Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:41 AM EST

PDB ID	:	3JCC
EMDB ID	:	EMD-6543
Title	:	Structure of Simian Immunodeficiency Virus Envelope Spikes bound with CD4 and Monoclonal Antibody 36D5
Authors	:	Hu, G.; Liu, J.; Roux, K.; Taylor, K.A.
Deposited on	:	2015-11-25
Resolution	:	Not provided
Based on initial model	:	4NCO

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

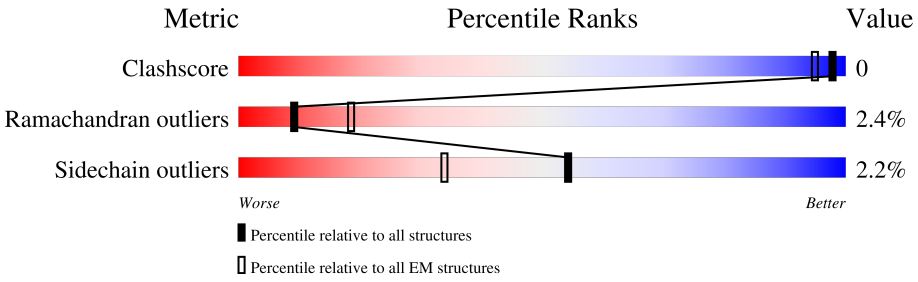
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 unknown.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	448	82% 11% • 6%
1	E	448	81% 12% • 6%
1	I	448	83% 10% • 6%
2	B	207	92% 5% •
3	C	232	93% • •
4	D	175	97% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14521 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3299	2065	581	626	27		
1	E	420	Total	C	N	O	S	0	0
			3299	2065	581	626	27		
1	I	420	Total	C	N	O	S	0	0
			3299	2065	581	626	27		

- Molecule 2 is a protein called Antibody 36D5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	202	Total	C	N	O	S	0	0
			1531	964	255	308	4		

- Molecule 3 is a protein called Antibody 36D5 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1729	1100	293	331	5		

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

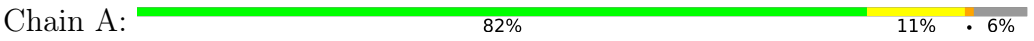
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1364	851	239	270	4		

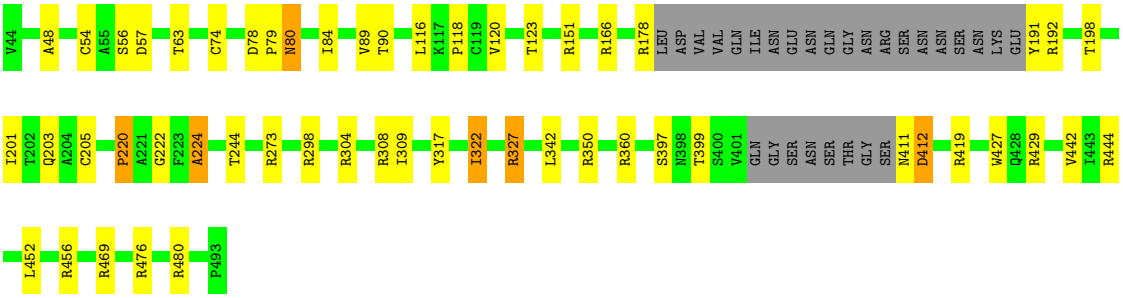
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Envelope glycoprotein gp120

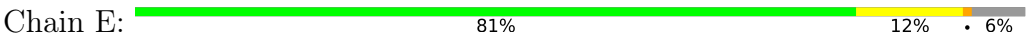
Chain A:

