wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:45 PM BST

PDB ID	:	2C7C
EMDB ID:	:	EMD-1180
Title	:	FITTED COORDINATES FOR GROEL-ATP7-GROES CRYO-EM COMPLEX (EMD-1180)
Authors	:	Ranson, N.A.; Clare, D.K.; Farr, G.W.; Houldershaw, D.; Horwich, A.L.; Saibil, H.R.
Deposited on	:	2005-11-22
Resolution	:	7.70 Å(reported)

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

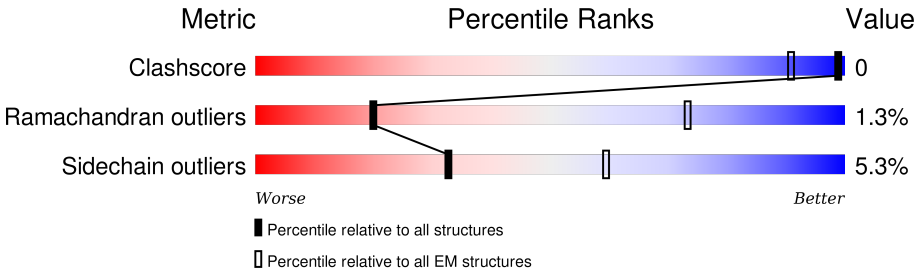
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 7.70 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	93% · ·
1	C	547	90% 5% ·
1	D	547	92% · ·
1	E	547	91% · ·
1	F	547	92% · ·
1	G	547	92% · ·
1	H	547	90% 5% ·
1	I	547	91% 5% ·

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Mol	Chain	Length	Quality of chain
1	J	547	90% 6%
1	K	547	89% 6%
1	L	547	90% 5%
1	M	547	90% 5%
1	N	547	90% 6%
2	O	97	85% 11%
2	P	97	77% 18%
2	Q	97	81% 14%
2	R	97	79% 15%
2	S	97	85% 10%
2	T	97	85% 10%
2	U	97	79% 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.

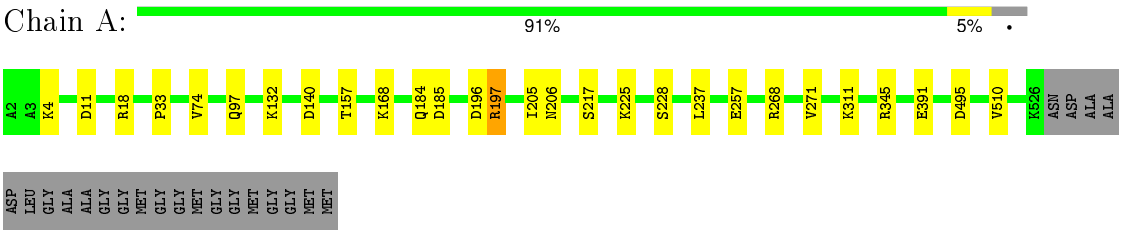
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	P	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	Q	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	R	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	S	93	Total	C	N	O	S	0	1
			680	432	112	135	1		
2	T	93	Total	C	N	O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

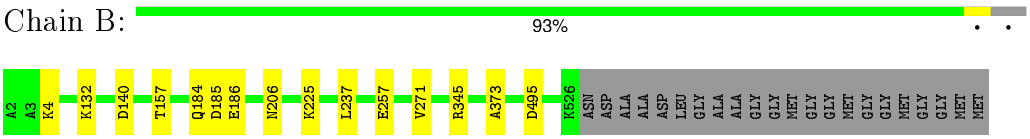
- Molecule 1: 60 KDA CHAPERONIN

Chain A:



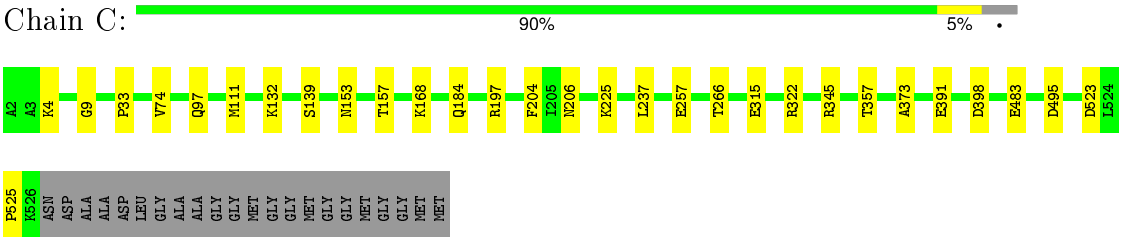
- Molecule 1: 60 KDA CHAPERONIN

Chain B:



