wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3DNO
EMDB ID:	:	EMD-5020
Title	:	Molecular structure for the HIV-1 gp120 trimer in the CD4-bound state
Authors	:	Borgnia, M.J.; Liu, J.; Bartesaghi, A.; Sapiro, G.; Subramaniam, S.
Deposited on	:	2008-07-02
Resolution	:	20.00 Å(reported)
Based on PDB ID	:	1GC1

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

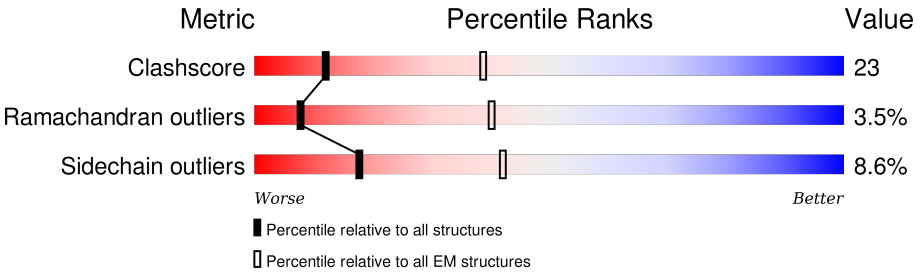
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 20.00 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	35	43% 46% 9% •
1	D	35	49% 40% 9% •
1	G	35	49% 40% 9% •
2	B	170	54% 40% 5% •
2	E	170	54% 41% 5% •
2	H	170	54% 40% 5% •
3	C	83	58% 36% 6%
3	F	83	58% 35% 7%
3	I	83	58% 35% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6738 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 HIV-1 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	35	Total	C	N	O	S	0	0
			293	186	47	56	4		
1	D	35	Total	C	N	O	S	0	0
			293	186	47	56	4		
1	G	35	Total	C	N	O	S	0	0
			293	186	47	56	4		

- Molecule 2 is a protein called HIV-1 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	170	Total	C	N	O	S	0	0
			1301	818	226	248	9		
2	E	170	Total	C	N	O	S	0	0
			1301	818	226	248	9		
2	H	170	Total	C	N	O	S	0	0
			1301	818	226	248	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	GLY	-	LINKER	UNP P04578
B	299	ALA	-	LINKER	UNP P04578
B	329	GLY	-	LINKER	UNP P04578
E	298	GLY	-	LINKER	UNP P04578
E	299	ALA	-	LINKER	UNP P04578
E	329	GLY	-	LINKER	UNP P04578
H	298	GLY	-	LINKER	UNP P04578
H	299	ALA	-	LINKER	UNP P04578
H	329	GLY	-	LINKER	UNP P04578

- Molecule 3 is a protein called HIV-1 envelope glycoprotein gp120.

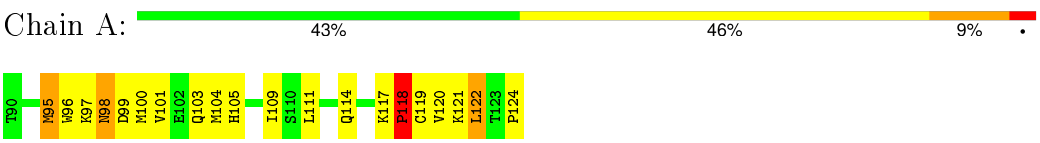
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	83	Total	C	N	O	S	0	0
			652	406	118	123	5		
3	F	83	Total	C	N	O	S	0	0
			652	406	118	123	5		
3	I	83	Total	C	N	O	S	0	0
			652	406	118	123	5		

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.

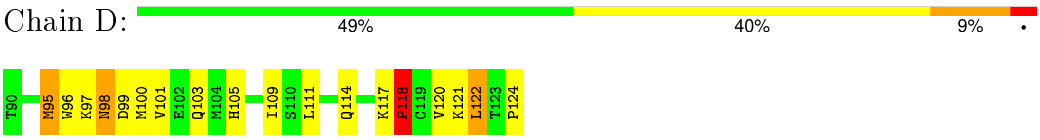
- Molecule 1: HIV-1 envelope glycoprotein gp120

Chain A:



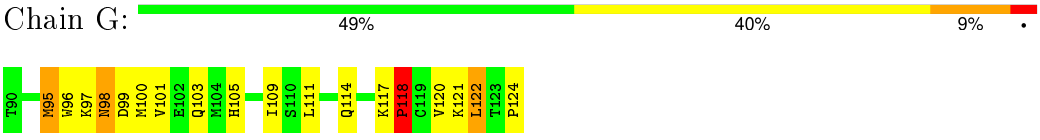
- Molecule 1: HIV-1 envelope glycoprotein gp120

Chain D:



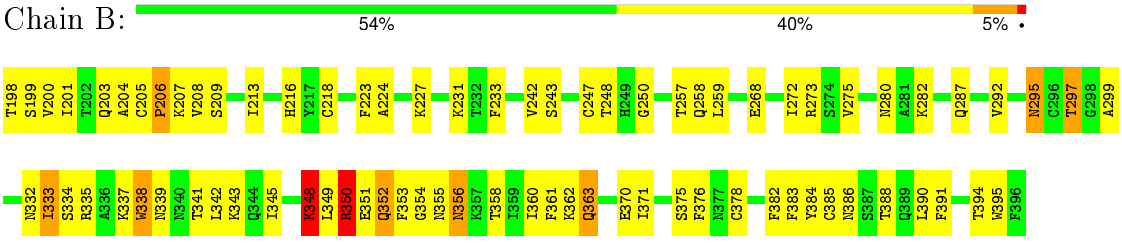
- Molecule 1: HIV-1 envelope glycoprotein gp120

Chain G:



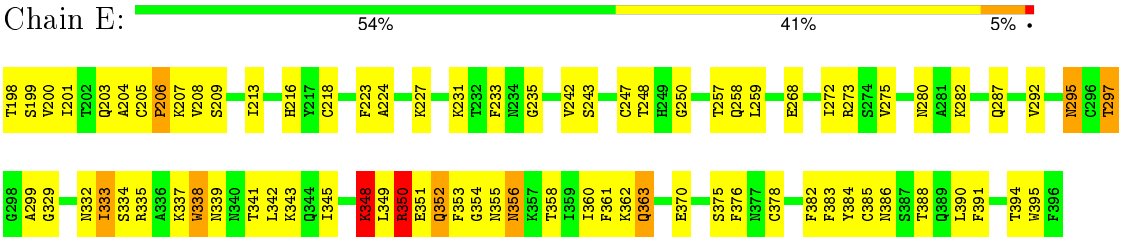
- Molecule 2: HIV-1 envelope glycoprotein gp120

Chain B:



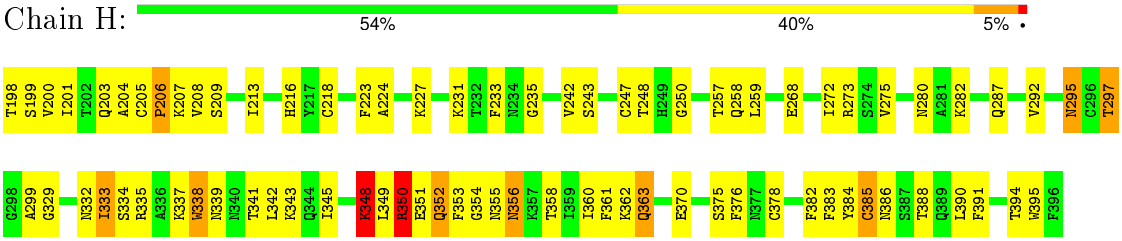
- Molecule 2: HIV-1 envelope glycoprotein gp120

Chain E:



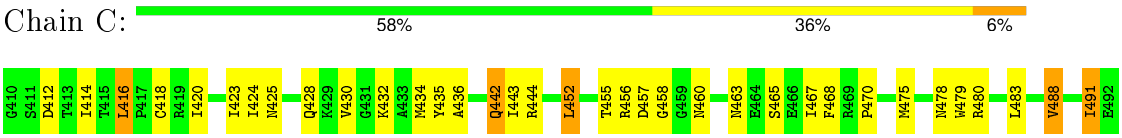
- Molecule 2: HIV-1 envelope glycoprotein gp120

Chain H:



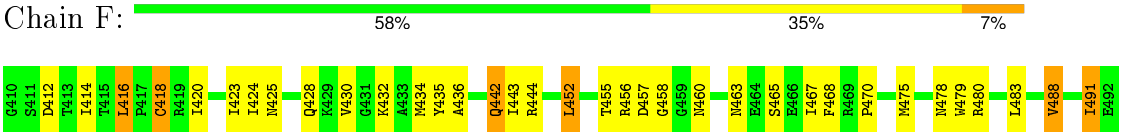
- Molecule 3: HIV-1 envelope glycoprotein gp120

Chain C:



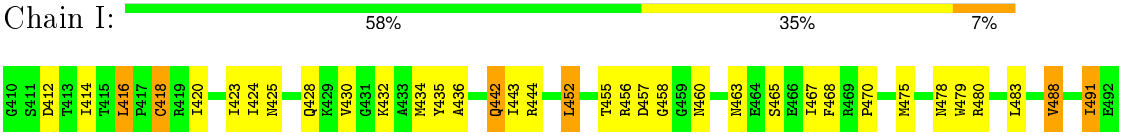
- Molecule 3: HIV-1 envelope glycoprotein gp120

Chain F:



- Molecule 3: HIV-1 envelope glycoprotein gp120

Chain I:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	No CTF correction applied	Depositor
Microscope	FEI Polara G2	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	8000	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	34000	Depositor
Image detector	CCD	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	0.41	0/300	0.82	0/406
1	D	0.42	0/300	0.81	0/406
1	G	0.42	0/300	0.81	0/406
2	B	0.39	0/1328	0.73	0/1805
2	E	0.40	0/1328	0.73	0/1805
2	H	0.40	0/1328	0.73	0/1805
3	C	0.37	0/663	0.70	0/890
3	F	0.38	0/663	0.70	0/890
3	I	0.38	0/663	0.70	0/890
All	All	0.39	0/6873	0.73	0/9303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	293	0	280	21	0
1	D	293	0	280	19	0
1	G	293	0	280	21	0
2	B	1301	0	1271	74	0
2	E	1301	0	1271	75	0
2	H	1301	0	1271	76	0
3	C	652	0	655	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	652	0	655	38	0
3	I	652	0	655	40	0
All	All	6738	0	6618	298	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 23.

