Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 30, 2019 – 10:03 AM EST

PDB ID	:	6GSH
EMDB ID:	:	EMD-0054
Title	:	Feline Calicivirus Strain F9
Authors	:	Conley, M.J.; Bhella, D.
Deposited on	:	2018-06-14
Resolution	:	3.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

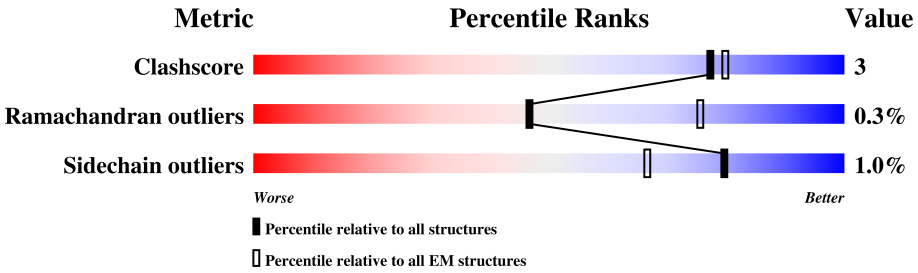
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 3.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	669	74% 5% 20%
1	B	669	73% 6% 21%
1	C	669	72% 7% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24297 atoms, of which 12040 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 VP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	533	Total	C	H	N	O	S	0	0
			8100	2606	4014	680	789	11		
1	B	530	Total	C	H	N	O	S	0	0
			8071	2596	4000	680	784	11		
1	C	534	Total	C	H	N	O	S	0	0
			8123	2612	4026	684	790	11		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	ASP	conflict	UNP A2T4P8
A	21	VAL	ILE	conflict	UNP A2T4P8
A	23	ASP	ASN	conflict	UNP A2T4P8
A	73	ALA	SER	conflict	UNP A2T4P8
A	82	ALA	SER	conflict	UNP A2T4P8
A	90	ALA	GLU	conflict	UNP A2T4P8
A	94	ILE	LEU	conflict	UNP A2T4P8
A	108	GLY	ASN	conflict	UNP A2T4P8
A	127	GLY	-	insertion	UNP A2T4P8
A	133	ALA	THR	conflict	UNP A2T4P8
A	139	PRO	MET	conflict	UNP A2T4P8
A	148	SER	ASN	conflict	UNP A2T4P8
A	149	ALA	THR	conflict	UNP A2T4P8
A	304	SER	THR	conflict	UNP A2T4P8
A	319	ALA	PRO	conflict	UNP A2T4P8
A	345	LYS	ARG	conflict	UNP A2T4P8
A	355	HIS	TYR	conflict	UNP A2T4P8
A	357	THR	SER	conflict	UNP A2T4P8
A	363	VAL	ILE	conflict	UNP A2T4P8
A	392	ILE	MET	conflict	UNP A2T4P8
A	402	ALA	SER	conflict	UNP A2T4P8
A	429	LYS	THR	conflict	UNP A2T4P8
A	440	ASN	ASP	conflict	UNP A2T4P8
A	441	LYS	GLN	conflict	UNP A2T4P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	442	SER	THR	conflict	UNP A2T4P8
A	447	THR	VAL	conflict	UNP A2T4P8
A	449	ALA	PRO	conflict	UNP A2T4P8
A	450	ALA	SER	conflict	UNP A2T4P8
A	451	GLY	ARG	conflict	UNP A2T4P8
A	452	TYR	PHE	conflict	UNP A2T4P8
A	454	GLY	ALA	conflict	UNP A2T4P8
A	456	ASP	ILE	conflict	UNP A2T4P8
A	457	VAL	THR	conflict	UNP A2T4P8
A	472	SER	ALA	conflict	UNP A2T4P8
A	493	LYS	ARG	conflict	UNP A2T4P8
A	494	VAL	GLU	conflict	UNP A2T4P8
A	495	ASP	ASN	conflict	UNP A2T4P8
A	497	ALA	LYS	conflict	UNP A2T4P8
A	498	ILE	LEU	conflict	UNP A2T4P8
A	499	GLU	ILE	conflict	UNP A2T4P8
A	506	MET	ALA	conflict	UNP A2T4P8
A	515	THR	ALA	conflict	UNP A2T4P8
A	519	LYS	ALA	conflict	UNP A2T4P8
A	529	SER	ALA	conflict	UNP A2T4P8
A	539	GLN	GLU	conflict	UNP A2T4P8
A	543	SER	ALA	conflict	UNP A2T4P8
A	603	PRO	ALA	conflict	UNP A2T4P8
A	615	SER	CYS	conflict	UNP A2T4P8
A	636	SER	ASN	conflict	UNP A2T4P8
A	665	SER	THR	conflict	UNP A2T4P8
B	13	ASN	ASP	conflict	UNP A2T4P8
B	21	VAL	ILE	conflict	UNP A2T4P8
B	23	ASP	ASN	conflict	UNP A2T4P8
B	73	ALA	SER	conflict	UNP A2T4P8
B	82	ALA	SER	conflict	UNP A2T4P8
B	90	ALA	GLU	conflict	UNP A2T4P8
B	94	ILE	LEU	conflict	UNP A2T4P8
B	108	GLY	ASN	conflict	UNP A2T4P8
B	127	GLY	-	insertion	UNP A2T4P8
B	133	ALA	THR	conflict	UNP A2T4P8
B	139	PRO	MET	conflict	UNP A2T4P8
B	148	SER	ASN	conflict	UNP A2T4P8
B	149	ALA	THR	conflict	UNP A2T4P8