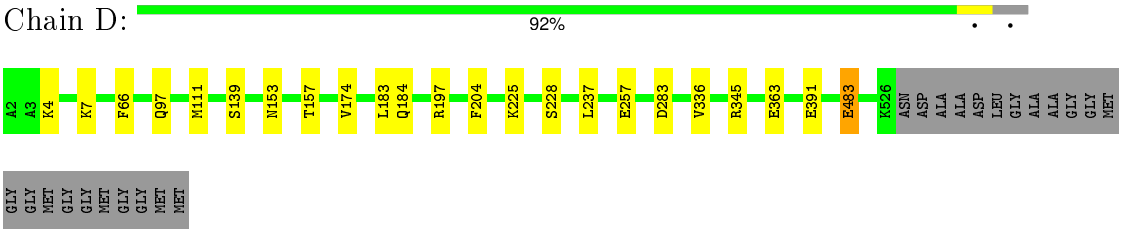
- Molecule 1: 60 KDA CHAPERONIN

Chain C:



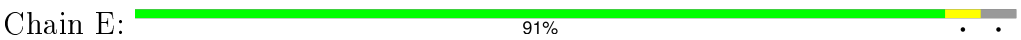
- Molecule 1: 60 KDA CHAPERONIN

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

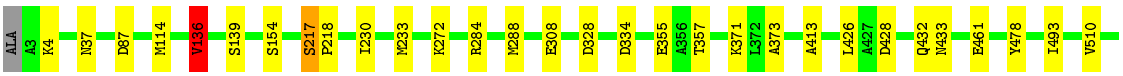
Chain J:

• Molecule 1: 60 KDA CHAPERONIN

Chain K:

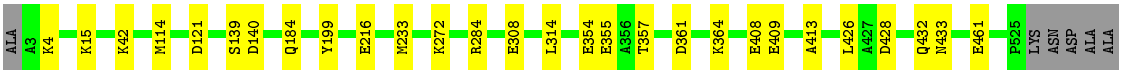
• Molecule 1: 60 KDA CHAPERONIN

Chain L:



• Molecule 1: 60 KDA CHAPERONIN

Chain M:

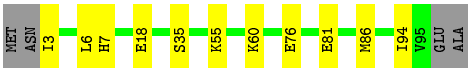


• Molecule 1: 60 KDA CHAPERONIN

Chain N:

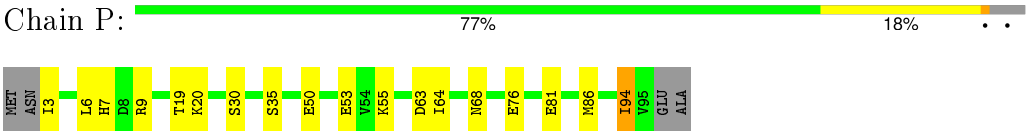
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain O:



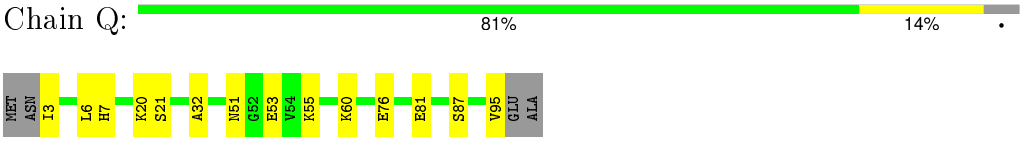
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain P:



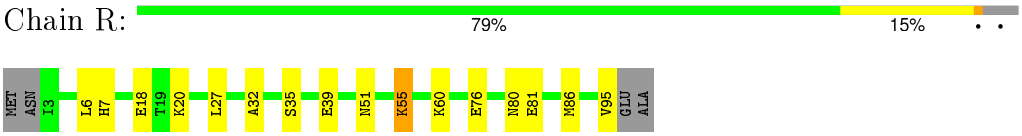
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain Q:



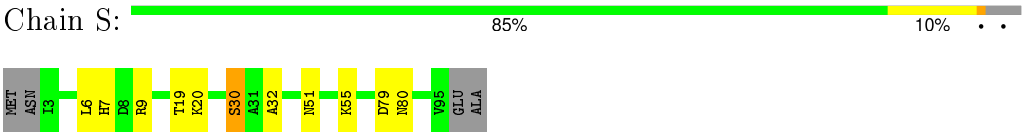
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain R:



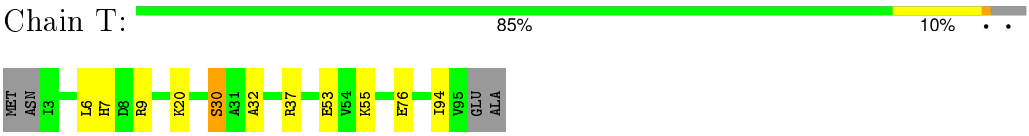
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

Chain S:



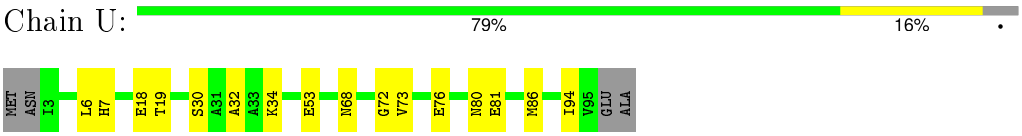
• Molecule 2: 10 KDA CHAPERONIN MOLECULE: GROES, PROTEIN CPN10, GROES PROTEIN

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)	1100	Depositor
Maximum defocus (nm)	3200	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	0.91	0/5165
1	C	0.59	0/3833	0.89	1/5165 (0.0%)
1	D	0.59	0/3833	0.90	1/5165 (0.0%)
1	E	0.59	0/3833	0.90	0/5165
1	F	0.59	0/3833	0.90	0/5165
1	G	0.60	0/3833	0.91	0/5165
1	H	0.59	0/3820	0.92	0/5146
1	I	0.60	0/3820	0.91	0/5146
1	J	0.60	0/3820	0.91	0/5146
1	K	0.60	0/3820	0.91	1/5146 (0.0%)
1	L	0.60	0/3820	0.91	0/5146
1	M	0.60	0/3820	0.90	0/5146
1	N	0.60	0/3820	0.91	0/5146
2	O	0.62	0/684	0.97	0/918
2	P	0.62	0/684	1.04	0/918
2	Q	0.63	0/684	0.99	0/918
2	R	0.62	0/684	1.01	1/918 (0.1%)
2	S	0.62	0/684	0.97	1/918 (0.1%)
2	T	0.63	0/684	0.99	0/918
2	U	0.63	0/684	1.00	0/918
All	All	0.60	0/58359	0.91	5/78603 (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	0	1
1	B	0	1
1	C	0	1
1	D	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	H	0	2
1	I	0	1
1	J	0	3
1	K	0	2
1	L	0	3
1	M	0	2
1	N	1	0
All	All	1	19

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	322	ARG	CD-NE-CZ	5.61	131.46	123.60
2	R	39	GLU	OE1-CD-OE2	-5.18	117.09	123.30
2	S	79	ASP	C-N-CA	5.11	134.48	121.70
1	D	483	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	K	285	ARG	CD-NE-CZ	5.00	130.60	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	N	120	ILE	CB

