wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:46 PM BST

PDB ID	:	3J41
EMDB ID:	:	EMD-5679
Title	:	Pseudo-atomic model of the Aquaporin-0/Calmodulin complex derived from electron microscopy
Authors	:	Reichow, S.L.; Clemens, D.M.; Freites, J.A.; Nemeth-Cahalan, K.L.; Heyden, M.; Tobias, D.J.; Hall, J.E.; Gonen, T.
Deposited on	:	2013-05-31
Resolution	:	25.00 Å(reported)
Based on PDB ID	:	1NWD, 2B6P

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

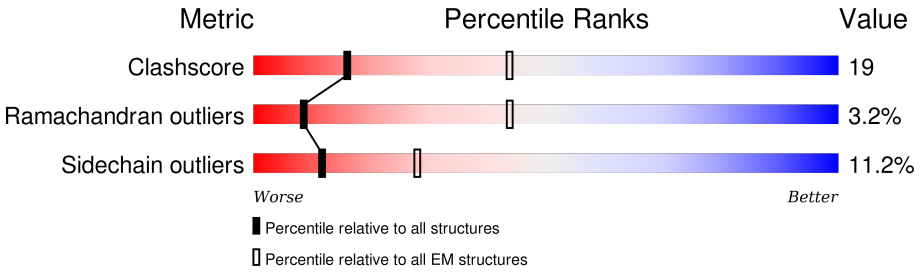
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 25.00 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	263	55% 28% 5% • 11%
1	B	263	56% 27% 6% • 11%
1	C	263	55% 27% 6% • 11%
1	D	263	56% 25% 6% • 11%
2	E	149	66% 24% 5% •
2	F	149	67% 23% 6% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9338 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 Lens fiber major intrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1768	1169	300	292	7		
1	B	233	Total	C	N	O	S	0	0
			1768	1169	300	292	7		
1	C	233	Total	C	N	O	S	0	0
			1768	1169	300	292	7		
1	D	233	Total	C	N	O	S	0	0
			1768	1169	300	292	7		

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	143	Total	C	N	O	S	0	0
			1129	692	182	246	9		
2	F	143	Total	C	N	O	S	0	0
			1129	692	182	246	9		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

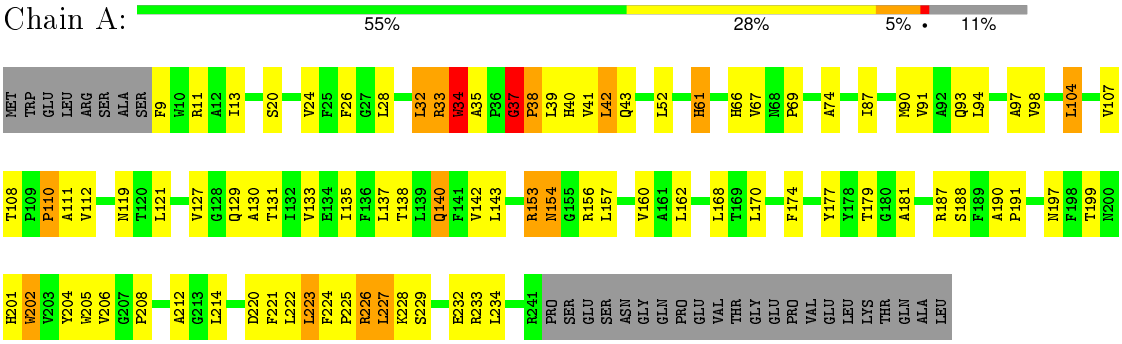
Mol	Chain	Residues	Atoms		AltConf
3	F	4	Total	Ca	0
			4	4	
3	E	4	Total	Ca	0
			4	4	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

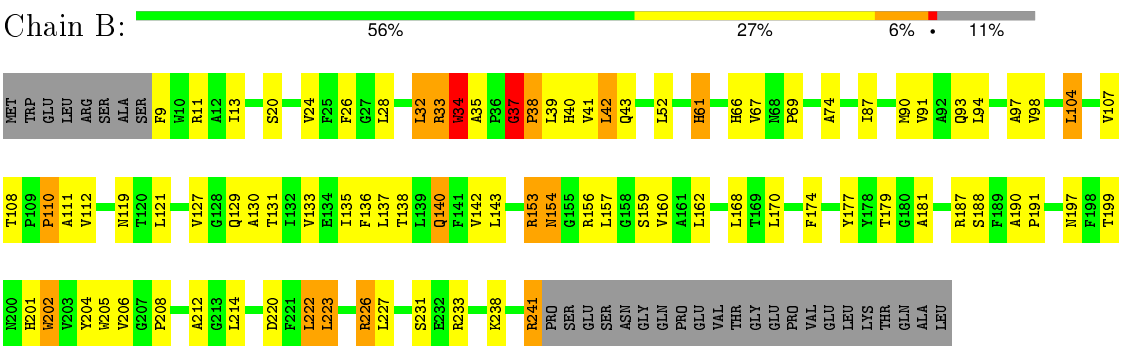
- Molecule 1: Lens fiber major intrinsic protein

Chain A:



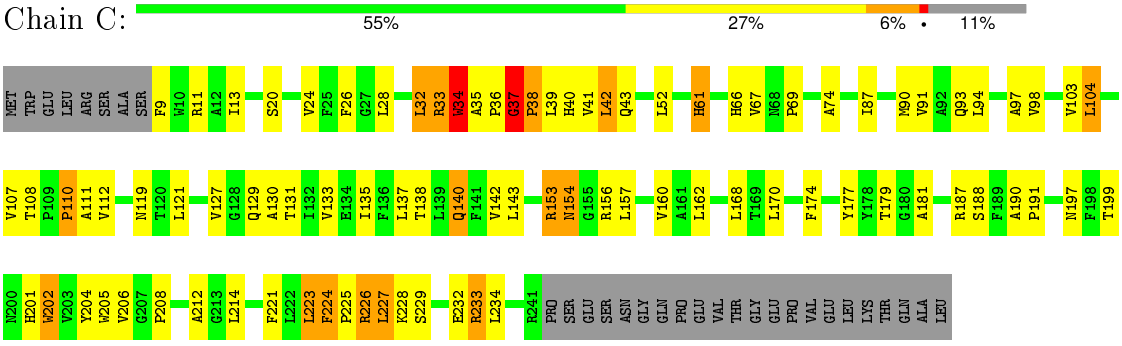
- Molecule 1: Lens fiber major intrinsic protein