B	304	SER	THR	conflict	UNP A2T4P8
B	319	ALA	PRO	conflict	UNP A2T4P8
B	345	LYS	ARG	conflict	UNP A2T4P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	355	HIS	TYR	conflict	UNP A2T4P8
B	357	THR	SER	conflict	UNP A2T4P8
B	363	VAL	ILE	conflict	UNP A2T4P8
B	392	ILE	MET	conflict	UNP A2T4P8
B	402	ALA	SER	conflict	UNP A2T4P8
B	429	LYS	THR	conflict	UNP A2T4P8
B	440	ASN	ASP	conflict	UNP A2T4P8
B	441	LYS	GLN	conflict	UNP A2T4P8
B	442	SER	THR	conflict	UNP A2T4P8
B	447	THR	VAL	conflict	UNP A2T4P8
B	449	ALA	PRO	conflict	UNP A2T4P8
B	450	ALA	SER	conflict	UNP A2T4P8
B	451	GLY	ARG	conflict	UNP A2T4P8
B	452	TYR	PHE	conflict	UNP A2T4P8
B	454	GLY	ALA	conflict	UNP A2T4P8
B	456	ASP	ILE	conflict	UNP A2T4P8
B	457	VAL	THR	conflict	UNP A2T4P8
B	472	SER	ALA	conflict	UNP A2T4P8
B	493	LYS	ARG	conflict	UNP A2T4P8
B	494	VAL	GLU	conflict	UNP A2T4P8
B	495	ASP	ASN	conflict	UNP A2T4P8
B	497	ALA	LYS	conflict	UNP A2T4P8
B	498	ILE	LEU	conflict	UNP A2T4P8
B	499	GLU	ILE	conflict	UNP A2T4P8
B	506	MET	ALA	conflict	UNP A2T4P8
B	515	THR	ALA	conflict	UNP A2T4P8
B	519	LYS	ALA	conflict	UNP A2T4P8
B	529	SER	ALA	conflict	UNP A2T4P8
B	539	GLN	GLU	conflict	UNP A2T4P8
B	543	SER	ALA	conflict	UNP A2T4P8
B	603	PRO	ALA	conflict	UNP A2T4P8
B	615	SER	CYS	conflict	UNP A2T4P8
B	636	SER	ASN	conflict	UNP A2T4P8
B	665	SER	THR	conflict	UNP A2T4P8
C	13	ASN	ASP	conflict	UNP A2T4P8
C	21	VAL	ILE	conflict	UNP A2T4P8
C	23	ASP	ASN	conflict	UNP A2T4P8
C	73	ALA	SER	conflict	UNP A2T4P8
C	82	ALA	SER	conflict	UNP A2T4P8
C	90	ALA	GLU	conflict	UNP A2T4P8
C	94	ILE	LEU	conflict	UNP A2T4P8
C	108	GLY	ASN	conflict	UNP A2T4P8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	127	GLY	-	insertion	UNP A2T4P8
C	133	ALA	THR	conflict	UNP A2T4P8
C	139	PRO	MET	conflict	UNP A2T4P8
C	148	SER	ASN	conflict	UNP A2T4P8
C	149	ALA	THR	conflict	UNP A2T4P8
C	304	SER	THR	conflict	UNP A2T4P8
C	319	ALA	PRO	conflict	UNP A2T4P8
C	345	LYS	ARG	conflict	UNP A2T4P8
C	355	HIS	TYR	conflict	UNP A2T4P8
C	357	THR	SER	conflict	UNP A2T4P8
C	363	VAL	ILE	conflict	UNP A2T4P8
C	392	ILE	MET	conflict	UNP A2T4P8
C	402	ALA	SER	conflict	UNP A2T4P8
C	429	LYS	THR	conflict	UNP A2T4P8
C	440	ASN	ASP	conflict	UNP A2T4P8
C	441	LYS	GLN	conflict	UNP A2T4P8
C	442	SER	THR	conflict	UNP A2T4P8
C	447	THR	VAL	conflict	UNP A2T4P8
C	449	ALA	PRO	conflict	UNP A2T4P8
C	450	ALA	SER	conflict	UNP A2T4P8
C	451	GLY	ARG	conflict	UNP A2T4P8
C	452	TYR	PHE	conflict	UNP A2T4P8
C	454	GLY	ALA	conflict	UNP A2T4P8
C	456	ASP	ILE	conflict	UNP A2T4P8
C	457	VAL	THR	conflict	UNP A2T4P8
C	472	SER	ALA	conflict	UNP A2T4P8
C	493	LYS	ARG	conflict	UNP A2T4P8
C	494	VAL	GLU	conflict	UNP A2T4P8
C	495	ASP	ASN	conflict	UNP A2T4P8
C	497	ALA	LYS	conflict	UNP A2T4P8
C	498	ILE	LEU	conflict	UNP A2T4P8
C	499	GLU	ILE	conflict	UNP A2T4P8
C	506	MET	ALA	conflict	UNP A2T4P8
C	515	THR	ALA	conflict	UNP A2T4P8
C	519	LYS	ALA	conflict	UNP A2T4P8
C	529	SER	ALA	conflict	UNP A2T4P8
C	539	GLN	GLU	conflict	UNP A2T4P8
C	543	SER	ALA	conflict	UNP A2T4P8
C	603	PRO	ALA	conflict	UNP A2T4P8
C	615	SER	CYS	conflict	UNP A2T4P8
C	636	SER	ASN	conflict	UNP A2T4P8
C	665	SER	THR	conflict	UNP A2T4P8