All (298) 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:124:PRO:HD2	2:B:198:THR:HA	1.52	0.91
1:D:124:PRO:HD2	2:E:198:THR:HA	1.52	0.90
1:G:124:PRO:HD2	2:H:198:THR:HA	1.52	0.90
2:B:363:GLN:HE21	3:C:470:PRO:HG3	1.43	0.82
2:H:363:GLN:HE21	3:I:470:PRO:HG3	1.43	0.81
2:E:363:GLN:HE21	3:F:470:PRO:HG3	1.44	0.81
2:H:349:LEU:HB3	3:I:468:PHE:CZ	2.17	0.80
2:B:349:LEU:HB3	3:C:468:PHE:CZ	2.17	0.80
2:E:349:LEU:HB3	3:F:468:PHE:CZ	2.17	0.79
2:B:348:LYS:HA	2:B:353:PHE:HA	1.67	0.76
2:H:348:LYS:HA	2:H:353:PHE:HA	1.67	0.74
2:B:280:ASN:HD22	3:C:458:GLY:HA3	1.53	0.74
2:E:348:LYS:HA	2:E:353:PHE:HA	1.67	0.73
2:E:280:ASN:HD22	3:F:458:GLY:HA3	1.53	0.73
2:H:280:ASN:HD22	3:I:458:GLY:HA3	1.53	0.72
2:E:335:ARG:CZ	3:F:412:ASP:HB3	2.21	0.70
2:B:335:ARG:CZ	3:C:412:ASP:HB3	2.21	0.70
2:H:335:ARG:CZ	3:I:412:ASP:HB3	2.21	0.70
2:H:350:ARG:HG3	3:I:456:ARG:HD2	1.75	0.69
2:B:350:ARG:HG3	3:C:456:ARG:HD2	1.75	0.68
2:B:350:ARG:HG3	3:C:456:ARG:CD	2.24	0.68
2:E:350:ARG:HG3	3:F:456:ARG:CD	2.24	0.68
2:E:350:ARG:HG3	3:F:456:ARG:HD2	1.75	0.68
2:H:350:ARG:HG3	3:I:456:ARG:CD	2.24	0.67
2:H:207:LYS:HD3	3:I:436:ALA:HB3	1.78	0.66
2:H:231:LYS:NZ	2:H:268:GLU:HG3	2.11	0.66
2:B:333:ILE:HD11	2:B:338:TRP:CG	2.31	0.66
2:E:360:ILE:HG12	2:E:394:THR:HG23	1.78	0.66
2:E:207:LYS:HD3	3:F:436:ALA:HB3	1.78	0.66
2:H:292:VAL:HG11	2:H:338:TRP:HD1	1.61	0.66
2:B:231:LYS:NZ	2:B:268:GLU:HG3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:333:ILE:HD11	2:H:338:TRP:CG	2.31	0.65
2:B:292:VAL:HG11	2:B:338:TRP:HD1	1.61	0.65
2:E:292:VAL:HG11	2:E:338:TRP:HD1	1.61	0.65
2:E:333:ILE:HD11	2:E:338:TRP:CG	2.31	0.65
2:B:358:THR:HB	3:C:465:SER:OG	1.97	0.65
2:E:231:LYS:NZ	2:E:268:GLU:HG3	2.11	0.65
2:B:207:LYS:HD3	3:C:436:ALA:HB3	1.78	0.65
2:H:360:ILE:HG12	2:H:394:THR:HG23	1.78	0.64
2:H:358:THR:HB	3:I:465:SER:OG	1.97	0.64
2:H:362:LYS:HE2	3:I:467:ILE:HG12	1.80	0.64
3:F:442:GLN:NE2	3:F:444:ARG:HD2	2.13	0.64
2:B:360:ILE:HG12	2:B:394:THR:HG23	1.78	0.64
2:E:358:THR:HB	3:F:465:SER:OG	1.96	0.64
3:I:442:GLN:NE2	3:I:444:ARG:HD2	2.13	0.63
3:C:442:GLN:NE2	3:C:444:ARG:HD2	2.13	0.63
2:E:362:LYS:HE2	3:F:467:ILE:HG12	1.80	0.63
2:B:362:LYS:HE2	3:C:467:ILE:HG12	1.80	0.62
2:E:333:ILE:HD11	2:E:338:TRP:CD1	2.36	0.60
2:B:333:ILE:HD11	2:B:338:TRP:CD1	2.36	0.60
2:H:355:ASN:O	2:H:356:ASN:HB2	2.02	0.60
2:H:333:ILE:HD11	2:H:338:TRP:CD1	2.36	0.59
2:E:218:CYS:HA	2:E:247:CYS:HA	1.83	0.59
1:A:95:MET:HE2	1:A:96:TRP:H	1.68	0.59
1:D:95:MET:HE2	1:D:96:TRP:H	1.68	0.59
2:E:355:ASN:O	2:E:356:ASN:HB2	2.01	0.59
1:D:118:PRO:C	2:E:205:CYS:SG	2.81	0.59
2:H:218:CYS:HA	2:H:247:CYS:HA	1.84	0.59
2:B:218:CYS:HA	2:B:247:CYS:HA	1.84	0.59
2:B:355:ASN:O	2:B:356:ASN:HB2	2.02	0.59
1:A:118:PRO:C	2:B:205:CYS:SG	2.81	0.59
1:G:118:PRO:C	2:H:205:CYS:SG	2.81	0.58
1:G:95:MET:HE2	1:G:96:TRP:H	1.68	0.58
1:D:118:PRO:HB3	3:F:435:TYR:CZ	2.39	0.58
2:E:343:LYS:HB3	2:E:395:TRP:CZ3	2.39	0.58
1:A:109:ILE:HG23	3:C:428:GLN:HG2	1.86	0.58
1:A:118:PRO:HD2	2:B:203:GLN:HE22	1.69	0.58
2:H:351:GLU:O	2:H:352:GLN:HB2	2.04	0.57
1:D:118:PRO:HD2	2:E:203:GLN:HE22	1.69	0.57
1:G:118:PRO:HB3	3:I:435:TYR:CZ	2.39	0.57
2:E:351:GLU:O	2:E:352:GLN:HB2	2.04	0.57
1:G:109:ILE:HG23	3:I:428:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:363:GLN:HG3	2:E:388:THR:HA	1.87	0.57
2:B:343:LYS:HB3	2:B:395:TRP:CZ3	2.39	0.57
2:H:343:LYS:HB3	2:H:395:TRP:CZ3	2.39	0.57
1:A:118:PRO:HB3	3:C:435:TYR:CZ	2.39	0.57