Chain B:



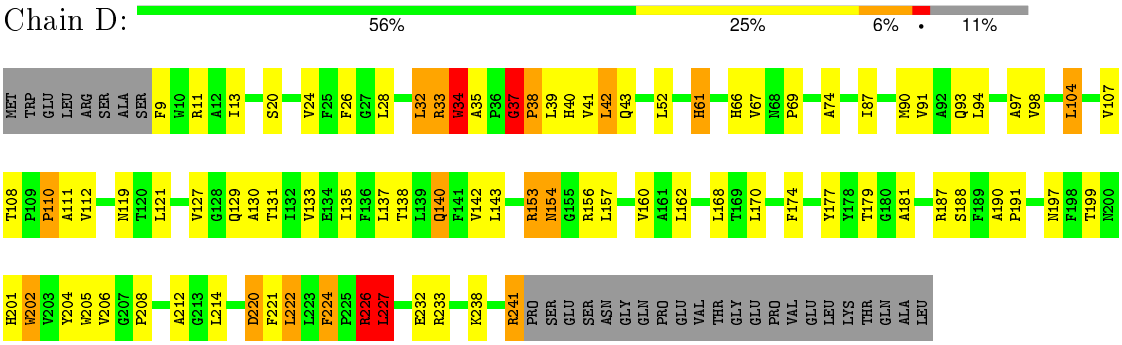
- Molecule 1: Lens fiber major intrinsic protein

Chain C:



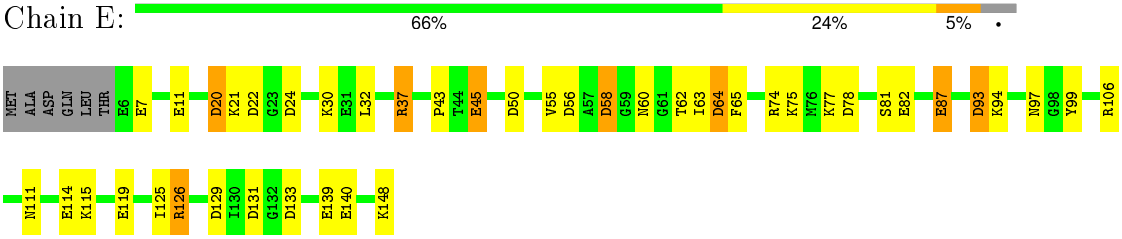
- Molecule 1: Lens fiber major intrinsic protein

Chain D:



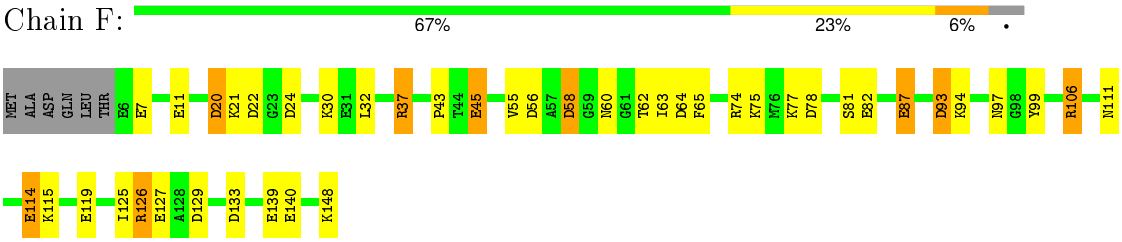
- Molecule 2: Calmodulin

Chain E:



- Molecule 2: Calmodulin

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	11720	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	CTF-TILT, each micrograph	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.46	0/1817	0.79	5/2478 (0.2%)
1	B	0.46	0/1817	0.79	4/2478 (0.2%)
1	C	0.46	0/1817	0.79	4/2478 (0.2%)
1	D	0.46	0/1817	0.78	3/2478 (0.1%)
2	E	0.74	0/1141	1.21	9/1529 (0.6%)
2	F	0.73	0/1141	1.21	9/1529 (0.6%)
All	All	0.54	0/9550	0.90	34/12970 (0.3%)

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	7
1	B	0	6
1	C	0	8
1	D	0	9
2	E	0	25
2	F	0	25
All	All	0	80

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	74	ARG	NE-CZ-NH1	9.93	125.27	120.30
2	E	74	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	B	37	GLY	N-CA-C	8.27	133.77	113.10
1	C	37	GLY	N-CA-C	8.21	133.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	GLY	N-CA-C	8.20	133.60	113.10
1	D	37	GLY	N-CA-C	8.20	133.60	113.10
2	E	93	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	F	93	ASP	CB-CG-OD2	-7.29	111.74	118.30
2	E	58	ASP	OD1-CG-OD2	-6.10	111.72	123.30
2	E	106	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	F	106	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	E	20	ASP	OD1-CG-OD2	-5.99	111.92	123.30
2	E	140	GLU	OE1-CD-OE2	-5.97	116.14	123.30
2	F	20	ASP	OD1-CG-OD2	-5.96	111.98	123.30
2	F	140	GLU	OE1-CD-OE2	-5.94	116.17	123.30
2	F	58	ASP	OD1-CG-OD2	-5.90	112.09	123.30
1	C	233	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	233	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	223	LEU	CB-CA-C	5.59	120.82	110.20
2	F	37	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	E	87	GLU	OE1-CD-OE2	-5.54	116.65	123.30
2	F	87	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	D	233	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	223	LEU	C-N-CA	5.28	134.91	121.70
2	E	126	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	223	LEU	CB-CA-C	5.22	120.13	110.20
2	E	37	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	233	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	F	126	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	226	ARG	C-N-CA	5.07	134.36	121.70
1	B	37	GLY	O-C-N	-5.07	111.47	121.10
1	D	37	GLY	O-C-N	-5.05	111.51	121.10
1	C	37	GLY	O-C-N	-5.03	111.54	121.10
1	A	37	GLY	O-C-N	-5.01	111.57	121.10