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

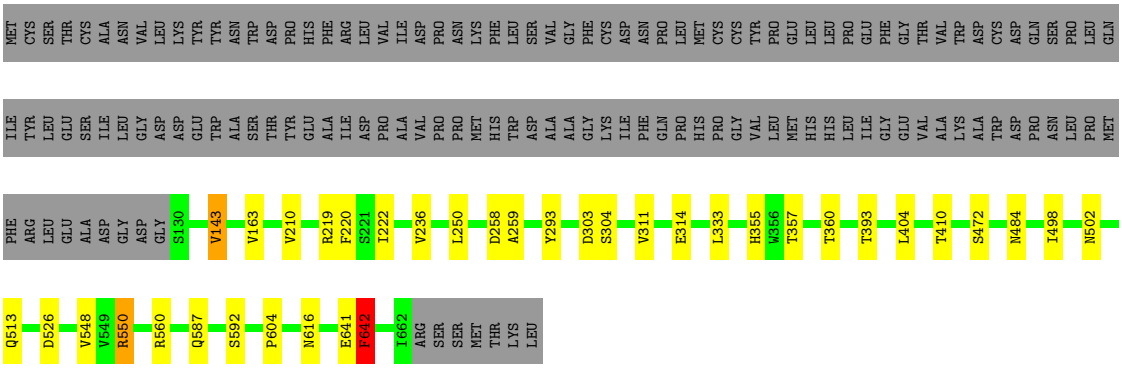
Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total K 1 1	0
2	A	1	Total K 1 1	0
2	C	1	Total K 1 1	0

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 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.

