	C	N	O	S	0	1
			3805	2397	622	766	20		
1	H	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	I	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	J	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	K	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	L	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	M	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		
1	N	523	Total	C	N	O	S	0	1
			3793	2389	620	764	20		

- Molecule 2 is a protein called 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN.

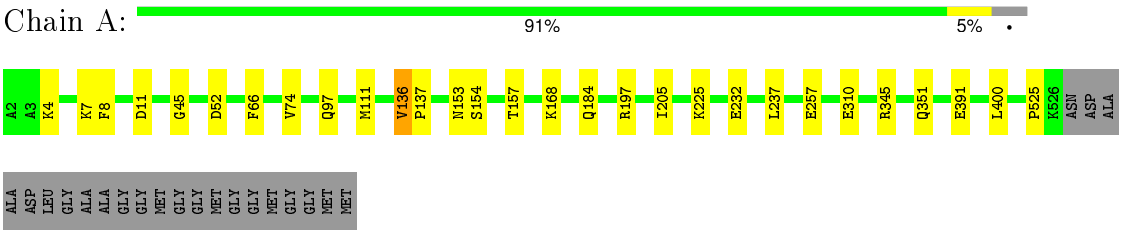
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	P	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	Q	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	R	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	S	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	T	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	U	93	Total	C	N	O	S	0	1
			680	432	112	135	1		

3 Residue-property plots (i)

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. 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.

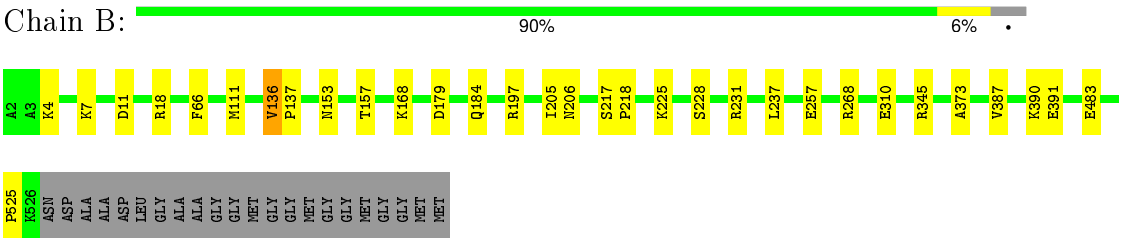
- Molecule 1: 60 KDA CHAPERONIN

Chain A:



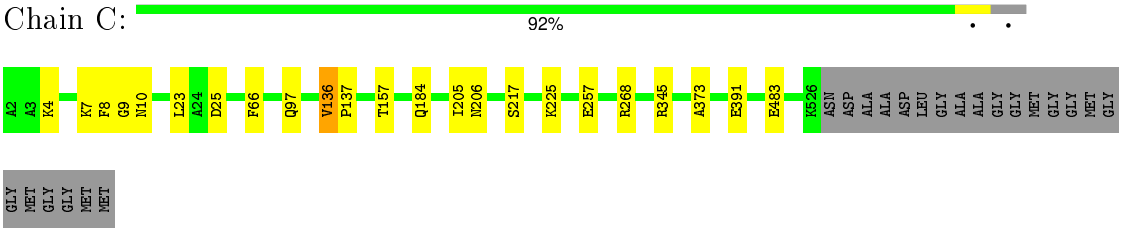
- Molecule 1: 60 KDA CHAPERONIN

Chain B:



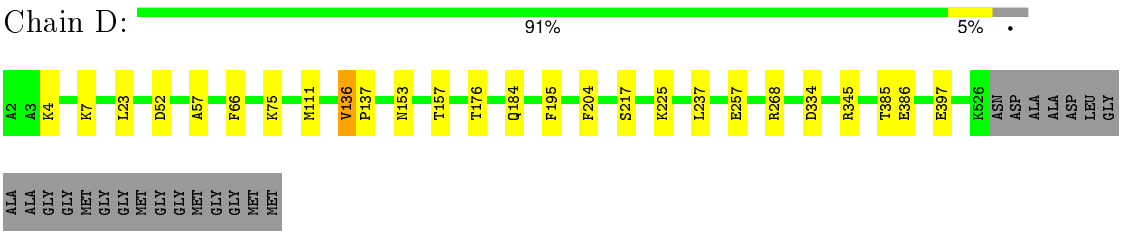
- Molecule 1: 60 KDA CHAPERONIN

Chain C:



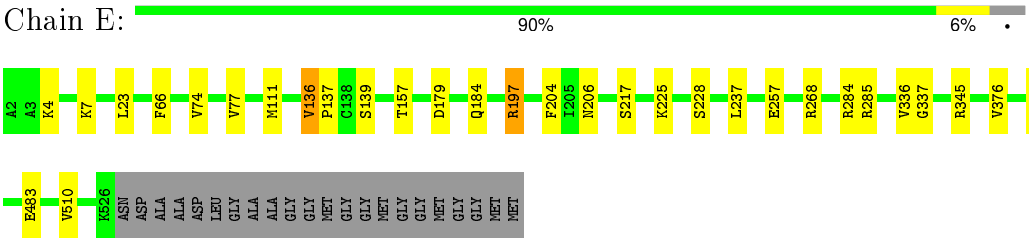
- Molecule 1: 60 KDA CHAPERONIN

Chain D:



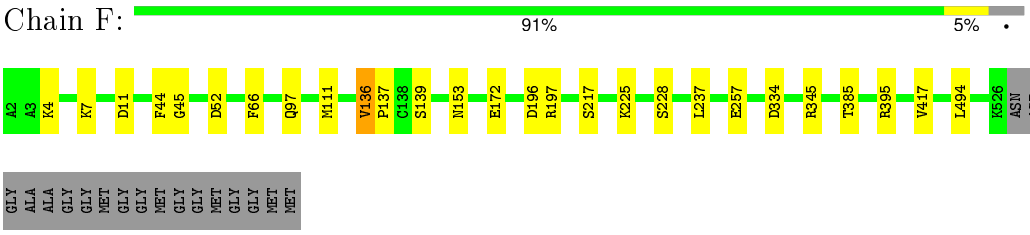
- Molecule 1: 60 KDA CHAPERONIN

Chain E:



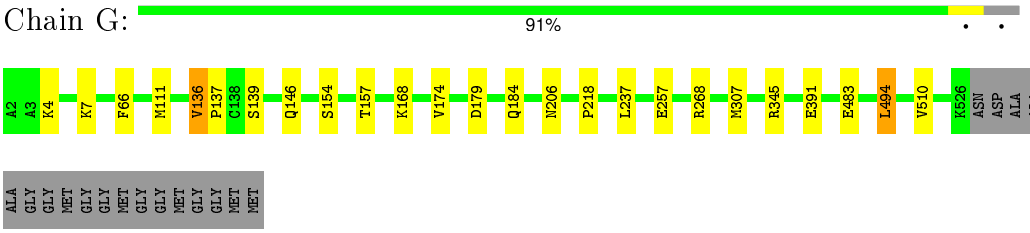
• Molecule 1: 60 KDA CHAPERONIN

Chain F:



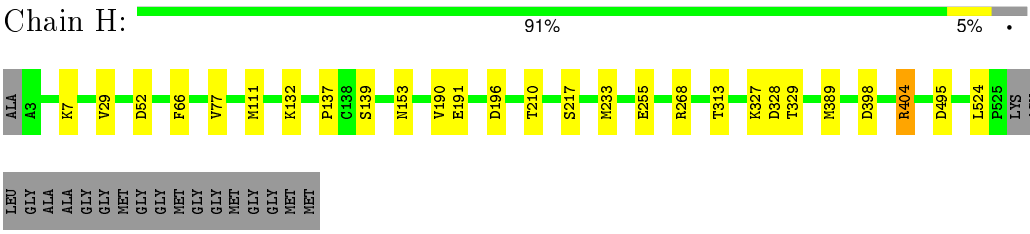
• Molecule 1: 60 KDA CHAPERONIN

Chain G:



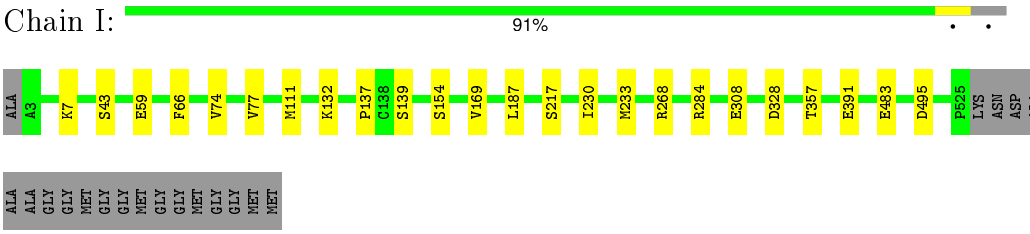
• Molecule 1: 60 KDA CHAPERONIN

Chain H:



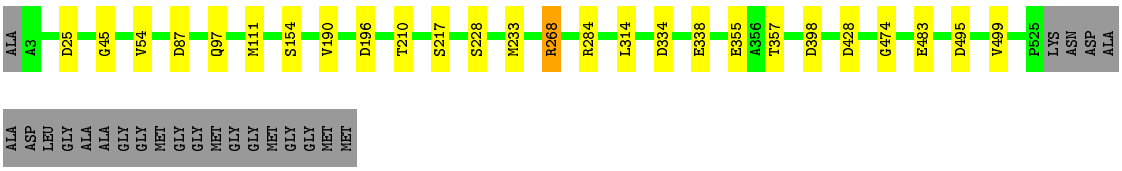
• Molecule 1: 60 KDA CHAPERONIN

Chain I:



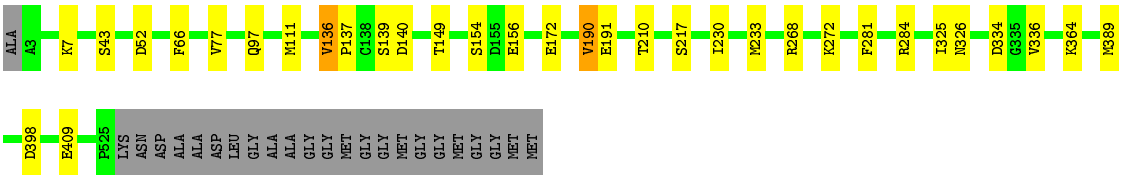
• Molecule 1: 60 KDA CHAPERONIN

Chain J:



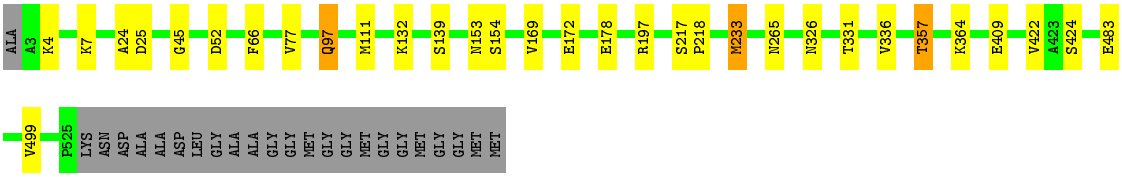
• Molecule 1: 60 KDA CHAPERONIN

Chain K:



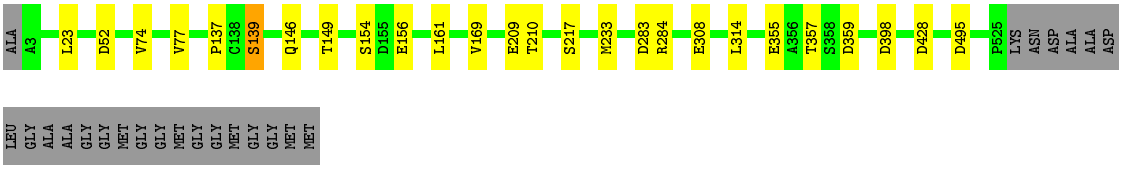
• Molecule 1: 60 KDA CHAPERONIN

Chain L:



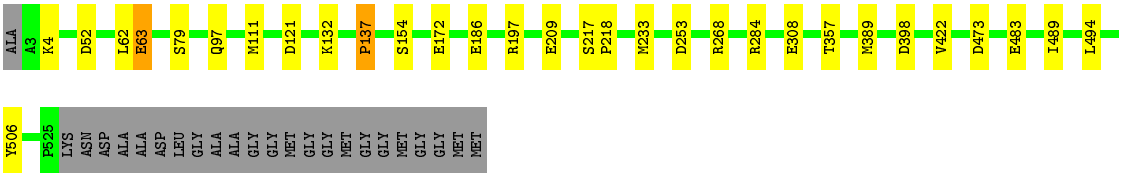
• Molecule 1: 60 KDA CHAPERONIN

Chain M:



• Molecule 1: 60 KDA CHAPERONIN

Chain N:



• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

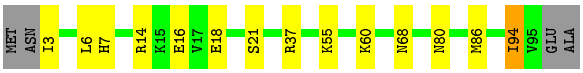
Chain O:

• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain P:

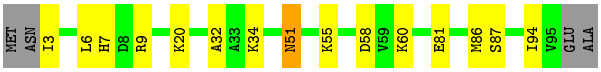
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain Q:



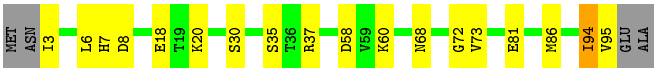
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain R:



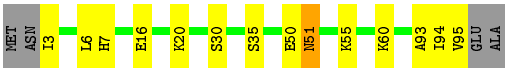
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain S:



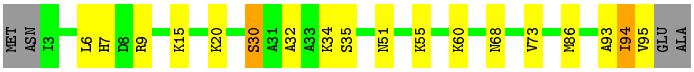
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain T:



• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain U:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL CORRECTION ON 2D CLASS AVERAGES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.60	0/3833	0.91	0/5165
1	B	0.60	0/3833	0.92	0/5165
1	C	0.60	0/3833	0.91	0/5165
1	D	0.60	0/3833	0.89	0/5165
1	E	0.60	0/3833	0.92	0/5165
1	F	0.59	0/3833	0.91	0/5165
1	G	0.60	0/3833	0.90	0/5165
1	H	0.60	0/3820	0.91	1/5146 (0.0%)
1	I	0.60	0/3820	0.92	0/5146
1	J	0.60	0/3820	0.90	0/5146
1	K	0.60	0/3820	0.91	0/5146
1	L	0.60	0/3820	0.92	0/5146
1	M	0.61	0/3820	0.91	0/5146
1	N	0.60	0/3820	0.92	2/5146 (0.0%)
2	O	0.64	0/684	0.99	1/918 (0.1%)
2	P	0.63	0/684	1.01	0/918
2	Q	0.64	0/684	1.01	1/918 (0.1%)
2	R	0.64	0/684	1.03	0/918
2	S	0.63	0/684	1.02	0/918
2	T	0.62	0/684	1.04	1/918 (0.1%)
2	U	0.63	0/684	1.00	0/918
All	All	0.60	0/58359	0.92	6/78603 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	3
1	B	2	3
1	C	2	3
1	D	2	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	2	3
1	F	2	3
1	G	2	5
1	J	0	1
1	K	0	1
1	L	0	4
1	N	0	3
2	P	0	1
2	T	0	1
2	U	0	1
All	All	14	35

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	50	GLU	C-N-CA	5.40	135.21	121.70
1	N	186	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	H	404	ARG	CD-NE-CZ	5.18	130.86	123.60
1	N	506	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	O	79	ASP	C-N-CA	5.05	134.32	121.70
2	Q	14	ARG	CD-NE-CZ	5.00	130.60	123.60

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	136	VAL	CA
1	A	137	PRO	CA
1	B	136	VAL	CA
1	B	137	PRO	CA
1	C	136	VAL	CA
1	C	137	PRO	CA
1	D	136	VAL	CA
1	D	137	PRO	CA
1	E	136	VAL	CA
1	E	137	PRO	CA
1	F	136	VAL	CA
1	F	137	PRO	CA
1	G	136	VAL	CA
1	G	137	PRO	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	VAL	Peptide
1	A	4	LYS	Peptide
1	A	8	PHE	Peptide
1	B	136	VAL	Peptide
1	B	218	PRO	Peptide
1	B	4	LYS	Peptide
1	C	136	VAL	Peptide
1	C	4	LYS	Peptide
1	C	8	PHE	Peptide
1	D	136	VAL	Peptide
1	D	195	PHE	Peptide
1	D	4	LYS	Peptide
1	E	136	VAL	Peptide
1	E	284	ARG	Peptide
1	E	4	LYS	Peptide
1	F	136	VAL	Peptide
1	F	172	GLU	Peptide
1	F	4	LYS	Peptide
1	G	136	VAL	Peptide
1	G	139	SER	Peptide
1	G	218	PRO	Peptide
1	G	307	MET	Peptide
1	G	4	LYS	Peptide
1	J	355	GLU	Peptide
1	K	136	VAL	Peptide
1	L	139	SER	Peptide
1	L	178	GLU	Peptide
1	L	218	PRO	Peptide
1	L	4	LYS	Peptide
1	N	218	PRO	Peptide
1	N	4	LYS	Peptide
1	N	63	GLU	Peptide
2	P	19	THR	Peptide
2	T	93	ALA	Peptide
2	U	93	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3805	0	3881	1	0
1	B	3805	0	3881	2	0
1	C	3805	0	3881	1	0
1	D	3805	0	3881	3	0
1	E	3805	0	3881	3	0
1	F	3805	0	3881	2	0
1	G	3805	0	3881	3	0
1	H	3793	0	3869	2	0
1	I	3793	0	3869	1	0
1	J	3793	0	3869	1	0
1	K	3793	0	3869	3	0
1	L	3793	0	3869	2	0
1	M	3793	0	3869	2	0
1	N	3793	0	3869	1	0
2	O	680	0	703	2	0
2	P	680	0	703	1	0
2	Q	680	0	703	1	0
2	R	680	0	703	3	0
2	S	680	0	703	3	0
2	T	680	0	703	3	0
2	U	680	0	703	2	0
All	All	57946	0	59171	33	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 0.