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ASP	Sidechain
1	A	221	PHE	Mainchain,Peptide
1	A	232	GLU	Sidechain
1	A	34	TRP	Mainchain,Peptide
1	A	37	GLY	Mainchain
1	B	220	ASP	Sidechain
1	B	222	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	B	241	ARG	Sidechain
1	B	34	TRP	Mainchain,Peptide
1	B	37	GLY	Mainchain
1	C	221	PHE	Mainchain,Peptide
1	C	224	PHE	Mainchain
1	C	232	GLU	Sidechain
1	C	233	ARG	Mainchain
1	C	34	TRP	Mainchain,Peptide
1	C	37	GLY	Mainchain
1	D	220	ASP	Sidechain
1	D	222	LEU	Mainchain
1	D	226	ARG	Peptide
1	D	227	LEU	Mainchain
1	D	232	GLU	Sidechain
1	D	241	ARG	Sidechain
1	D	34	TRP	Mainchain,Peptide
1	D	37	GLY	Mainchain
2	E	114	GLU	Sidechain
2	E	119	GLU	Sidechain
2	E	125	ILE	Mainchain
2	E	126	ARG	Peptide
2	E	129	ASP	Sidechain
2	E	133	ASP	Sidechain
2	E	20	ASP	Sidechain
2	E	24	ASP	Sidechain
2	E	37	ARG	Sidechain
2	E	43	PRO	Peptide
2	E	45	GLU	Mainchain
2	E	50	ASP	Sidechain
2	E	55	VAL	Mainchain
2	E	56	ASP	Sidechain
2	E	58	ASP	Sidechain
2	E	63	ILE	Mainchain
2	E	64	ASP	Sidechain
2	E	7	GLU	Sidechain
2	E	78	ASP	Mainchain,Peptide
2	E	82	GLU	Sidechain
2	E	87	GLU	Sidechain,Mainchain
2	E	93	ASP	Sidechain
2	E	99	TYR	Sidechain
2	F	106	ARG	Sidechain
2	F	114	GLU	Sidechain

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Mol	Chain	Res	Type	Group
2	F	119	GLU	Sidechain
2	F	125	ILE	Mainchain
2	F	126	ARG	Peptide
2	F	127	GLU	Sidechain
2	F	129	ASP	Sidechain
2	F	133	ASP	Sidechain
2	F	20	ASP	Sidechain
2	F	24	ASP	Sidechain
2	F	37	ARG	Sidechain
2	F	43	PRO	Peptide
2	F	45	GLU	Mainchain
2	F	55	VAL	Mainchain
2	F	56	ASP	Sidechain
2	F	58	ASP	Sidechain
2	F	63	ILE	Mainchain
2	F	7	GLU	Sidechain
2	F	78	ASP	Mainchain,Peptide
2	F	82	GLU	Sidechain
2	F	87	GLU	Sidechain,Mainchain
2	F	93	ASP	Sidechain
2	F	99	TYR	Sidechain

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	1768	0	1805	97	0
1	B	1768	0	1805	97	0
1	C	1768	0	1805	101	0
1	D	1768	0	1805	94	0
2	E	1129	0	1058	2	0
2	F	1129	0	1058	2	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
All	All	9338	0	9336	351	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 19.