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	LYS	Peptide
1	B	4	LYS	Peptide
1	C	4	LYS	Peptide
1	D	183	LEU	Peptide
1	D	4	LYS	Peptide
1	G	4	LYS	Peptide
1	H	4	LYS	Peptide
1	H	8	PHE	Peptide
1	I	4	LYS	Peptide
1	J	179	ASP	Peptide
1	J	255	GLU	Peptide
1	J	4	LYS	Peptide
1	K	218	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	K	4	LYS	Peptide
1	L	136	VAL	Peptide
1	L	373	ALA	Peptide
1	L	4	LYS	Peptide
1	M	4	LYS	Peptide
1	M	408	GLU	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	0	0
1	C	3805	0	3881	2	0
1	D	3805	0	3881	1	0
1	E	3805	0	3881	2	0
1	F	3805	0	3881	0	0
1	G	3805	0	3881	1	0
1	H	3793	0	3869	2	0
1	I	3793	0	3869	0	0
1	J	3793	0	3869	1	0
1	K	3793	0	3869	1	0
1	L	3793	0	3869	1	0
1	M	3793	0	3869	1	0
1	N	3793	0	3869	0	0
2	O	680	0	703	1	0
2	P	680	0	703	2	0
2	Q	680	0	703	2	0
2	R	680	0	703	2	0
2	S	680	0	703	0	0
2	T	680	0	703	0	0
2	U	680	0	703	0	0
All	All	57946	0	59171	16	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 (16) 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:M:314:LEU:H	1:M:314:LEU:HD12	1.70	0.55
1:D:7:LYS:HE2	1:D:66:PHE:CE2	2.43	0.54
1:E:7:LYS:HE2	1:E:66:PHE:CE2	2.46	0.50
1:H:7:LYS:HE2	1:H:66:PHE:CE2	2.47	0.50
1:A:510:VAL:HG23	1:G:385:THR:HG21	1.94	0.50
1:E:360:TYR:CE2	1:E:364:LYS:HE2	2.51	0.45
1:C:204:PHE:CG	1:C:266:THR:HG21	2.51	0.45
1:H:230:ILE:H	1:H:230:ILE:HD12	1.82	0.44
2:R:55:LYS:HE3	2:R:55:LYS:H	1.82	0.44
2:O:3:ILE:HA	2:P:94:ILE:O	2.19	0.42
2:Q:3:ILE:HA	2:R:95:VAL:N	2.34	0.41
1:C:204:PHE:CD2	1:C:266:THR:HG21	2.55	0.41
1:J:7:LYS:HE2	1:J:66:PHE:CE2	2.55	0.41
1:K:65:LYS:HE3	1:K:525:PRO:N	2.36	0.41
2:P:3:ILE:N	2:Q:95:VAL:N	2.69	0.41
1:L:217:SER:N	1:L:218:PRO:HD3	2.36	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%)	490 (94%)	29 (6%)	4 (1%)	24	69
1	B	523/547 (96%)	492 (94%)	30 (6%)	1 (0%)	52	86
1	C	523/547 (96%)	493 (94%)	23 (4%)	7 (1%)	15	60
1	D	523/547 (96%)	494 (94%)	25 (5%)	4 (1%)	24	69
1	E	523/547 (96%)	495 (95%)	22 (4%)	6 (1%)	17	63
1	F	523/547 (96%)	481 (92%)	38 (7%)	4 (1%)	24	69
1	G	523/547 (96%)	491 (94%)	28 (5%)	4 (1%)	24	69
1	H	521/547 (95%)	471 (90%)	44 (8%)	6 (1%)	16	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	521/547 (95%)	481 (92%)	35 (7%)	5 (1%)	19	65
1	J	521/547 (95%)	475 (91%)	42 (8%)	4 (1%)	24	69
1	K	521/547 (95%)	482 (92%)	35 (7%)	4 (1%)	24	69
1	L	521/547 (95%)	479 (92%)	33 (6%)	9 (2%)	11	55
1	M	521/547 (95%)	479 (92%)	39 (8%)	3 (1%)	30	74
1	N	521/547 (95%)	479 (92%)	31 (6%)	11 (2%)	9	50
2	O	91/97 (94%)	73 (80%)	15 (16%)	3 (3%)	5	40
2	P	91/97 (94%)	71 (78%)	15 (16%)	5 (6%)	2	29
2	Q	91/97 (94%)	74 (81%)	14 (15%)	3 (3%)	5	40
2	R	91/97 (94%)	74 (81%)	13 (14%)	4 (4%)	3	33
2	S	91/97 (94%)	70 (77%)	16 (18%)	5 (6%)	2	29
2	T	91/97 (94%)	73 (80%)	14 (15%)	4 (4%)	3	33
2	U	91/97 (94%)	73 (80%)	11 (12%)	7 (8%)	1	20
All	All	7945/8337 (95%)	7290 (92%)	552 (7%)	103 (1%)	20	60