All (33) 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:J:314:LEU:H	1:J:314:LEU:HD12	1.69	0.56
2:R:3:ILE:HA	2:S:95:VAL:N	2.23	0.53
1:D:385:THR:HG21	1:E:510:VAL:HG23	1.92	0.52
1:E:7:LYS:HE2	1:E:66:PHE:CE2	2.45	0.52
1:B:387:VAL:HA	1:B:390:LYS:HE3	1.91	0.52
1:G:7:LYS:HE2	1:G:66:PHE:CE2	2.47	0.50
1:F:385:THR:HG21	1:G:510:VAL:HG23	1.92	0.50
1:E:7:LYS:HE2	1:E:66:PHE:CD2	2.47	0.49
1:I:7:LYS:HE2	1:I:66:PHE:CE2	2.47	0.49
1:M:149:THR:HG22	1:M:156:GLU:HA	1.95	0.48
1:K:190:VAL:HG22	1:K:191:GLU:H	1.79	0.47
1:N:489:ILE:HD13	1:N:494:LEU:HD21	1.95	0.47
1:H:7:LYS:HE2	1:H:66:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HE2	1:B:66:PHE:CE2	2.49	0.47
1:A:7:LYS:HE2	1:A:66:PHE:CE2	2.50	0.47
2:O:60:LYS:HE3	2:O:60:LYS:N	2.31	0.46
1:M:314:LEU:H	1:M:314:LEU:HD12	1.80	0.46
2:Q:3:ILE:HA	2:R:94:ILE:O	2.17	0.45
1:F:7:LYS:HE2	1:F:66:PHE:CE2	2.51	0.45
2:T:3:ILE:HA	2:U:95:VAL:N	2.31	0.44
1:L:7:LYS:HE2	1:L:66:PHE:CE2	2.51	0.44
2:T:3:ILE:HA	2:U:94:ILE:O	2.16	0.44
2:R:3:ILE:HA	2:S:94:ILE:O	2.18	0.43
1:G:146:GLN:HE21	1:G:494:LEU:HD21	1.82	0.43
1:D:7:LYS:HE2	1:D:66:PHE:CE2	2.55	0.42
1:K:7:LYS:HE2	1:K:66:PHE:CE2	2.54	0.42
2:O:3:ILE:HA	2:P:95:VAL:N	2.33	0.42
1:H:190:VAL:HG22	1:H:191:GLU:H	1.85	0.42
1:L:24:ALA:HB3	1:L:97:GLN:HE21	1.85	0.42
1:C:7:LYS:HE2	1:C:66:PHE:CE2	2.56	0.41
2:S:3:ILE:HA	2:T:95:VAL:N	2.36	0.41
1:K:149:THR:HG22	1:K:156:GLU:HA	2.03	0.40
1:D:57:ALA:O	1:D:75:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	523/547 (96%)	488 (93%)	28 (5%)	7 (1%)	15	60
1	B	523/547 (96%)	490 (94%)	25 (5%)	8 (2%)	13	57
1	C	523/547 (96%)	486 (93%)	30 (6%)	7 (1%)	15	60
1	D	523/547 (96%)	491 (94%)	28 (5%)	4 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	523/547 (96%)	483 (92%)	32 (6%)	8 (2%)	13	57
1	F	523/547 (96%)	485 (93%)	30 (6%)	8 (2%)	13	57
1	G	523/547 (96%)	488 (93%)	31 (6%)	4 (1%)	24	69
1	H	521/547 (95%)	476 (91%)	38 (7%)	7 (1%)	15	60
1	I	521/547 (95%)	486 (93%)	29 (6%)	6 (1%)	16	61
1	J	521/547 (95%)	489 (94%)	23 (4%)	9 (2%)	11	55
1	K	521/547 (95%)	477 (92%)	33 (6%)	11 (2%)	9	50
1	L	521/547 (95%)	473 (91%)	39 (8%)	9 (2%)	11	55
1	M	521/547 (95%)	486 (93%)	29 (6%)	6 (1%)	16	61
1	N	521/547 (95%)	478 (92%)	36 (7%)	7 (1%)	15	60
2	O	91/97 (94%)	65 (71%)	21 (23%)	5 (6%)	2	29
2	P	91/97 (94%)	70 (77%)	16 (18%)	5 (6%)	2	29
2	Q	91/97 (94%)	70 (77%)	16 (18%)	5 (6%)	2	29
2	R	91/97 (94%)	70 (77%)	18 (20%)	3 (3%)	5	40
2	S	91/97 (94%)	70 (77%)	15 (16%)	6 (7%)	1	24
2	T	91/97 (94%)	71 (78%)	15 (16%)	5 (6%)	2	29
2	U	91/97 (94%)	70 (77%)	15 (16%)	6 (7%)	1	24
All	All	7945/8337 (95%)	7262 (91%)	547 (7%)	136 (2%)	16	55