2:H:273:ARG:HH22	2:H:287:GLN:NE2	2.03	0.57
1:G:118:PRO:HD2	2:H:203:GLN:HE22	1.69	0.56
1:D:109:ILE:HG23	3:F:428:GLN:HG2	1.86	0.56
2:B:273:ARG:HH22	2:B:287:GLN:NE2	2.04	0.56
2:E:273:ARG:HH22	2:E:287:GLN:NE2	2.04	0.56
2:H:363:GLN:HG3	2:H:388:THR:HA	1.88	0.56
2:B:351:GLU:O	2:B:352:GLN:HB2	2.05	0.56
2:B:363:GLN:HG3	2:B:388:THR:HA	1.87	0.56
1:D:105:HIS:HA	3:F:479:TRP:HE1	1.72	0.55
2:H:338:TRP:HZ3	2:H:390:LEU:O	1.90	0.55
2:E:352:GLN:HA	2:E:352:GLN:NE2	2.22	0.55
2:E:204:ALA:O	2:E:206:PRO:HD3	2.07	0.54
2:B:338:TRP:HZ3	2:B:390:LEU:O	1.90	0.54
3:F:457:ASP:HB2	3:F:467:ILE:HB	1.90	0.54
1:G:105:HIS:HA	3:I:479:TRP:HE1	1.73	0.54
2:H:349:LEU:O	2:H:351:GLU:N	2.41	0.54
2:B:352:GLN:NE2	2:B:352:GLN:HA	2.23	0.54
2:B:204:ALA:O	2:B:206:PRO:HD3	2.07	0.54
1:A:105:HIS:HA	3:C:479:TRP:HE1	1.72	0.54
2:E:349:LEU:O	2:E:351:GLU:N	2.41	0.54
2:H:352:GLN:NE2	2:H:352:GLN:HA	2.22	0.54
2:B:349:LEU:O	2:B:351:GLU:N	2.41	0.54
2:E:338:TRP:HZ3	2:E:390:LEU:O	1.90	0.54
2:E:335:ARG:NE	3:F:412:ASP:HB3	2.23	0.53
2:B:349:LEU:HD13	3:C:468:PHE:CD1	2.43	0.53
2:B:335:ARG:NE	3:C:412:ASP:HB3	2.23	0.53
1:A:111:LEU:O	1:A:114:GLN:HG2	2.09	0.53
2:H:204:ALA:O	2:H:206:PRO:HD3	2.07	0.53
2:H:335:ARG:NE	3:I:412:ASP:HB3	2.24	0.53
2:E:349:LEU:HD13	3:F:468:PHE:CD1	2.43	0.53
3:C:457:ASP:HB2	3:C:467:ILE:HB	1.90	0.53
2:H:349:LEU:HD13	3:I:468:PHE:CD1	2.43	0.53
2:E:224:ALA:HB2	3:F:491:ILE:HG13	1.91	0.53
2:H:231:LYS:HD2	2:H:268:GLU:HG3	1.90	0.53
1:G:111:LEU:O	1:G:114:GLN:HG2	2.09	0.52
3:I:457:ASP:HB2	3:I:467:ILE:HB	1.90	0.52
2:H:224:ALA:HB2	3:I:491:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:LEU:O	1:D:114:GLN:HG2	2.09	0.52
2:E:378:CYS:HB3	2:E:383:PHE:CE1	2.44	0.52
2:H:378:CYS:HB3	2:H:383:PHE:CD1	2.45	0.52
2:H:231:LYS:HZ2	2:H:268:GLU:HG3	1.73	0.52
2:B:378:CYS:HB3	2:B:383:PHE:CD1	2.45	0.52
2:B:378:CYS:HB3	2:B:383:PHE:CE1	2.45	0.52
1:G:120:VAL:HG12	1:G:121:LYS:N	2.25	0.52
2:E:378:CYS:HB3	2:E:383:PHE:CD1	2.45	0.52
2:B:231:LYS:HD2	2:B:268:GLU:HG3	1.91	0.52
2:H:378:CYS:HB3	2:H:383:PHE:CE1	2.45	0.52
2:B:339:ASN:HA	2:B:342:LEU:HD12	1.92	0.52
2:E:339:ASN:HA	2:E:342:LEU:HD12	1.92	0.52
2:E:231:LYS:HD2	2:E:268:GLU:HG3	1.91	0.51
2:B:233:PHE:O	2:B:273:ARG:NH1	2.44	0.51
1:D:117:LYS:O	2:E:206:PRO:HD2	2.10	0.51
1:A:120:VAL:HG12	1:A:121:LYS:N	2.25	0.51
2:H:297:THR:HA	3:I:443:ILE:O	2.11	0.51
2:B:384:TYR:OH	3:C:424:ILE:HG22	2.11	0.51
2:E:370:GLU:HA	2:E:375:SER:OG	2.10	0.51
3:I:475:MET:O	3:I:478:ASN:HB2	2.11	0.51
2:E:384:TYR:OH	3:F:424:ILE:HG22	2.11	0.51
2:H:341:THR:O	2:H:345:ILE:HG13	2.10	0.51
2:B:341:THR:O	2:B:345:ILE:HG13	2.11	0.51
2:B:224:ALA:HB2	3:C:491:ILE:HG13	1.91	0.51
1:G:117:LYS:O	2:H:206:PRO:HD2	2.10	0.51
2:H:370:GLU:HA	2:H:375:SER:OG	2.10	0.51
2:H:275:VAL:HB	2:H:282:LYS:HD3	1.93	0.51
2:H:384:TYR:OH	3:I:424:ILE:HG22	2.11	0.51
2:H:233:PHE:O	2:H:273:ARG:NH1	2.44	0.51
3:C:475:MET:O	3:C:478:ASN:HB2	2.11	0.51
1:D:120:VAL:HG12	1:D:121:LYS:N	2.25	0.51
2:E:341:THR:O	2:E:345:ILE:HG13	2.11	0.51
2:E:297:THR:HA	3:F:443:ILE:O	2.11	0.51
2:E:350:ARG:C	2:E:350:ARG:HD3	2.32	0.51
2:B:275:VAL:HB	2:B:282:LYS:HD3	1.93	0.51
1:A:117:LYS:O	2:B:206:PRO:HD2	2.10	0.50
2:E:208:VAL:HG22	2:E:209:SER:H	1.76	0.50
2:H:208:VAL:HG22	2:H:209:SER:H	1.76	0.50
2:E:233:PHE:O	2:E:273:ARG:NH1	2.44	0.50
3:F:475:MET:O	3:F:478:ASN:HB2	2.11	0.50
2:H:350:ARG:C	2:H:350:ARG:HD3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:ARG:C	2:H:352:GLN:N	2.63	0.50