All (351) 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:B:133:VAL:HG23	1:C:107:VAL:HG11	1.56	0.88
1:A:133:VAL:HG23	1:B:107:VAL:HG11	1.56	0.86
1:C:133:VAL:HG23	1:D:107:VAL:HG11	1.57	0.86
1:A:107:VAL:HG11	1:D:133:VAL:HG23	1.56	0.86
1:C:154:ASN:HB2	1:C:157:LEU:HG	1.58	0.85
1:A:154:ASN:HB2	1:A:157:LEU:HG	1.58	0.85
1:B:154:ASN:HB2	1:B:157:LEU:HG	1.58	0.84
1:D:154:ASN:HB2	1:D:157:LEU:HG	1.58	0.82
1:D:197:ASN:OD1	1:D:199:THR:HG22	1.81	0.80
1:B:197:ASN:OD1	1:B:199:THR:HG22	1.81	0.80
1:A:197:ASN:OD1	1:A:199:THR:HG22	1.81	0.80
1:C:197:ASN:OD1	1:C:199:THR:HG22	1.81	0.80
1:A:37:GLY:HA3	1:A:177:TYR:HE1	1.48	0.79
1:D:37:GLY:HA3	1:D:177:TYR:HE1	1.48	0.78
1:B:37:GLY:HA3	1:B:177:TYR:HE1	1.48	0.78
1:C:37:GLY:HA3	1:C:177:TYR:HE1	1.48	0.77
1:C:33:ARG:HG3	1:C:34:TRP:N	2.04	0.72
1:D:33:ARG:HG3	1:D:34:TRP:N	2.04	0.72
1:B:33:ARG:HG3	1:B:34:TRP:N	2.04	0.71
1:C:153:ARG:HE	1:C:154:ASN:CG	1.94	0.71
1:D:153:ARG:HE	1:D:154:ASN:CG	1.94	0.71
1:A:153:ARG:HE	1:A:154:ASN:CG	1.94	0.70
1:B:153:ARG:HE	1:B:154:ASN:CG	1.94	0.70
1:B:104:LEU:O	1:B:108:THR:HG22	1.92	0.70
1:A:38:PRO:O	1:B:43:GLN:NE2	2.25	0.70
1:C:104:LEU:O	1:C:108:THR:HG22	1.92	0.70
1:C:38:PRO:O	1:D:43:GLN:NE2	2.26	0.69
1:D:104:LEU:O	1:D:108:THR:HG22	1.92	0.69
1:A:104:LEU:O	1:A:108:THR:HG22	1.92	0.69
1:A:33:ARG:HG3	1:A:34:TRP:N	2.04	0.69
1:A:43:GLN:NE2	1:D:38:PRO:O	2.26	0.69
1:D:67:VAL:HG12	1:D:67:VAL:O	1.93	0.68
1:B:38:PRO:O	1:C:43:GLN:NE2	2.27	0.68
1:C:67:VAL:O	1:C:67:VAL:HG12	1.93	0.68
1:A:67:VAL:HG12	1:A:67:VAL:O	1.93	0.68
1:B:67:VAL:HG12	1:B:67:VAL:O	1.93	0.68
1:D:61:HIS:CD2	1:D:61:HIS:H	2.13	0.66
1:D:190:ALA:HB3	1:D:191:PRO:HD3	1.78	0.66
1:B:190:ALA:HB3	1:B:191:PRO:HD3	1.78	0.65
1:C:190:ALA:HB3	1:C:191:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:HIS:H	1:B:61:HIS:CD2	2.13	0.64
1:A:190:ALA:HB3	1:A:191:PRO:HD3	1.78	0.64
1:B:154:ASN:CB	1:B:157:LEU:HG	2.28	0.64
1:C:61:HIS:CD2	1:C:61:HIS:H	2.13	0.64
1:C:33:ARG:HH21	1:C:40:HIS:HA	1.62	0.64
1:D:154:ASN:CB	1:D:157:LEU:HG	2.28	0.64
1:D:33:ARG:HH21	1:D:40:HIS:HA	1.62	0.64
1:A:61:HIS:H	1:A:61:HIS:CD2	2.13	0.64
1:A:129:GLN:HB3	1:B:107:VAL:HG13	1.80	0.64
1:C:154:ASN:CB	1:C:157:LEU:HG	2.28	0.63
1:C:133:VAL:O	1:C:137:LEU:HG	1.99	0.63
1:A:33:ARG:HH21	1:A:40:HIS:HA	1.62	0.63
1:B:133:VAL:O	1:B:137:LEU:HG	1.98	0.63
1:A:107:VAL:HG13	1:D:129:GLN:HB3	1.80	0.63
1:D:133:VAL:O	1:D:137:LEU:HG	1.98	0.63
1:B:33:ARG:HH21	1:B:40:HIS:HA	1.62	0.63
1:A:154:ASN:CB	1:A:157:LEU:HG	2.28	0.62
1:A:133:VAL:O	1:A:137:LEU:HG	1.99	0.62
1:B:9:PHE:CE1	1:B:13:ILE:HD11	2.35	0.62
1:A:9:PHE:CE1	1:A:13:ILE:HD11	2.35	0.62
1:A:121:LEU:CD1	1:A:179:THR:HG22	2.30	0.61
1:A:202:TRP:CZ2	1:A:206:VAL:HG21	2.35	0.61
1:D:188:SER:O	1:D:191:PRO:HD2	2.01	0.61
1:A:202:TRP:CE2	1:A:206:VAL:HG21	2.35	0.61
1:B:121:LEU:CD1	1:B:179:THR:HG22	2.31	0.61
1:D:202:TRP:CE2	1:D:206:VAL:HG21	2.36	0.61
1:B:129:GLN:HB3	1:C:107:VAL:HG13	1.81	0.61
1:C:9:PHE:CE1	1:C:13:ILE:HD11	2.35	0.61
1:D:9:PHE:CE1	1:D:13:ILE:HD11	2.35	0.61
1:B:24:VAL:CG1	1:B:28:LEU:HD22	2.31	0.61
1:D:24:VAL:CG1	1:D:28:LEU:HD22	2.31	0.61
1:B:202:TRP:CZ2	1:B:206:VAL:HG21	2.35	0.61
1:A:24:VAL:CG1	1:A:28:LEU:HD22	2.31	0.61
1:D:202:TRP:CZ2	1:D:206:VAL:HG21	2.35	0.61
1:C:202:TRP:CZ2	1:C:206:VAL:HG21	2.35	0.61
1:D:121:LEU:CD1	1:D:179:THR:HG22	2.30	0.61
1:C:188:SER:O	1:C:191:PRO:HD2	2.01	0.61
1:A:133:VAL:HG23	1:B:107:VAL:CG1	2.31	0.60
1:C:129:GLN:HB3	1:D:107:VAL:HG13	1.81	0.60
1:A:188:SER:O	1:A:191:PRO:HD2	2.00	0.60
1:B:188:SER:O	1:B:191:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LEU:CD1	1:C:179:THR:HG22	2.31	0.60
1:C:24:VAL:CG1	1:C:28:LEU:HD22	2.31	0.60
1:B:133:VAL:HG23	1:C:107:VAL:CG1	2.31	0.60
1:B:202:TRP:CE2	1:B:206:VAL:HG21	2.36	0.60
1:C:202:TRP:CE2	1:C:206:VAL:HG21	2.35	0.60
1:C:201:HIS:CE1	1:C:205:TRP:HE1	2.21	0.59
1:C:133:VAL:HG23	1:D:107:VAL:CG1	2.32	0.59
1:B:201:HIS:CE1	1:B:205:TRP:HE1	2.21	0.59
1:D:201:HIS:CE1	1:D:205:TRP:HE1	2.21	0.59
1:A:201:HIS:CE1	1:A:205:TRP:HE1	2.21	0.58
1:B:131:THR:O	1:B:135:ILE:HG13	2.04	0.58
1:D:131:THR:O	1:D:135:ILE:HG13	2.04	0.58
1:A:38:PRO:HB3	1:B:39:LEU:HD11	1.86	0.58
1:C:142:VAL:HG21	1:C:212:ALA:HA	1.86	0.57
1:C:28:LEU:O	1:C:32:LEU:HD13	2.04	0.57
1:B:142:VAL:HG21	1:B:212:ALA:HA	1.86	0.57
1:D:142:VAL:HG21	1:D:212:ALA:HA	1.86	0.57
1:D:69:PRO:HB3	1:D:90:MET:HE2	1.84	0.57
1:A:28:LEU:O	1:A:32:LEU:HD13	2.04	0.57
1:C:24:VAL:HG12	1:C:28:LEU:HD22	1.87	0.57
1:B:20:SER:HA	1:B:67:VAL:HG13	1.87	0.57
1:A:142:VAL:HG21	1:A:212:ALA:HA	1.86	0.57
1:A:32:LEU:O	1:A:33:ARG:HB3	2.05	0.57
1:C:32:LEU:O	1:C:33:ARG:CB	2.53	0.57
1:D:28:LEU:O	1:D:32:LEU:HD13	2.04	0.57
1:D:32:LEU:O	1:D:33:ARG:CB	2.53	0.57
1:D:32:LEU:O	1:D:33:ARG:HB3	2.05	0.57
1:C:32:LEU:O	1:C:33:ARG:HB3	2.05	0.57
1:A:131:THR:O	1:A:135:ILE:HG13	2.04	0.57
1:C:20:SER:HA	1:C:67:VAL:HG13	1.86	0.57
1:D:20:SER:HA	1:D:67:VAL:HG13	1.87	0.57
1:C:69:PRO:HB3	1:C:90:MET:HE2	1.86	0.57
1:B:24:VAL:HG12	1:B:28:LEU:HD22	1.87	0.56
1:B:32:LEU:O	1:B:33:ARG:HB3	2.05	0.56
1:B:28:LEU:O	1:B:32:LEU:HD13	2.04	0.56
1:B:32:LEU:O	1:B:33:ARG:CB	2.53	0.56
1:C:131:THR:O	1:C:135:ILE:HG13	2.04	0.56
1:B:38:PRO:HB3	1:C:39:LEU:HD11	1.87	0.56
1:C:38:PRO:HB3	1:D:39:LEU:HD11	1.86	0.56