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	B	137	PRO
1	C	137	PRO
1	C	483	GLU
1	D	137	PRO
1	E	137	PRO
1	E	197	ARG
1	E	285	ARG
1	F	137	PRO
1	G	137	PRO
1	H	217	SER
1	H	524	LEU
1	I	154	SER
1	I	217	SER

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Mol	Chain	Res	Type
1	J	217	SER
1	K	154	SER
1	K	217	SER
1	K	334	ASP
1	L	154	SER
1	M	154	SER
1	N	137	PRO
1	N	483	GLU
2	O	80	ASN
2	P	32	ALA
2	P	80	ASN
2	Q	21	SER
2	R	32	ALA
2	R	51	ASN
2	S	73	VAL
2	T	16	GLU
2	T	35	SER
2	T	51	ASN
2	U	73	VAL
1	A	154	SER
1	B	153	ASN
1	B	310	GLU
1	C	9	GLY
1	D	334	ASP
1	E	139	SER
1	E	483	GLU
1	I	139	SER
1	I	483	GLU
1	J	154	SER
1	J	268	ARG
1	J	334	ASP
1	K	210	THR
1	L	217	SER
1	L	233	MET
1	L	409	GLU
1	L	483	GLU
1	M	217	SER
1	N	63	GLU
1	N	154	SER
2	Q	80	ASN
2	Q	94	ILE
2	S	7	HIS

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Mol	Chain	Res	Type
2	S	18	GLU
2	T	7	HIS
2	U	94	ILE
1	A	153	ASN
1	B	373	ALA
1	D	153	ASN
1	F	139	SER
1	F	334	ASP
1	G	174	VAL
1	I	43	SER
1	J	483	GLU
1	K	139	SER
1	K	409	GLU
1	M	139	SER
2	O	7	HIS
2	O	18	GLU
2	P	7	HIS
2	Q	18	GLU
2	S	35	SER
2	U	35	SER
1	A	45	GLY
1	A	525	PRO
1	B	483	GLU
1	C	10	ASN
1	D	217	SER
1	E	336	VAL
1	F	153	ASN
1	F	196	ASP
1	G	154	SER
1	H	139	SER
1	J	210	THR
1	J	474	GLY
1	K	190	VAL
1	K	281	PHE
1	L	45	GLY
1	N	62	LEU
1	N	217	SER
2	O	8	ASP
2	P	94	ILE
2	Q	7	HIS
2	R	7	HIS
2	S	8	ASP