2:B:297:THR:HA	3:C:443:ILE:O	2.11	0.50
3:C:460:ASN:ND2	3:C:463:ASN:HB3	2.27	0.50
2:B:350:ARG:HD3	2:B:350:ARG:C	2.32	0.50
2:B:370:GLU:HA	2:B:375:SER:OG	2.10	0.50
3:F:460:ASN:ND2	3:F:463:ASN:HB3	2.27	0.50
2:H:339:ASN:HA	2:H:342:LEU:HD12	1.92	0.50
2:B:350:ARG:C	2:B:352:GLN:N	2.63	0.49
2:H:216:HIS:CE1	2:H:250:GLY:HA2	2.48	0.49
3:I:460:ASN:ND2	3:I:463:ASN:HB3	2.27	0.49
2:E:275:VAL:HB	2:E:282:LYS:HD3	1.93	0.49
2:B:208:VAL:HG22	2:B:209:SER:H	1.77	0.49
2:H:361:PHE:HD2	2:H:395:TRP:HE1	1.61	0.49
2:E:216:HIS:CE1	2:E:250:GLY:HA2	2.48	0.48
2:B:231:LYS:HZ2	2:B:268:GLU:HG3	1.75	0.48
2:B:361:PHE:HD2	2:B:395:TRP:HE1	1.61	0.48
2:E:376:PHE:HE2	2:E:378:CYS:HB2	1.79	0.48
2:B:216:HIS:CE1	2:B:250:GLY:HA2	2.48	0.48
2:E:231:LYS:HZ2	2:E:268:GLU:HG3	1.78	0.48
2:E:350:ARG:C	2:E:352:GLN:N	2.64	0.48
2:E:361:PHE:HD2	2:E:395:TRP:HE1	1.61	0.48
2:H:376:PHE:HE2	2:H:378:CYS:HB2	1.78	0.48
2:B:391:PHE:CE1	3:C:452:LEU:HD21	2.49	0.48
2:H:201:ILE:HG22	2:H:203:GLN:HG3	1.96	0.47
2:B:376:PHE:HE2	2:B:378:CYS:HB2	1.78	0.47
2:E:375:SER:HA	2:E:383:PHE:O	2.14	0.47
2:B:375:SER:HA	2:B:383:PHE:O	2.14	0.47
2:E:257:THR:O	2:E:259:LEU:N	2.48	0.47
2:E:391:PHE:CE1	3:F:452:LEU:HD21	2.49	0.47
3:I:430:VAL:O	3:I:430:VAL:HG12	2.15	0.47
2:H:375:SER:HA	2:H:383:PHE:O	2.14	0.47
2:H:391:PHE:CE1	3:I:452:LEU:HD21	2.49	0.47
2:B:201:ILE:HG22	2:B:203:GLN:HG3	1.96	0.46
1:D:118:PRO:HB3	3:F:435:TYR:CE2	2.50	0.46
2:E:382:PHE:O	3:F:420:ILE:HA	2.16	0.46
3:F:430:VAL:HG12	3:F:430:VAL:O	2.15	0.46
2:B:382:PHE:O	3:C:420:ILE:HA	2.16	0.46
2:E:201:ILE:HG22	2:E:203:GLN:HG3	1.96	0.46
1:A:118:PRO:HB3	3:C:435:TYR:CE2	2.50	0.46
2:H:334:SER:HB2	2:H:337:LYS:HB2	1.98	0.46
2:H:382:PHE:O	3:I:420:ILE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:LYS:O	2:H:242:VAL:HG23	2.16	0.46
1:D:101:VAL:HG11	3:F:480:ARG:HH21	1.81	0.46
1:G:118:PRO:HB3	3:I:435:TYR:CE2	2.50	0.46
1:A:100:MET:HB2	3:C:483:LEU:HD13	1.98	0.46
2:B:227:LYS:O	2:B:242:VAL:HG23	2.16	0.46
2:B:280:ASN:ND2	3:C:458:GLY:HA3	2.27	0.46
3:F:442:GLN:HE22	3:F:444:ARG:HD2	1.80	0.46
2:E:227:LYS:O	2:E:242:VAL:HG23	2.16	0.45
1:G:100:MET:HB2	3:I:483:LEU:HD13	1.98	0.45
2:H:231:LYS:HD2	2:H:268:GLU:CG	2.46	0.45
2:H:272:ILE:O	2:H:273:ARG:HG3	2.16	0.45
1:D:121:LYS:HG3	2:E:200:VAL:HG12	1.98	0.45
3:C:430:VAL:O	3:C:430:VAL:HG12	2.16	0.45
1:D:100:MET:HB2	3:F:483:LEU:HD13	1.98	0.45
2:B:335:ARG:HA	3:C:414:ILE:HG13	1.99	0.45
2:H:335:ARG:HA	3:I:414:ILE:HG13	1.99	0.45
2:E:231:LYS:HD2	2:E:268:GLU:CG	2.47	0.45
1:A:121:LYS:HG3	2:B:200:VAL:HG12	1.99	0.45
2:E:334:SER:HB2	2:E:337:LYS:HB2	1.98	0.45
1:G:101:VAL:HG11	3:I:480:ARG:HH21	1.81	0.45
2:E:272:ILE:O	2:E:273:ARG:HG3	2.16	0.45
2:E:335:ARG:HA	3:F:414:ILE:HG13	1.99	0.45
2:B:231:LYS:HD2	2:B:268:GLU:CG	2.47	0.45
1:G:121:LYS:HG3	2:H:200:VAL:HG12	1.98	0.45
1:A:101:VAL:HG11	3:C:480:ARG:HH21	1.81	0.44
2:B:334:SER:HB2	2:B:337:LYS:HB2	1.98	0.44
2:B:386:ASN:O	3:C:416:LEU:HG	2.18	0.44
2:B:272:ILE:O	2:B:273:ARG:HG3	2.16	0.44
2:E:223:PHE:HB3	3:F:488:VAL:HG22	1.99	0.44
2:H:223:PHE:HB3	3:I:488:VAL:HG22	1.99	0.44
2:E:351:GLU:OE1	2:E:354:GLY:HA3	2.18	0.44
2:H:351:GLU:OE1	2:H:354:GLY:HA3	2.18	0.44
2:E:386:ASN:O	3:F:416:LEU:HG	2.18	0.44
2:H:386:ASN:O	3:I:416:LEU:HG	2.18	0.44
2:H:376:PHE:CE2	2:H:378:CYS:HB2	2.53	0.43
1:A:105:HIS:HA	3:C:479:TRP:NE1	2.34	0.43
2:E:376:PHE:CE2	2:E:378:CYS:HB2	2.54	0.43
2:H:257:THR:O	2:H:259:LEU:N	2.47	0.43
2:B:371:ILE:HA	2:B:371:ILE:HD13	1.79	0.43