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	C	483	GLU
1	H	154	SER
1	H	483	GLU
1	I	154	SER
1	J	483	GLU
1	K	66	PHE
1	K	154	SER
1	L	136	VAL
1	L	154	SER
1	M	409	GLU
1	N	154	SER
1	N	409	GLU
2	O	7	HIS
2	P	53	GLU
2	Q	7	HIS
2	Q	32	ALA
2	R	7	HIS
2	S	32	ALA

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Mol	Chain	Res	Type
2	S	80	ASN
2	T	32	ALA
2	U	73	VAL
1	C	9	GLY
1	C	139	SER
1	D	483	GLU
1	E	154	SER
1	E	310	GLU
1	F	179	ASP
1	F	336	VAL
1	G	483	GLU
1	H	217	SER
1	J	139	SER
1	K	139	SER
1	L	139	SER
1	N	217	SER
1	N	334	ASP
2	R	32	ALA
2	S	7	HIS
2	T	7	HIS
2	T	30	SER
2	U	7	HIS
2	U	19	THR
1	E	153	ASN
1	F	153	ASN
1	H	139	SER
1	I	139	SER
1	I	409	GLU
1	M	139	SER
1	M	413	ALA
1	N	139	SER
1	N	208	PRO
1	N	327	LYS
2	O	18	GLU
2	P	7	HIS
2	P	19	THR
2	Q	21	SER
2	U	18	GLU
2	U	32	ALA
2	U	94	ILE
1	A	33	PRO
1	C	153	ASN

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Mol	Chain	Res	Type
1	D	139	SER
1	D	153	ASN
1	E	217	SER
1	E	334	ASP
1	E	374	GLY
1	H	334	ASP
1	I	357	THR
1	I	371	LYS
1	J	154	SER
1	J	217	SER
1	L	413	ALA
1	N	413	ALA
2	R	18	GLU
2	R	80	ASN
2	S	19	THR
2	S	30	SER
1	C	33	PRO
1	C	373	ALA
1	C	525	PRO
1	G	217	SER
1	G	367	GLU
1	G	373	ALA
1	L	217	SER
1	L	328	ASP
1	L	334	ASP
1	N	483	GLU
2	O	94	ILE
2	P	50	GLU
1	A	217	SER
1	B	373	ALA
1	K	356	ALA
1	L	371	LYS
1	N	268	ARG
1	N	336	VAL
2	T	94	ILE
2	U	72	GLY
1	A	205	ILE
1	D	336	VAL
1	H	493	ILE
1	L	493	ILE
1	F	9	GLY
2	P	64	ILE

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%)	381 (94%)	23 (6%)	25 62
1	B	404/414 (98%)	391 (97%)	13 (3%)	46 76
1	C	404/414 (98%)	385 (95%)	19 (5%)	32 68
1	D	404/414 (98%)	389 (96%)	15 (4%)	41 73
1	E	404/414 (98%)	388 (96%)	16 (4%)	38 71
1	F	404/414 (98%)	388 (96%)	16 (4%)	38 71
1	G	404/414 (98%)	390 (96%)	14 (4%)	43 74
1	H	403/414 (97%)	383 (95%)	20 (5%)	30 66
1	I	403/414 (97%)	383 (95%)	20 (5%)	30 66
1	J	403/414 (97%)	381 (94%)	22 (6%)	27 63
1	K	403/414 (97%)	378 (94%)	25 (6%)	23 60
1	L	403/414 (97%)	384 (95%)	19 (5%)	32 68
1	M	403/414 (97%)	381 (94%)	22 (6%)	27 63
1	N	403/414 (97%)	382 (95%)	21 (5%)	29 65
2	O	76/80 (95%)	69 (91%)	7 (9%)	11 43
2	P	76/80 (95%)	64 (84%)	12 (16%)	3 21
2	Q	76/80 (95%)	67 (88%)	9 (12%)	6 32
2	R	76/80 (95%)	66 (87%)	10 (13%)	5 28
2	S	76/80 (95%)	70 (92%)	6 (8%)	15 51
2	T	76/80 (95%)	68 (90%)	8 (10%)	8 36
2	U	76/80 (95%)	67 (88%)	9 (12%)	6 32
All	All	6181/6356 (97%)	5855 (95%)	326 (5%)	33 64