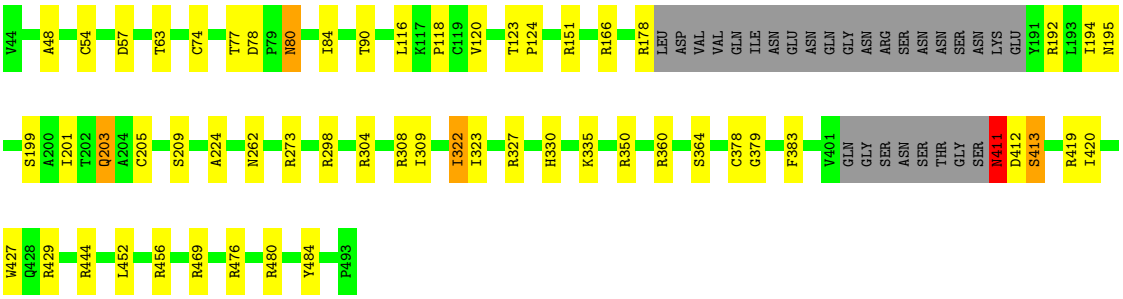




- Molecule 1: Envelope glycoprotein gp120

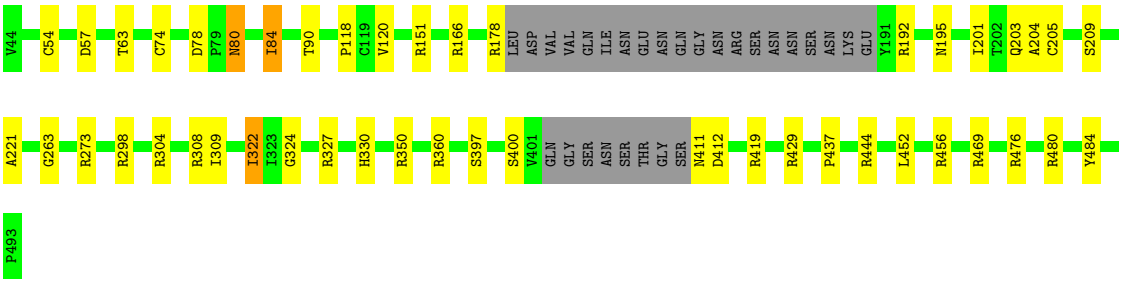
Chain E:





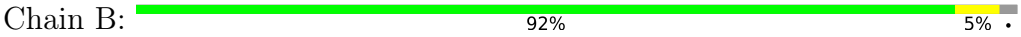
- Molecule 1: Envelope glycoprotein gp120

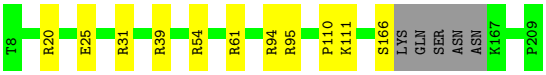
Chain I:



• Molecule 2: Antibody 36D5 light chain

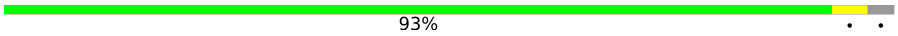
Chain B:

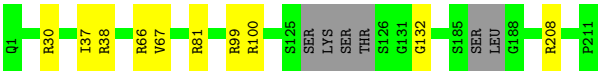




• Molecule 3: Antibody 36D5 heavy chain

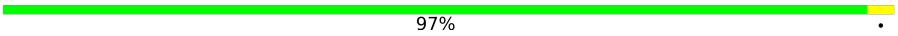
Chain C:

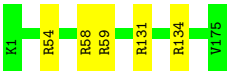




• Molecule 4: T-cell surface glycoprotein CD4

Chain D:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1796	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	31000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/3369	1.11	24/4574 (0.5%)
1	E	0.63	0/3369	1.08	26/4574 (0.6%)
1	I	0.63	0/3369	1.09	20/4574 (0.4%)
2	B	0.62	0/1573	0.98	9/2154 (0.4%)
3	C	0.62	0/1777	0.98	8/2427 (0.3%)
4	D	0.53	0/1383	0.95	6/1863 (0.3%)
All	All	0.62	0/14840	1.05	93/20166 (0.5%)

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	1	5
1	E	1	5
1	I	1	2
2	B	0	2
3	C	0	1
All	All	3	15