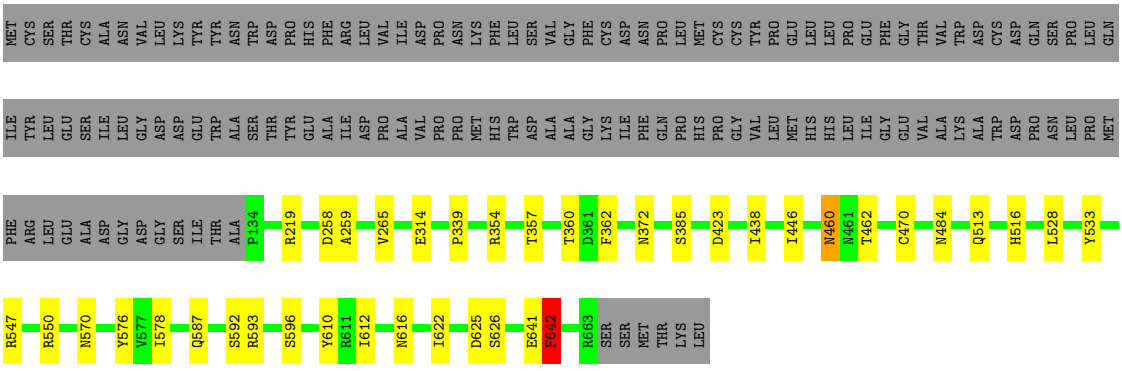
• Molecule 1: VP1

Chain A:



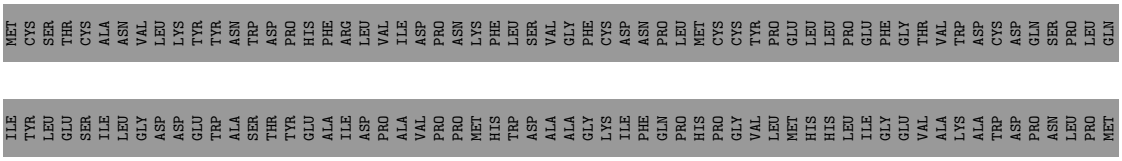
• Molecule 1: VP1

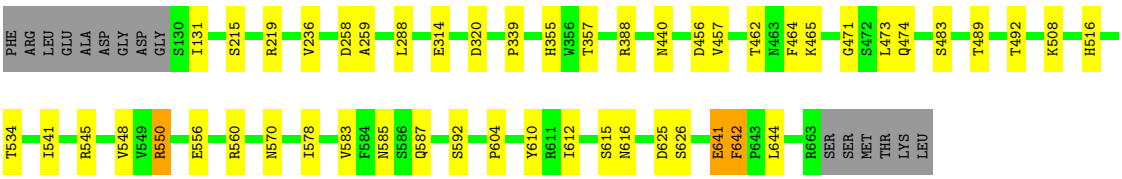
Chain B:



• Molecule 1: VP1

Chain C:




PHE
ARG
LEU
GLU
ALA
ASP
GLY
ASP
GLY
S130
I131
S215
R219
V236
D258
A259
L288
E314
D320
P339
H355
W356
T357
R388
N440
D456
V457
T462
N463
F464
K465
G471
S472
L473
Q474
S483
T489
T492
K508
H516
T534
I541
R545
V548
V549
R550
E556
R560
N570
I578
V583
F584
N585
S586
Q587
S592
P604
Y610
R611
I612
S615
M616
D625
S626
E641
F642
P643
L644
R663
SER
SER
MET
THR
LYS
LEU

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was implemented through Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.45	0/4188	0.63	1/5711 (0.0%)
1	B	0.44	0/4173	0.62	1/5688 (0.0%)
1	C	0.47	0/4199	0.63	0/5725
All	All	0.45	0/12560	0.63	2/17124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	642	PHE	N-CA-C	5.97	127.11	111.00
1	A	642	PHE	N-CA-C	5.75	126.54	111.00

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	4086	4014	4017	22	0
1	B	4071	4000	4003	28	0
1	C	4097	4026	4030	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12257	12040	12050	78	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 3.