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Mol	Chain	Res	Type
2	T	94	ILE
2	U	7	HIS
2	U	30	SER
1	A	310	GLU
1	B	231	ARG
1	C	217	SER
1	C	373	ALA
1	E	217	SER
1	F	217	SER
1	H	29	VAL
1	H	327	LYS
1	K	136	VAL
1	L	357	THR
1	M	209	GLU
1	N	209	GLU
2	U	32	ALA
1	B	525	PRO
1	E	337	GLY
1	F	395	ARG
1	G	483	GLU
1	H	210	THR
1	J	45	GLY
1	L	169	VAL
1	M	210	THR
1	A	205	ILE
1	F	45	GLY
1	H	137	PRO
1	K	336	VAL
2	O	94	ILE
1	K	137	PRO
1	L	336	VAL
1	C	205	ILE
1	J	190	VAL
2	P	48	ILE
1	B	205	ILE
1	I	137	PRO
2	S	72	GLY
1	M	137	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	404/414 (98%)	386 (96%)	18 (4%)	34	69
1	B	404/414 (98%)	386 (96%)	18 (4%)	34	69
1	C	404/414 (98%)	392 (97%)	12 (3%)	48	77
1	D	404/414 (98%)	389 (96%)	15 (4%)	41	73
1	E	404/414 (98%)	383 (95%)	21 (5%)	29	65
1	F	404/414 (98%)	390 (96%)	14 (4%)	43	74
1	G	404/414 (98%)	391 (97%)	13 (3%)	46	76
1	H	403/414 (97%)	387 (96%)	16 (4%)	38	71
1	I	403/414 (97%)	387 (96%)	16 (4%)	38	71
1	J	403/414 (97%)	387 (96%)	16 (4%)	38	71
1	K	403/414 (97%)	386 (96%)	17 (4%)	36	70
1	L	403/414 (97%)	385 (96%)	18 (4%)	34	69
1	M	403/414 (97%)	385 (96%)	18 (4%)	34	69
1	N	403/414 (97%)	384 (95%)	19 (5%)	32	68
2	O	76/80 (95%)	69 (91%)	7 (9%)	11	43
2	P	76/80 (95%)	69 (91%)	7 (9%)	11	43
2	Q	76/80 (95%)	68 (90%)	8 (10%)	8	36
2	R	76/80 (95%)	65 (86%)	11 (14%)	4	24
2	S	76/80 (95%)	66 (87%)	10 (13%)	5	28
2	T	76/80 (95%)	70 (92%)	6 (8%)	15	51
2	U	76/80 (95%)	65 (86%)	11 (14%)	4	24
All	All	6181/6356 (97%)	5890 (95%)	291 (5%)	37	68

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP

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Mol	Chain	Res	Type
1	A	52	ASP
1	A	74	VAL
1	A	97	GLN
1	A	111	MET
1	A	136	VAL
1	A	157	THR
1	A	168	LYS
1	A	184	GLN
1	A	197	ARG
1	A	225	LYS
1	A	232	GLU
1	A	237	LEU
1	A	257	GLU
1	A	345	ARG
1	A	351	GLN
1	A	391	GLU
1	A	400	LEU
1	B	11	ASP
1	B	18	ARG
1	B	111	MET
1	B	136	VAL
1	B	157	THR
1	B	168	LYS
1	B	179	ASP
1	B	184	GLN
1	B	197	ARG
1	B	206	ASN
1	B	217	SER
1	B	225	LYS
1	B	228	SER
1	B	237	LEU
1	B	257	GLU
1	B	268	ARG
1	B	345	ARG
1	B	391	GLU
1	C	23	LEU
1	C	25	ASP
1	C	97	GLN
1	C	136	VAL
1	C	157	THR
1	C	184	GLN
1	C	206	ASN

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Mol	Chain	Res	Type
1	C	225	LYS
1	C	257	GLU
1	C	268	ARG
1	C	345	ARG
1	C	391	GLU
1	D	23	LEU
1	D	52	ASP
1	D	111	MET
1	D	136	VAL
1	D	157	THR
1	D	176	THR
1	D	184	GLN
1	D	204	PHE
1	D	225	LYS
1	D	237	LEU
1	D	257	GLU
1	D	268	ARG
1	D	345	ARG
1	D	386	GLU
1	D	397	GLU
1	E	23	LEU
1	E	74	VAL
1	E	77	VAL
1	E	111	MET
1	E	136	VAL
1	E	157	THR
1	E	179	ASP
1	E	184	GLN
1	E	197	ARG
1	E	204	PHE
1	E	206	ASN
1	E	225	LYS
1	E	228	SER
1	E	237	LEU
1	E	257	GLU
1	E	268	ARG
1	E	345	ARG
1	E	376	VAL
1	E	391	GLU
1	E	463	SER
1	E	473	ASP
1	F	11	ASP

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Mol	Chain	Res	Type
1	F	44	PHE
1	F	52	ASP
1	F	97	GLN
1	F	111	MET
1	F	136	VAL
1	F	197	ARG
1	F	225	LYS
1	F	228	SER
1	F	237	LEU
1	F	257	GLU
1	F	345	ARG
1	F	417	VAL
1	F	494	LEU
1	G	111	MET
1	G	136	VAL
1	G	157	THR
1	G	168	LYS
1	G	179	ASP
1	G	184	GLN
1	G	206	ASN
1	G	237	LEU
1	G	257	GLU
1	G	268	ARG
1	G	345	ARG
1	G	391	GLU
1	G	494	LEU
1	H	52	ASP
1	H	77	VAL
1	H	111	MET
1	H	132	LYS
1	H	153	ASN
1	H	196	ASP
1	H	233	MET
1	H	255	GLU
1	H	268	ARG
1	H	313	THR
1	H	328	ASP
1	H	329	THR
1	H	389	MET
1	H	398	ASP
1	H	404	ARG
1	H	495	ASP