1:C:140:GLN:HG2	1:D:26:PHE:CZ	2.40	0.56
1:A:140:GLN:HG2	1:B:26:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLN:HG2	1:C:26:PHE:CZ	2.40	0.56
1:C:107:VAL:O	1:C:107:VAL:HG12	2.06	0.56
1:A:32:LEU:O	1:A:33:ARG:CB	2.53	0.56
1:A:20:SER:HA	1:A:67:VAL:HG13	1.87	0.56
1:A:121:LEU:CD1	1:A:130:ALA:HB1	2.36	0.56
1:D:24:VAL:HG12	1:D:28:LEU:HD22	1.87	0.56
1:A:26:PHE:CZ	1:D:140:GLN:HG2	2.41	0.56
1:A:37:GLY:HA3	1:A:177:TYR:CE1	2.36	0.56
1:A:107:VAL:O	1:A:107:VAL:HG12	2.06	0.56
1:A:24:VAL:HG12	1:A:28:LEU:HD22	1.87	0.56
1:B:121:LEU:CD1	1:B:130:ALA:HB1	2.36	0.56
1:C:121:LEU:CD1	1:C:130:ALA:HB1	2.36	0.56
1:B:37:GLY:HA3	1:B:177:TYR:CE1	2.36	0.55
1:D:121:LEU:CD1	1:D:130:ALA:HB1	2.36	0.55
1:D:107:VAL:HG12	1:D:107:VAL:O	2.06	0.55
1:B:61:HIS:H	1:B:61:HIS:HD2	1.54	0.55
1:C:52:LEU:HD22	1:C:168:LEU:HD22	1.89	0.55
1:A:110:PRO:C	1:A:112:VAL:H	2.10	0.55
1:B:107:VAL:HG12	1:B:107:VAL:O	2.06	0.55
1:A:107:VAL:CG1	1:D:133:VAL:HG23	2.31	0.55
1:D:110:PRO:C	1:D:112:VAL:H	2.10	0.55
1:A:52:LEU:HD22	1:A:168:LEU:HD22	1.89	0.55
1:A:37:GLY:N	1:A:38:PRO:HD3	2.22	0.54
1:D:37:GLY:N	1:D:38:PRO:HD3	2.22	0.54
1:A:39:LEU:HD11	1:D:38:PRO:HB3	1.88	0.54
1:C:61:HIS:HD2	1:C:61:HIS:H	1.53	0.54
1:B:110:PRO:C	1:B:112:VAL:H	2.10	0.54
1:C:37:GLY:HA3	1:C:177:TYR:CE1	2.36	0.54
1:C:110:PRO:C	1:C:112:VAL:H	2.09	0.54
1:D:37:GLY:HA3	1:D:177:TYR:CE1	2.36	0.54
1:B:110:PRO:O	1:B:112:VAL:N	2.38	0.54
1:B:52:LEU:HD22	1:B:168:LEU:HD22	1.89	0.54
1:B:69:PRO:HB3	1:B:90:MET:HE2	1.88	0.54
1:B:37:GLY:N	1:B:38:PRO:HD3	2.23	0.54
1:D:52:LEU:HD22	1:D:168:LEU:HD22	1.89	0.54
1:C:37:GLY:N	1:C:38:PRO:HD3	2.22	0.54
1:D:121:LEU:HD12	1:D:179:THR:HG22	1.91	0.53
1:A:61:HIS:HD2	1:A:61:HIS:H	1.54	0.53
1:A:121:LEU:HD12	1:A:179:THR:HG22	1.91	0.53
1:C:121:LEU:HD12	1:C:179:THR:HG22	1.91	0.53
1:D:33:ARG:HG3	1:D:34:TRP:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD12	1:B:179:THR:HG22	1.91	0.52
1:B:33:ARG:HG3	1:B:34:TRP:H	1.75	0.52
1:D:61:HIS:HD2	1:D:61:HIS:H	1.54	0.52
1:D:110:PRO:O	1:D:111:ALA:HB3	2.11	0.51
1:A:110:PRO:O	1:A:112:VAL:N	2.38	0.51
1:A:121:LEU:HD11	1:A:130:ALA:HB1	1.93	0.51
1:D:32:LEU:O	1:D:33:ARG:HG2	2.11	0.51
1:C:24:VAL:HG21	1:C:97:ALA:CB	2.40	0.51
1:D:121:LEU:HD11	1:D:130:ALA:HB1	1.93	0.51
1:C:121:LEU:HD11	1:C:130:ALA:HB1	1.93	0.51
1:A:110:PRO:O	1:A:111:ALA:HB3	2.11	0.51
1:D:24:VAL:HG21	1:D:97:ALA:CB	2.40	0.51
1:B:121:LEU:HD11	1:B:130:ALA:HB1	1.93	0.51
1:C:32:LEU:O	1:C:33:ARG:HG2	2.11	0.51
1:B:24:VAL:HG21	1:B:97:ALA:CB	2.40	0.50
1:C:33:ARG:HG3	1:C:34:TRP:H	1.74	0.50
1:C:110:PRO:O	1:C:111:ALA:HB3	2.10	0.50
1:A:24:VAL:HG21	1:A:97:ALA:CB	2.40	0.50
1:A:223:LEU:HD23	1:A:224:PHE:H	1.76	0.50
1:A:32:LEU:O	1:A:33:ARG:HG2	2.11	0.50
1:B:32:LEU:O	1:B:33:ARG:HG2	2.11	0.50
1:B:110:PRO:O	1:B:111:ALA:HB3	2.11	0.50
1:A:33:ARG:HG3	1:A:34:TRP:H	1.74	0.50
1:D:137:LEU:HD21	1:D:174:PHE:HD2	1.77	0.49
1:C:143:LEU:HD12	1:C:143:LEU:O	2.12	0.49
1:A:143:LEU:HD12	1:A:143:LEU:O	2.12	0.49
1:B:143:LEU:O	1:B:143:LEU:HD12	2.12	0.49
1:A:153:ARG:HH21	1:A:154:ASN:ND2	2.10	0.49
1:C:110:PRO:O	1:C:112:VAL:N	2.38	0.49
1:D:143:LEU:HD12	1:D:143:LEU:O	2.12	0.49
2:F:139:GLU:CD	2:F:139:GLU:H	2.16	0.49
1:B:153:ARG:HH21	1:B:154:ASN:ND2	2.10	0.49
1:C:137:LEU:HD21	1:C:174:PHE:HD2	1.77	0.49
1:D:153:ARG:HH21	1:D:154:ASN:ND2	2.10	0.49
2:E:139:GLU:CD	2:E:139:GLU:H	2.16	0.49
1:A:153:ARG:HE	1:A:154:ASN:CB	2.26	0.49
1:D:153:ARG:HE	1:D:154:ASN:CB	2.26	0.48
1:D:110:PRO:O	1:D:112:VAL:N	2.38	0.48
1:B:87:ILE:O	1:B:91:VAL:HG23	2.13	0.48
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.79	0.48
1:C:87:ILE:O	1:C:91:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:HH21	1:C:154:ASN:ND2	2.10	0.48
1:B:28:LEU:HD21	1:B:191:PRO:HG3	1.95	0.48
1:A:87:ILE:O	1:A:91:VAL:HG23	2.13	0.48
1:C:28:LEU:HD21	1:C:191:PRO:HG3	1.95	0.48
1:C:11:ARG:HH11	1:C:11:ARG:HG2	1.78	0.48
1:A:137:LEU:HD21	1:A:174:PHE:HD2	1.77	0.48
1:A:11:ARG:HG2	1:A:11:ARG:HH11	1.79	0.48
1:B:153:ARG:HE	1:B:154:ASN:CB	2.26	0.48
1:C:153:ARG:HE	1:C:154:ASN:CB	2.26	0.48
1:B:11:ARG:HH11	1:B:11:ARG:HG2	1.79	0.48
1:B:137:LEU:HD21	1:B:174:PHE:HD2	1.77	0.47
1:D:87:ILE:O	1:D:91:VAL:HG23	2.13	0.47
1:A:28:LEU:HD21	1:A:191:PRO:HG3	1.95	0.47
1:B:37:GLY:HA2	1:B:41:VAL:HG23	1.97	0.47
1:D:39:LEU:HD12	1:D:40:HIS:N	2.30	0.47
1:A:69:PRO:HB3	1:A:90:MET:HE2	1.95	0.47
1:A:153:ARG:HH21	1:A:154:ASN:CG	2.18	0.47
1:D:28:LEU:HD21	1:D:191:PRO:HG3	1.95	0.47
1:C:37:GLY:HA2	1:C:41:VAL:HG23	1.97	0.47
1:C:74:ALA:HB2	1:C:212:ALA:HB1	1.96	0.47
1:A:37:GLY:HA2	1:A:41:VAL:HG23	1.97	0.47
1:B:153:ARG:HH21	1:B:154:ASN:CG	2.18	0.47
1:B:39:LEU:HD12	1:B:40:HIS:N	2.30	0.46
1:B:74:ALA:HB2	1:B:212:ALA:HB1	1.96	0.46
1:A:133:VAL:CG2	1:B:107:VAL:HG11	2.39	0.46
1:D:121:LEU:N	1:D:121:LEU:HD22	2.31	0.46
1:D:153:ARG:HH21	1:D:154:ASN:CG	2.18	0.46
1:C:153:ARG:HH21	1:C:154:ASN:CG	2.18	0.46
1:D:33:ARG:CG	1:D:34:TRP:H	2.29	0.46
1:D:121:LEU:HD12	1:D:130:ALA:CB	2.46	0.46
1:A:138:THR:OG1	1:A:208:PRO:HA	2.16	0.46
1:A:39:LEU:HD12	1:A:40:HIS:N	2.30	0.46
1:C:39:LEU:HD12	1:C:40:HIS:N	2.30	0.46
1:B:121:LEU:N	1:B:121:LEU:HD22	2.31	0.46
1:D:37:GLY:HA2	1:D:41:VAL:HG23	1.97	0.46
1:A:121:LEU:HD12	1:A:130:ALA:CB	2.46	0.46
1:D:138:THR:OG1	1:D:208:PRO:HA	2.16	0.46