All (326) 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	18	ARG
1	A	74	VAL
1	A	97	GLN
1	A	132	LYS
1	A	140	ASP
1	A	157	THR
1	A	168	LYS
1	A	184	GLN
1	A	185	ASP
1	A	196	ASP
1	A	197	ARG
1	A	206	ASN
1	A	225	LYS
1	A	228	SER
1	A	237	LEU
1	A	257	GLU
1	A	268	ARG
1	A	271	VAL
1	A	311	LYS
1	A	345	ARG
1	A	391	GLU
1	A	495	ASP
1	B	132	LYS
1	B	140	ASP
1	B	157	THR
1	B	184	GLN
1	B	185	ASP
1	B	186	GLU
1	B	206	ASN
1	B	225	LYS
1	B	237	LEU
1	B	257	GLU
1	B	271	VAL
1	B	345	ARG
1	B	495	ASP
1	C	74	VAL
1	C	97	GLN
1	C	111	MET
1	C	132	LYS
1	C	157	THR
1	C	168	LYS
1	C	184	GLN

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Mol	Chain	Res	Type
1	C	197	ARG
1	C	206	ASN
1	C	225	LYS
1	C	237	LEU
1	C	257	GLU
1	C	315	GLU
1	C	345	ARG
1	C	357	THR
1	C	391	GLU
1	C	398	ASP
1	C	495	ASP
1	C	523	ASP
1	D	97	GLN
1	D	111	MET
1	D	157	THR
1	D	174	VAL
1	D	184	GLN
1	D	197	ARG
1	D	204	PHE
1	D	225	LYS
1	D	228	SER
1	D	237	LEU
1	D	257	GLU
1	D	283	ASP
1	D	345	ARG
1	D	363	GLU
1	D	391	GLU
1	E	11	ASP
1	E	52	ASP
1	E	111	MET
1	E	153	ASN
1	E	157	THR
1	E	168	LYS
1	E	184	GLN
1	E	185	ASP
1	E	197	ARG
1	E	225	LYS
1	E	237	LEU
1	E	257	GLU
1	E	345	ARG
1	E	391	GLU
1	E	495	ASP

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Mol	Chain	Res	Type
1	E	523	ASP
1	F	11	ASP
1	F	25	ASP
1	F	132	LYS
1	F	157	THR
1	F	176	THR
1	F	184	GLN
1	F	185	ASP
1	F	197	ARG
1	F	206	ASN
1	F	225	LYS
1	F	237	LEU
1	F	257	GLU
1	F	345	ARG
1	F	369	VAL
1	F	391	GLU
1	F	417	VAL
1	G	52	ASP
1	G	111	MET
1	G	132	LYS
1	G	157	THR
1	G	179	ASP
1	G	184	GLN
1	G	197	ARG
1	G	206	ASN
1	G	225	LYS
1	G	228	SER
1	G	237	LEU
1	G	257	GLU
1	G	345	ARG
1	G	391	GLU
1	H	37	ASN
1	H	42	LYS
1	H	61	GLU
1	H	87	ASP
1	H	114	MET
1	H	184	GLN
1	H	230	ILE
1	H	233	MET
1	H	272	LYS
1	H	284	ARG
1	H	288	MET

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Mol	Chain	Res	Type
1	H	357	THR
1	H	364	LYS
1	H	378	VAL
1	H	389	MET
1	H	426	LEU
1	H	432	GLN
1	H	433	ASN
1	H	441	LYS
1	H	523	ASP
1	I	37	ASN
1	I	42	LYS
1	I	107	VAL
1	I	114	MET
1	I	185	ASP
1	I	188	ASP
1	I	197	ARG
1	I	233	MET
1	I	272	LYS
1	I	284	ARG
1	I	288	MET
1	I	302	SER
1	I	364	LYS
1	I	389	MET
1	I	421	ARG
1	I	426	LEU
1	I	432	GLN
1	I	500	THR
1	I	504	LEU
1	I	523	ASP
1	J	21	ASN
1	J	42	LYS
1	J	140	ASP
1	J	230	ILE
1	J	233	MET
1	J	272	LYS
1	J	284	ARG
1	J	288	MET
1	J	311	LYS
1	J	351	GLN
1	J	357	THR
1	J	364	LYS
1	J	385	THR