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	298	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	298	ARG	NE-CZ-NH1	9.81	125.21	120.30
4	D	54	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	E	444	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	I	166	ARG	NE-CZ-NH2	9.12	124.86	120.30
2	B	61	ARG	NE-CZ-NH1	9.03	124.81	120.30
4	D	58	ARG	NE-CZ-NH1	8.95	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	99	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	I	350	ARG	NE-CZ-NH1	8.85	124.72	120.30
4	D	59	ARG	NE-CZ-NH1	8.78	124.69	120.30
3	C	208	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	E	350	ARG	NE-CZ-NH1	8.73	124.67	120.30
2	B	39	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	I	298	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	I	429	ARG	NE-CZ-NH2	8.69	124.65	120.30
1	A	476	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	A	360	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	B	31	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	308	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	178	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	E	192	ARG	NE-CZ-NH2	8.37	124.49	120.30
1	E	327	ARG	NE-CZ-NH2	8.35	124.47	120.30
2	B	20	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	I	456	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	273	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	E	480	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	E	308	ARG	NE-CZ-NH2	8.12	124.36	120.30
3	C	30	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	B	54	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	I	476	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	E	166	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	166	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	E	360	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	I	444	ARG	NE-CZ-NH1	7.90	124.25	120.30
3	C	81	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	I	273	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	E	429	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	A	429	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	A	469	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	I	308	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	I	304	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	A	327	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	350	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	151	ARG	NE-CZ-NH2	7.56	124.08	120.30
2	B	94	ARG	NE-CZ-NH1	7.55	124.08	120.30
3	C	38	ARG	NE-CZ-NH1	7.53	124.07	120.30
3	C	66	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	I	192	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	I	327	ARG	NE-CZ-NH2	7.51	124.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	151	ARG	NE-CZ-NH2	7.51	124.06	120.30
4	D	131	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	I	419	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	A	192	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	A	456	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	I	360	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	E	419	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	I	469	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	304	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	E	304	ARG	NE-CZ-NH2	7.03	123.82	120.30
4	D	134	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	I	151	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	I	178	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	444	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	178	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	E	476	ARG	NE-CZ-NH2	6.79	123.70	120.30
2	B	95	ARG	NE-CZ-NH2	6.78	123.69	120.30
3	C	100	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	E	456	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	E	411	ASN	N-CA-C	6.47	128.48	111.00
1	A	480	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	E	273	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	E	412	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	298	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	I	54	CYS	CA-CB-SG	6.08	124.94	114.00
1	E	327	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	419	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	E	469	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	I	480	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	54	CYS	CA-CB-SG	5.88	124.58	114.00
2	B	31	ARG	NE-CZ-NH2	-5.79	117.41	120.30
4	D	131	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	E	298	ARG	NE-CZ-NH2	-5.49	117.55	120.30
2	B	111	LYS	N-CA-C	5.41	125.60	111.00
1	A	469	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	192	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	79	PRO	N-CA-C	5.36	126.03	112.10
1	E	74	CYS	CA-CB-SG	5.32	123.57	114.00
1	E	54	CYS	CA-CB-SG	5.31	123.56	114.00
1	A	220	PRO	N-CA-C	5.27	125.80	112.10
1	E	80	ASN	N-CA-C	5.06	124.67	111.00
1	I	74	CYS	CA-CB-SG	5.03	123.06	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	CYS	CA-CB-SG	5.00	123.00	114.00
3	C	81	ARG	NE-CZ-NH1	-5.00	117.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	411	ASN	CA
1	E	411	ASN	CA
1	I	411	ASN	CA