1:C:61:HIS:N	1:C:61:HIS:CD2	2.84	0.46
1:A:121:LEU:HD22	1:A:121:LEU:N	2.31	0.46
1:D:74:ALA:HB2	1:D:212:ALA:HB1	1.96	0.46
1:A:74:ALA:HB2	1:A:212:ALA:HB1	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:TRP:CH2	1:C:206:VAL:HG21	2.52	0.45
1:D:202:TRP:CH2	1:D:206:VAL:HG21	2.52	0.45
1:A:37:GLY:O	1:A:41:VAL:HG23	2.16	0.45
1:B:119:ASN:ND2	1:B:188:SER:OG	2.50	0.45
1:B:119:ASN:HB3	1:B:204:TYR:CZ	2.52	0.45
1:C:119:ASN:HB3	1:C:204:TYR:CZ	2.52	0.45
1:C:37:GLY:O	1:C:41:VAL:HG23	2.16	0.45
1:B:121:LEU:HD12	1:B:130:ALA:CB	2.46	0.45
1:C:133:VAL:HG13	1:C:174:PHE:HE2	1.82	0.45
1:D:37:GLY:O	1:D:41:VAL:HG23	2.16	0.45
1:C:33:ARG:CG	1:C:34:TRP:H	2.28	0.45
1:D:133:VAL:HG13	1:D:174:PHE:HE2	1.82	0.45
1:B:37:GLY:O	1:B:41:VAL:HG23	2.16	0.45
1:A:119:ASN:ND2	1:A:188:SER:OG	2.50	0.45
1:D:119:ASN:HB3	1:D:204:TYR:CZ	2.52	0.45
1:B:202:TRP:CH2	1:B:206:VAL:HG21	2.52	0.45
1:C:121:LEU:HD12	1:C:130:ALA:CB	2.46	0.45
1:A:33:ARG:CG	1:A:34:TRP:H	2.28	0.45
1:D:119:ASN:ND2	1:D:188:SER:OG	2.50	0.45
1:C:121:LEU:N	1:C:121:LEU:HD22	2.31	0.45
1:B:33:ARG:CG	1:B:34:TRP:H	2.29	0.45
1:B:138:THR:OG1	1:B:208:PRO:HA	2.16	0.45
1:C:138:THR:OG1	1:C:208:PRO:HA	2.16	0.45
1:A:133:VAL:HG13	1:A:174:PHE:HE2	1.82	0.44
1:C:119:ASN:ND2	1:C:188:SER:OG	2.50	0.44
1:C:24:VAL:HG21	1:C:97:ALA:HB1	2.00	0.44
1:A:94:LEU:O	1:A:98:VAL:HG23	2.17	0.44
2:F:94:LYS:HE2	2:F:94:LYS:HA	1.99	0.44
2:E:94:LYS:HE2	2:E:94:LYS:HA	1.99	0.44
1:B:24:VAL:HG21	1:B:97:ALA:HB1	2.00	0.44
1:C:24:VAL:O	1:C:28:LEU:HB2	2.17	0.44
1:A:202:TRP:CH2	1:A:206:VAL:HG21	2.52	0.44
1:A:156:ARG:HB3	1:B:160:VAL:HG13	1.99	0.44
1:A:119:ASN:HB3	1:A:204:TYR:CZ	2.52	0.44
1:A:24:VAL:O	1:A:28:LEU:HB2	2.17	0.44
1:D:24:VAL:HG21	1:D:97:ALA:HB1	1.99	0.44
1:C:94:LEU:O	1:C:98:VAL:HG23	2.17	0.44
1:B:24:VAL:O	1:B:28:LEU:HB2	2.17	0.44
1:A:24:VAL:HG21	1:A:97:ALA:HB1	1.99	0.44
1:B:61:HIS:CD2	1:B:61:HIS:N	2.84	0.44
1:B:94:LEU:O	1:B:98:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:CG2	1:C:107:VAL:HG11	2.39	0.44
1:D:110:PRO:C	1:D:112:VAL:N	2.72	0.44
1:B:156:ARG:HB3	1:C:160:VAL:HG13	1.99	0.44
1:B:133:VAL:HG13	1:B:174:PHE:HE2	1.82	0.44
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.83	0.44
1:C:110:PRO:C	1:C:112:VAL:N	2.71	0.43
1:D:94:LEU:O	1:D:98:VAL:HG23	2.17	0.43
1:D:33:ARG:HH11	1:D:33:ARG:HG2	1.83	0.43
1:C:33:ARG:HG2	1:C:33:ARG:HH11	1.84	0.43
1:D:90:MET:HA	1:D:93:GLN:NE2	2.34	0.43
1:D:24:VAL:O	1:D:28:LEU:HB2	2.17	0.43
1:D:137:LEU:HD21	1:D:174:PHE:CD2	2.54	0.43
1:B:119:ASN:HB3	1:B:204:TYR:CE1	2.54	0.43
1:B:33:ARG:HH11	1:B:33:ARG:HG2	1.83	0.43
1:B:121:LEU:HD12	1:B:130:ALA:HB1	2.00	0.43
1:C:156:ARG:HB3	1:D:160:VAL:HG13	1.99	0.43
1:A:119:ASN:HB3	1:A:204:TYR:CE1	2.54	0.43
1:A:121:LEU:HD12	1:A:130:ALA:HB1	2.01	0.43
1:C:90:MET:HA	1:C:93:GLN:NE2	2.34	0.43
1:A:110:PRO:C	1:A:112:VAL:N	2.72	0.43
1:B:37:GLY:O	1:B:41:VAL:CG2	2.67	0.43
1:D:121:LEU:HD12	1:D:130:ALA:HB1	2.00	0.43
1:C:223:LEU:HD23	1:C:224:PHE:H	1.83	0.43
1:A:37:GLY:O	1:A:41:VAL:CG2	2.67	0.43
1:B:90:MET:HA	1:B:93:GLN:NE2	2.34	0.43
1:A:160:VAL:HG13	1:D:156:ARG:HB3	1.99	0.43
1:C:119:ASN:HB3	1:C:204:TYR:CE1	2.54	0.42
1:C:69:PRO:HB3	1:C:90:MET:CE	2.49	0.42
1:A:90:MET:HA	1:A:93:GLN:NE2	2.34	0.42
1:A:137:LEU:HD21	1:A:174:PHE:CD2	2.54	0.42
1:D:37:GLY:O	1:D:41:VAL:CG2	2.67	0.42
1:D:119:ASN:HB3	1:D:204:TYR:CE1	2.54	0.42
1:B:137:LEU:HD21	1:B:174:PHE:CD2	2.54	0.42
1:A:129:GLN:CB	1:B:107:VAL:HG13	2.49	0.42
1:C:37:GLY:O	1:C:41:VAL:CG2	2.67	0.42
1:B:129:GLN:CB	1:C:107:VAL:HG13	2.49	0.42
1:A:225:PRO:HA	1:A:226:ARG:HB3	2.01	0.42
1:C:42:LEU:HD11	1:D:42:LEU:HD13	2.02	0.42
1:B:110:PRO:C	1:B:112:VAL:N	2.72	0.42
1:A:69:PRO:HB3	1:A:90:MET:CE	2.49	0.42
1:C:223:LEU:HB3	1:D:11:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PRO:HA	1:C:226:ARG:HB3	2.01	0.42
1:C:121:LEU:HD12	1:C:130:ALA:HB1	2.01	0.41
1:A:107:VAL:HG13	1:D:129:GLN:CB	2.49	0.41
1:A:121:LEU:CD1	1:A:130:ALA:CB	2.99	0.41
1:C:137:LEU:HD21	1:C:174:PHE:CD2	2.54	0.41
1:D:121:LEU:CD1	1:D:130:ALA:CB	2.98	0.41
1:B:69:PRO:HB3	1:B:90:MET:CE	2.49	0.41
1:B:32:LEU:O	1:B:33:ARG:CG	2.69	0.41
1:C:32:LEU:O	1:C:33:ARG:CG	2.69	0.41
1:A:32:LEU:O	1:A:33:ARG:CG	2.69	0.41
1:A:42:LEU:HD11	1:B:42:LEU:HD13	2.02	0.41
1:C:38:PRO:HB3	1:D:39:LEU:CD1	2.51	0.41
1:D:32:LEU:O	1:D:33:ARG:CG	2.69	0.41
1:C:121:LEU:CD1	1:C:130:ALA:CB	2.99	0.41
1:B:129:GLN:HB3	1:C:107:VAL:CG1	2.50	0.41
1:B:42:LEU:HD11	1:C:42:LEU:HD13	2.02	0.41
1:A:107:VAL:CG1	1:D:129:GLN:HB3	2.50	0.40
1:C:38:PRO:HB2	1:C:39:LEU:H	1.68	0.40
1:D:201:HIS:HE1	1:D:205:TRP:HE1	1.69	0.40
1:D:220:ASP:CB	1:D:221:PHE:HA	2.51	0.40
1:A:157:LEU:O	1:B:159:SER:HB2	2.22	0.40
1:A:38:PRO:HB2	1:A:39:LEU:H	1.68	0.40
1:B:136:PHE:CZ	1:C:103:VAL:HG11	2.56	0.40
1:C:37:GLY:N	1:C:38:PRO:CD	2.85	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	231/263 (88%)	209 (90%)	15 (6%)	7 (3%)	5 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	231/263 (88%)	205 (89%)	17 (7%)	9 (4%)	4 36
1	C	231/263 (88%)	209 (90%)	14 (6%)	8 (4%)	4 39
1	D	231/263 (88%)	203 (88%)	18 (8%)	10 (4%)	3 34
2	E	141/149 (95%)	119 (84%)	20 (14%)	2 (1%)	14 58
2	F	141/149 (95%)	121 (86%)	18 (13%)	2 (1%)	14 58
All	All	1206/1350 (89%)	1066 (88%)	102 (8%)	38 (3%)	8 41