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Mol	Chain	Res	Type
1	J	409	GLU
1	J	421	ARG
1	J	426	LEU
1	J	433	ASN
1	J	435	ASP
1	J	436	GLN
1	J	461	GLU
1	J	499	VAL
1	J	522	THR
1	K	21	ASN
1	K	37	ASN
1	K	42	LYS
1	K	52	ASP
1	K	114	MET
1	K	115	ASP
1	K	129	GLU
1	K	216	GLU
1	K	230	ILE
1	K	233	MET
1	K	259	LEU
1	K	272	LYS
1	K	284	ARG
1	K	288	MET
1	K	310	GLU
1	K	364	LYS
1	K	389	MET
1	K	391	GLU
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	460	GLU
1	K	461	GLU
1	K	509	SER
1	K	510	VAL
1	L	37	ASN
1	L	87	ASP
1	L	114	MET
1	L	136	VAL
1	L	230	ILE
1	L	233	MET
1	L	272	LYS
1	L	284	ARG

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Mol	Chain	Res	Type
1	L	288	MET
1	L	308	GLU
1	L	355	GLU
1	L	357	THR
1	L	426	LEU
1	L	428	ASP
1	L	432	GLN
1	L	433	ASN
1	L	461	GLU
1	L	478	TYR
1	L	510	VAL
1	M	15	LYS
1	M	42	LYS
1	M	114	MET
1	M	121	ASP
1	M	140	ASP
1	M	184	GLN
1	M	199	TYR
1	M	216	GLU
1	M	233	MET
1	M	272	LYS
1	M	284	ARG
1	M	308	GLU
1	M	354	GLU
1	M	355	GLU
1	M	357	THR
1	M	361	ASP
1	M	364	LYS
1	M	426	LEU
1	M	428	ASP
1	M	432	GLN
1	M	433	ASN
1	M	461	GLU
1	N	37	ASN
1	N	42	LYS
1	N	52	ASP
1	N	76	GLU
1	N	87	ASP
1	N	107	VAL
1	N	114	MET
1	N	140	ASP
1	N	169	VAL

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Mol	Chain	Res	Type
1	N	191	GLU
1	N	197	ARG
1	N	230	ILE
1	N	233	MET
1	N	272	LYS
1	N	288	MET
1	N	359	ASP
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	435	ASP
2	O	6	LEU
2	O	35	SER
2	O	55	LYS
2	O	60	LYS
2	O	76	GLU
2	O	81	GLU
2	O	86	MET
2	P	6	LEU
2	P	9	ARG
2	P	20	LYS
2	P	30	SER
2	P	35	SER
2	P	55	LYS
2	P	63	ASP
2	P	68	ASN
2	P	76	GLU
2	P	81	GLU
2	P	86	MET
2	P	94	ILE
2	Q	6	LEU
2	Q	20	LYS
2	Q	51	ASN
2	Q	53	GLU
2	Q	55	LYS
2	Q	60	LYS
2	Q	76	GLU
2	Q	81	GLU
2	Q	87	SER
2	R	6	LEU
2	R	20	LYS

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Mol	Chain	Res	Type
2	R	27	LEU
2	R	35	SER
2	R	51	ASN
2	R	55	LYS
2	R	60	LYS
2	R	76	GLU
2	R	81	GLU
2	R	86	MET
2	S	6	LEU
2	S	9	ARG
2	S	20	LYS
2	S	30	SER
2	S	51	ASN
2	S	55	LYS
2	T	6	LEU
2	T	9	ARG
2	T	20	LYS
2	T	30	SER
2	T	37	ARG
2	T	53	GLU
2	T	55	LYS
2	T	76	GLU
2	U	6	LEU
2	U	30	SER
2	U	34	LYS
2	U	53	GLU
2	U	68	ASN
2	U	76	GLU
2	U	80	ASN
2	U	81	GLU
2	U	86	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	97	GLN
1	L	432	GLN
1	L	436	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.