2:E:280:ASN:ND2	3:F:458:GLY:HA3	2.27	0.43
3:I:442:GLN:HE22	3:I:444:ARG:HD2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:THR:O	2:B:259:LEU:N	2.48	0.43
1:D:122:LEU:HG	2:E:199:SER:OG	2.19	0.43
3:F:414:ILE:HG22	3:F:416:LEU:HD13	2.01	0.43
2:B:223:PHE:HB3	3:C:488:VAL:HG22	1.99	0.43
2:B:351:GLU:OE1	2:B:354:GLY:HA3	2.18	0.43
1:G:105:HIS:HA	3:I:479:TRP:NE1	2.34	0.43
3:C:442:GLN:HE22	3:C:444:ARG:HD2	1.80	0.43
2:B:376:PHE:CE2	2:B:378:CYS:HB2	2.54	0.43
2:H:329:GLY:O	3:I:418:CYS:N	2.47	0.42
3:C:414:ILE:HG22	3:C:416:LEU:HD13	2.01	0.42
1:A:122:LEU:HG	2:B:199:SER:OG	2.19	0.42
2:H:280:ASN:ND2	3:I:458:GLY:HA3	2.27	0.42
3:I:414:ILE:HG22	3:I:416:LEU:HD13	2.01	0.42
1:G:122:LEU:HG	2:H:199:SER:OG	2.19	0.42
1:A:118:PRO:HB2	1:A:119:CYS:H	1.63	0.42
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.87	0.42
3:C:425:ASN:OD1	3:C:432:LYS:HE2	2.20	0.42
2:E:257:THR:C	2:E:259:LEU:H	2.23	0.42
3:I:425:ASN:OD1	3:I:432:LYS:HE2	2.19	0.42
1:D:105:HIS:HA	3:F:479:TRP:NE1	2.33	0.42
3:I:423:ILE:HG22	3:I:432:LYS:HD2	2.02	0.42
3:F:423:ILE:HD13	3:F:434:MET:HB2	2.02	0.42
2:B:333:ILE:HD11	2:B:338:TRP:HB2	2.02	0.42
2:E:257:THR:HG21	2:E:370:GLU:O	2.20	0.42
2:E:242:VAL:HG22	2:E:243:SER:N	2.35	0.42
2:H:363:GLN:NE2	3:I:470:PRO:HG3	2.23	0.41
1:A:100:MET:O	1:A:104:MET:N	2.49	0.41
2:H:257:THR:HG21	2:H:370:GLU:O	2.20	0.41
2:H:242:VAL:HG22	2:H:243:SER:N	2.35	0.41
2:H:355:ASN:O	2:H:356:ASN:CB	2.69	0.41
2:H:257:THR:C	2:H:259:LEU:H	2.23	0.41
2:B:242:VAL:HG22	2:B:243:SER:N	2.35	0.41
2:B:295:ASN:OD1	2:B:295:ASN:N	2.53	0.41
2:E:295:ASN:N	2:E:295:ASN:OD1	2.54	0.41
1:G:97:LYS:HG3	1:G:98:ASN:ND2	2.36	0.41
1:A:97:LYS:HG3	1:A:98:ASN:ND2	2.36	0.41
1:D:97:LYS:HG3	1:D:98:ASN:N	2.36	0.41
2:H:333:ILE:HD11	2:H:338:TRP:HB2	2.02	0.41
3:F:425:ASN:OD1	3:F:432:LYS:HE2	2.20	0.41
2:H:295:ASN:OD1	2:H:295:ASN:N	2.53	0.41
2:H:385:CYS:HA	3:I:418:CYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:THR:HG21	2:B:370:GLU:O	2.21	0.41
1:G:122:LEU:N	1:G:122:LEU:HD23	2.36	0.41
3:I:423:ILE:HD13	3:I:434:MET:HB2	2.02	0.41
1:A:97:LYS:HG3	1:A:98:ASN:N	2.36	0.41
2:E:349:LEU:HA	2:E:349:LEU:HD23	1.87	0.41
2:B:257:THR:C	2:B:259:LEU:H	2.23	0.41
3:C:423:ILE:HG22	3:C:432:LYS:HD2	2.02	0.41
1:G:105:HIS:O	1:G:109:ILE:HG13	2.22	0.41
2:E:235:GLY:H	2:E:273:ARG:HD3	1.86	0.41
1:G:97:LYS:HG3	1:G:98:ASN:N	2.36	0.41
1:D:122:LEU:N	1:D:122:LEU:HD23	2.36	0.40
3:C:423:ILE:HD13	3:C:434:MET:HB2	2.02	0.40
1:D:97:LYS:HG3	1:D:98:ASN:ND2	2.36	0.40
2:E:333:ILE:HD11	2:E:338:TRP:HB2	2.02	0.40
2:E:338:TRP:CZ3	2:E:390:LEU:O	2.74	0.40
1:A:120:VAL:HG12	1:A:121:LYS:H	1.86	0.40
3:F:423:ILE:HG22	3:F:432:LYS:HD2	2.02	0.40
2:E:329:GLY:O	3:F:418:CYS:N	2.47	0.40
2:B:355:ASN:O	2:B:356:ASN:CB	2.69	0.40
2:H:235:GLY:H	2:H:273:ARG:HD3	1.86	0.40
1:G:120:VAL:HG12	1:G:121:LYS:H	1.85	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	33/35 (94%)	21 (64%)	10 (30%)	2 (6%)	2 26
1	D	33/35 (94%)	22 (67%)	9 (27%)	2 (6%)	2 26
1	G	33/35 (94%)	21 (64%)	10 (30%)	2 (6%)	2 26
2	B	168/170 (99%)	139 (83%)	21 (12%)	8 (5%)	3 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	168/170 (99%)	139 (83%)	21 (12%)	8 (5%)	3 32
2	H	168/170 (99%)	139 (83%)	21 (12%)	8 (5%)	3 32
3	C	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
3	F	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
3	I	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
All	All	846/864 (98%)	703 (83%)	113 (13%)	30 (4%)	8 39