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	38	PRO
1	A	154	ASN
1	A	227	LEU
1	B	33	ARG
1	B	38	PRO
1	B	154	ASN
1	B	226	ARG
1	B	227	LEU
1	C	33	ARG
1	C	38	PRO
1	C	154	ASN
1	C	227	LEU
1	D	33	ARG
1	D	38	PRO
1	D	154	ASN
1	D	227	LEU
1	D	226	ARG
2	E	81	SER
2	E	97	ASN
2	F	81	SER
2	F	97	ASN
1	A	181	ALA
1	B	181	ALA
1	C	181	ALA
1	C	226	ARG
1	D	181	ALA
1	B	222	LEU
1	D	222	LEU
1	C	35	ALA

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Mol	Chain	Res	Type
1	D	35	ALA
1	D	224	PHE
1	A	35	ALA
1	A	110	PRO
1	B	35	ALA
1	B	110	PRO
1	C	110	PRO
1	D	110	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	179/205 (87%)	160 (89%)	19 (11%)	8 36
1	B	179/205 (87%)	160 (89%)	19 (11%)	8 36
1	C	179/205 (87%)	160 (89%)	19 (11%)	8 36
1	D	179/205 (87%)	160 (89%)	19 (11%)	8 36
2	E	122/127 (96%)	106 (87%)	16 (13%)	5 28
2	F	122/127 (96%)	106 (87%)	16 (13%)	5 28
All	All	960/1074 (89%)	852 (89%)	108 (11%)	12 33