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ALA	Peptide
1	A	317	TYR	Sidechain
1	A	327	ARG	Sidechain
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
2	B	110	PRO	Peptide
2	B	166	SER	Peptide
3	C	132	GLY	Peptide
1	E	124	PRO	Peptide
1	E	199	SER	Peptide
1	E	203	GLN	Peptide
1	E	224	ALA	Peptide
1	E	78	ASP	Peptide
1	I	78	ASP	Peptide
1	I	80	ASN	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	3299	0	3241	4	0
1	E	3299	0	3241	6	0
1	I	3299	0	3241	2	0
2	B	1531	0	1473	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1729	0	1701	0	0
4	D	1364	0	1389	0	0
All	All	14521	0	14286	12	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 (12) 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:A:120:VAL:HG12	1:A:201:ILE:HG22	1.67	0.77
1:E:120:VAL:HG13	1:E:203:GLN:HA	1.84	0.60
1:I:120:VAL:HG12	1:I:201:ILE:HG22	1.85	0.58
1:E:120:VAL:HG12	1:E:201:ILE:HG22	1.91	0.50
1:I:120:VAL:HG13	1:I:203:GLN:HA	1.94	0.48
1:E:378:CYS:HB3	1:E:383:PHE:CE1	2.50	0.46
1:A:120:VAL:HG13	1:A:203:GLN:HA	1.97	0.46
1:A:116:LEU:HD22	1:A:120:VAL:HG11	1.98	0.45
1:E:116:LEU:HD22	1:E:120:VAL:HG11	1.97	0.44
1:E:322:ILE:HG22	1:E:323:ILE:H	1.82	0.43
1:A:224:ALA:HB1	1:A:244:THR:HG23	2.01	0.43
1:E:335:LYS:HB2	1:E:413:SER:HA	2.02	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	418/448 (93%)	359 (86%)	43 (10%)	16 (4%)	3 3
1	E	418/448 (93%)	363 (87%)	42 (10%)	13 (3%)	4 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	418/448 (93%)	352 (84%)	51 (12%)	15 (4%)	3 3
2	B	200/207 (97%)	194 (97%)	6 (3%)	0	100 100
3	C	224/232 (97%)	218 (97%)	6 (3%)	0	100 100
4	D	173/175 (99%)	170 (98%)	3 (2%)	0	100 100
All	All	1851/1958 (94%)	1656 (90%)	151 (8%)	44 (2%)	9 6

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	220	PRO
1	A	322	ILE
1	A	412	ASP
1	E	57	ASP
1	E	84	ILE
1	E	195	ASN
1	E	322	ILE
1	I	57	ASP
1	I	84	ILE
1	I	322	ILE
1	A	80	ASN
1	A	90	THR
1	A	118	PRO
1	A	198	THR
1	E	205	CYS
1	E	411	ASN
1	I	118	PRO
1	I	195	ASN
1	I	204	ALA
1	I	221	ALA
1	I	263	GLY
1	I	412	ASP
1	A	48	ALA
1	A	57	ASP
1	E	63	THR
1	E	262	ASN
1	I	90	THR
1	I	324	GLY
1	A	63	THR
1	A	427	TRP
1	E	90	THR

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Mol	Chain	Res	Type
1	E	118	PRO
1	E	379	GLY
1	I	63	THR
1	I	80	ASN
1	E	48	ALA
1	E	427	TRP
1	I	205	CYS
1	A	205	CYS
1	A	222	GLY
1	A	442	VAL
1	I	437	PRO
1	A	89	VAL

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	375/400 (94%)	364 (97%)	11 (3%)	42	42
1	E	375/400 (94%)	362 (96%)	13 (4%)	36	36
1	I	375/400 (94%)	365 (97%)	10 (3%)	44	44
2	B	171/176 (97%)	170 (99%)	1 (1%)	86	86
3	C	196/202 (97%)	194 (99%)	2 (1%)	76	76
4	D	159/159 (100%)	159 (100%)	0	100	100
All	All	1651/1737 (95%)	1614 (98%)	37 (2%)	54	52

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	A	123	THR
1	A	191	TYR
1	A	309	ILE
1	A	322	ILE
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	397	SER
1	A	399	THR
1	A	411	ASN
1	A	412	ASP
1	A	452	LEU
2	B	25	GLU
3	C	37	ILE
3	C	67	VAL
1	E	77	THR
1	E	80	ASN
1	E	123	THR
1	E	194	ILE
1	E	209	SER
1	E	309	ILE
1	E	330	HIS
1	E	364	SER
1	E	411	ASN
1	E	413	SER
1	E	420	ILE
1	E	452	LEU
1	E	484	TYR
1	I	84	ILE
1	I	209	SER
1	I	309	ILE
1	I	322	ILE
1	I	330	HIS
1	I	397	SER
1	I	400	SER
1	I	411	ASN
1	I	452	LEU
1	I	484	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	133	ASN
1	A	216	HIS
4	D	164	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 monosaccharides 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 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-6543. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis (i)

This section contains the results of statistical analysis of the tomogram.

7.1 Map-value distribution (i)

This section was not generated.

8 Map-model fit

This section was not generated.