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	118	PRO
2	B	258	GLN
2	B	350	ARG
2	B	352	GLN
1	D	99	ASP
1	D	118	PRO
2	E	258	GLN
2	E	350	ARG
2	E	352	GLN
1	G	99	ASP
1	G	118	PRO
2	H	258	GLN
2	H	350	ARG
2	H	352	GLN
2	B	248	THR
2	B	348	LYS
2	E	248	THR
2	E	348	LYS
2	H	248	THR
2	H	348	LYS
2	B	356	ASN
2	E	356	ASN
2	H	356	ASN
2	B	299	ALA
2	E	299	ALA
2	H	299	ALA
2	B	206	PRO
2	H	206	PRO
2	E	206	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	35/35 (100%)	30 (86%)	5 (14%)	4	25
1	D	35/35 (100%)	30 (86%)	5 (14%)	4	25
1	G	35/35 (100%)	30 (86%)	5 (14%)	4	25
2	B	149/149 (100%)	139 (93%)	10 (7%)	20	57
2	E	149/149 (100%)	139 (93%)	10 (7%)	20	57
2	H	149/149 (100%)	139 (93%)	10 (7%)	20	57
3	C	72/72 (100%)	65 (90%)	7 (10%)	10	40
3	F	72/72 (100%)	65 (90%)	7 (10%)	10	40
3	I	72/72 (100%)	65 (90%)	7 (10%)	10	40
All	All	768/768 (100%)	702 (91%)	66 (9%)	18	47