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Mol	Chain	Res	Type
1	I	59	GLU
1	I	74	VAL
1	I	77	VAL
1	I	111	MET
1	I	132	LYS
1	I	169	VAL
1	I	187	LEU
1	I	230	ILE
1	I	233	MET
1	I	268	ARG
1	I	284	ARG
1	I	308	GLU
1	I	328	ASP
1	I	357	THR
1	I	391	GLU
1	I	495	ASP
1	J	25	ASP
1	J	54	VAL
1	J	87	ASP
1	J	97	GLN
1	J	111	MET
1	J	196	ASP
1	J	228	SER
1	J	233	MET
1	J	268	ARG
1	J	284	ARG
1	J	338	GLU
1	J	357	THR
1	J	398	ASP
1	J	428	ASP
1	J	495	ASP
1	J	499	VAL
1	K	43	SER
1	K	52	ASP
1	K	77	VAL
1	K	97	GLN
1	K	111	MET
1	K	140	ASP
1	K	172	GLU
1	K	230	ILE
1	K	233	MET
1	K	268	ARG

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Mol	Chain	Res	Type
1	K	272	LYS
1	K	284	ARG
1	K	325	ILE
1	K	326	ASN
1	K	364	LYS
1	K	389	MET
1	K	398	ASP
1	L	25	ASP
1	L	52	ASP
1	L	77	VAL
1	L	97	GLN
1	L	111	MET
1	L	132	LYS
1	L	153	ASN
1	L	172	GLU
1	L	197	ARG
1	L	233	MET
1	L	265	ASN
1	L	326	ASN
1	L	331	THR
1	L	357	THR
1	L	364	LYS
1	L	422	VAL
1	L	424	SER
1	L	499	VAL
1	M	23	LEU
1	M	52	ASP
1	M	74	VAL
1	M	77	VAL
1	M	139	SER
1	M	146	GLN
1	M	161	LEU
1	M	169	VAL
1	M	233	MET
1	M	283	ASP
1	M	284	ARG
1	M	308	GLU
1	M	355	GLU
1	M	357	THR
1	M	359	ASP
1	M	398	ASP
1	M	428	ASP

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Mol	Chain	Res	Type
1	M	495	ASP
1	N	52	ASP
1	N	79	SER
1	N	97	GLN
1	N	111	MET
1	N	121	ASP
1	N	132	LYS
1	N	137	PRO
1	N	172	GLU
1	N	197	ARG
1	N	233	MET
1	N	253	ASP
1	N	268	ARG
1	N	284	ARG
1	N	308	GLU
1	N	357	THR
1	N	389	MET
1	N	398	ASP
1	N	422	VAL
1	N	473	ASP
2	O	6	LEU
2	O	8	ASP
2	O	30	SER
2	O	51	ASN
2	O	55	LYS
2	O	60	LYS
2	O	87	SER
2	P	6	LEU
2	P	20	LYS
2	P	55	LYS
2	P	60	LYS
2	P	86	MET
2	P	87	SER
2	P	94	ILE
2	Q	6	LEU
2	Q	16	GLU
2	Q	37	ARG
2	Q	55	LYS
2	Q	60	LYS
2	Q	68	ASN
2	Q	86	MET
2	Q	94	ILE

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Mol	Chain	Res	Type
2	R	6	LEU
2	R	9	ARG
2	R	20	LYS
2	R	34	LYS
2	R	51	ASN
2	R	55	LYS
2	R	58	ASP
2	R	60	LYS
2	R	81	GLU
2	R	86	MET
2	R	87	SER
2	S	6	LEU
2	S	20	LYS
2	S	30	SER
2	S	37	ARG
2	S	58	ASP
2	S	60	LYS
2	S	68	ASN
2	S	81	GLU
2	S	86	MET
2	S	94	ILE
2	T	6	LEU
2	T	20	LYS
2	T	30	SER
2	T	51	ASN
2	T	55	LYS
2	T	60	LYS
2	U	6	LEU
2	U	9	ARG
2	U	15	LYS
2	U	20	LYS
2	U	30	SER
2	U	34	LYS
2	U	51	ASN
2	U	55	LYS
2	U	60	LYS
2	U	68	ASN
2	U	86	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	I	194	GLN

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

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.