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	34	TRP
1	A	42	LEU
1	A	61	HIS
1	A	66	HIS
1	A	104	LEU
1	A	127	VAL
1	A	140	GLN
1	A	153	ARG
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	170	LEU
1	A	187	ARG
1	A	202	TRP
1	A	214	LEU
1	A	222	LEU
1	A	227	LEU
1	A	228	LYS
1	A	229	SER
1	A	234	LEU
1	B	32	LEU
1	B	34	TRP
1	B	42	LEU
1	B	61	HIS
1	B	66	HIS
1	B	104	LEU
1	B	127	VAL
1	B	140	GLN
1	B	153	ARG
1	B	162	LEU
1	B	170	LEU
1	B	187	ARG
1	B	202	TRP
1	B	214	LEU
1	B	223	LEU
1	B	226	ARG
1	B	231	SER
1	B	238	LYS
1	B	241	ARG
1	C	32	LEU
1	C	34	TRP
1	C	36	PRO
1	C	42	LEU
1	C	61	HIS
1	C	66	HIS
1	C	104	LEU
1	C	127	VAL
1	C	140	GLN
1	C	153	ARG
1	C	162	LEU
1	C	170	LEU
1	C	187	ARG
1	C	202	TRP

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	227	LEU
1	C	228	LYS
1	C	229	SER
1	C	234	LEU
1	D	32	LEU
1	D	34	TRP
1	D	42	LEU
1	D	61	HIS
1	D	66	HIS
1	D	104	LEU
1	D	127	VAL
1	D	140	GLN
1	D	153	ARG
1	D	162	LEU
1	D	170	LEU
1	D	187	ARG
1	D	202	TRP
1	D	214	LEU
1	D	224	PHE
1	D	226	ARG
1	D	227	LEU
1	D	238	LYS
1	D	241	ARG
2	E	11	GLU
2	E	21	LYS
2	E	22	ASP
2	E	30	LYS
2	E	32	LEU
2	E	45	GLU
2	E	60	ASN
2	E	62	THR
2	E	64	ASP
2	E	65	PHE
2	E	75	LYS
2	E	77	LYS
2	E	111	ASN
2	E	115	LYS
2	E	131	ASP
2	E	148	LYS
2	F	11	GLU
2	F	21	LYS

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Mol	Chain	Res	Type
2	F	22	ASP
2	F	30	LYS
2	F	32	LEU
2	F	45	GLU
2	F	60	ASN
2	F	62	THR
2	F	64	ASP
2	F	65	PHE
2	F	75	LYS
2	F	77	LYS
2	F	111	ASN
2	F	114	GLU
2	F	115	LYS
2	F	148	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	66	HIS
1	A	80	GLN
1	A	93	GLN
1	A	119	ASN
1	A	140	GLN
1	A	201	HIS
1	B	61	HIS
1	B	66	HIS
1	B	80	GLN
1	B	93	GLN
1	B	119	ASN
1	B	140	GLN
1	B	201	HIS
1	C	61	HIS
1	C	66	HIS
1	C	80	GLN
1	C	93	GLN
1	C	119	ASN
1	C	140	GLN
1	C	201	HIS
1	D	61	HIS
1	D	66	HIS
1	D	80	GLN

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Mol	Chain	Res	Type
1	D	93	GLN
1	D	119	ASN
1	D	140	GLN
1	D	201	HIS

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.