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	MET
1	A	98	ASN
1	A	103	GLN
1	A	118	PRO
1	A	122	LEU
2	B	213	ILE
2	B	295	ASN
2	B	297	THR
2	B	332	ASN
2	B	333	ILE
2	B	338	TRP
2	B	348	LYS
2	B	350	ARG
2	B	363	GLN
2	B	385	CYS
3	C	416	LEU
3	C	418	CYS
3	C	442	GLN

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Mol	Chain	Res	Type
3	C	452	LEU
3	C	455	THR
3	C	488	VAL
3	C	491	ILE
1	D	95	MET
1	D	98	ASN
1	D	103	GLN
1	D	118	PRO
1	D	122	LEU
2	E	213	ILE
2	E	295	ASN
2	E	297	THR
2	E	332	ASN
2	E	333	ILE
2	E	338	TRP
2	E	348	LYS
2	E	350	ARG
2	E	363	GLN
2	E	385	CYS
3	F	416	LEU
3	F	418	CYS
3	F	442	GLN
3	F	452	LEU
3	F	455	THR
3	F	488	VAL
3	F	491	ILE
1	G	95	MET
1	G	98	ASN
1	G	103	GLN
1	G	118	PRO
1	G	122	LEU
2	H	213	ILE
2	H	295	ASN
2	H	297	THR
2	H	332	ASN
2	H	333	ILE
2	H	338	TRP
2	H	348	LYS
2	H	350	ARG
2	H	363	GLN
2	H	385	CYS
3	I	416	LEU

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Mol	Chain	Res	Type
3	I	418	CYS
3	I	442	GLN
3	I	452	LEU
3	I	455	THR
3	I	488	VAL
3	I	491	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
2	B	203	GLN
2	B	287	GLN
2	B	352	GLN
2	B	355	ASN
2	B	363	GLN
2	B	389	GLN
3	C	442	GLN
3	C	462	ASN
3	C	478	ASN
1	D	98	ASN
2	E	203	GLN
2	E	287	GLN
2	E	352	GLN
2	E	355	ASN
2	E	363	GLN
2	E	389	GLN
3	F	442	GLN
3	F	462	ASN
3	F	478	ASN
1	G	98	ASN
2	H	203	GLN
2	H	287	GLN
2	H	352	GLN
2	H	355	ASN
2	H	363	GLN
2	H	389	GLN
3	I	442	GLN
3	I	462	ASN
3	I	478	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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.