All (78) 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:360:THR:O	1:B:642:PHE:CE1	1.87	1.26
1:C:616:ASN:ND2	1:C:641:GLU:OE2	1.93	1.01
1:B:446:ILE:O	1:B:576:TYR:OH	1.83	0.96
1:B:360:THR:O	1:B:642:PHE:CD1	2.31	0.83
1:C:473:LEU:O	1:C:483:SER:OG	1.97	0.81
1:C:570:ASN:OD1	1:C:585:ASN:ND2	2.15	0.78
1:A:587:GLN:OE1	1:A:592:SER:OG	2.03	0.77
1:A:502:ASN:OD1	1:A:550:ARG:NH2	2.19	0.75
1:B:372:ASN:OD1	1:B:385:SER:OG	2.08	0.71
1:A:548:VAL:O	1:A:550:ARG:NH2	2.25	0.69
1:C:548:VAL:O	1:C:550:ARG:NH1	2.26	0.69
1:A:472:SER:OG	1:A:484:ASN:O	2.12	0.68
1:B:616:ASN:HB2	1:B:641:GLU:OE2	1.94	0.67
1:B:438:ILE:HD12	1:B:576:TYR:CE2	2.30	0.66
1:A:560:ARG:NH2	1:A:604:PRO:O	2.29	0.65
1:A:616:ASN:OD1	1:A:641:GLU:HG3	1.97	0.65
1:A:513:GLN:NE2	1:A:526:ASP:OD1	2.30	0.64
1:B:360:THR:O	1:B:642:PHE:CZ	2.47	0.64
1:C:560:ARG:NH2	1:C:604:PRO:O	2.31	0.64
1:B:484:ASN:O	1:B:513:GLN:NE2	2.31	0.63
1:B:593:ARG:O	1:B:596:SER:OG	2.14	0.63
1:C:642:PHE:O	1:C:644:LEU:N	2.34	0.60
1:C:641:GLU:N	1:C:641:GLU:OE1	2.36	0.58
1:C:465:LYS:O	1:C:534:THR:OG1	2.04	0.58
1:B:339:PRO:O	1:B:610:TYR:OH	2.21	0.57
1:C:615:SER:HB2	1:C:641:GLU:HG2	1.86	0.56
1:C:339:PRO:O	1:C:610:TYR:OH	2.18	0.56
1:B:612:ILE:CD1	1:B:622:ILE:HD12	2.37	0.55
1:A:393:THR:OG1	1:A:410:THR:OG1	2.26	0.54
1:B:438:ILE:HD12	1:B:576:TYR:HE2	1.74	0.53
1:B:533:TYR:OH	1:B:547:ARG:NH1	2.40	0.52
1:B:587:GLN:OE1	1:B:592:SER:OG	2.16	0.52
1:A:404:LEU:HD11	1:A:498:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG23	1:A:333:LEU:HD22	1.92	0.51
1:C:612:ILE:HG23	1:C:644:LEU:HD13	1.92	0.51
1:B:357:THR:O	1:B:570:ASN:ND2	2.44	0.50
1:A:404:LEU:HD11	1:A:498:ILE:CG2	2.41	0.50
1:C:258:ASP:OD1	1:C:259:ALA:N	2.45	0.50
1:B:258:ASP:OD1	1:B:259:ALA:N	2.45	0.50
1:B:362:PHE:N	1:B:362:PHE:CD1	2.79	0.49
1:B:460:ASN:ND2	1:B:462:THR:HG22	2.27	0.49
1:A:355:HIS:CD2	1:A:357:THR:HG23	2.48	0.49
1:C:578:ILE:O	1:C:578:ILE:HG22	2.13	0.48
1:A:219:ARG:NH2	1:A:314:GLU:OE1	2.45	0.47
1:C:587:GLN:OE1	1:C:592:SER:OG	2.13	0.47
1:B:265:VAL:HG12	1:C:131:ILE:HD11	1.96	0.47
1:A:404:LEU:O	1:A:404:LEU:HD13	2.13	0.47
1:C:560:ARG:NH1	1:C:625:ASP:OD1	2.49	0.46
1:C:462:THR:HG22	1:C:464:PHE:H	1.80	0.46
1:A:250:LEU:HD13	1:A:293:TYR:CD1	2.50	0.46
1:B:470:CYS:CB	1:B:528:LEU:HD12	2.45	0.46
1:C:215:SER:OG	1:C:320:ASP:OD1	2.24	0.45
1:A:258:ASP:OD1	1:A:259:ALA:N	2.50	0.45
1:B:219:ARG:NH2	1:B:314:GLU:OE1	2.50	0.44
1:B:578:ILE:HG22	1:B:578:ILE:O	2.17	0.44
1:B:642:PHE:O	1:B:642:PHE:CD2	2.71	0.44
1:C:236:VAL:HG23	1:C:236:VAL:O	2.18	0.44
1:A:236:VAL:HG23	1:A:236:VAL:O	2.18	0.44
1:B:438:ILE:HD12	1:B:576:TYR:CD2	2.52	0.44
1:C:492:THR:HG22	1:C:508:LYS:HE2	1.98	0.44
1:B:354:ARG:NH1	1:B:423:ASP:OD1	2.51	0.44
1:C:616:ASN:CG	1:C:641:GLU:OE2	2.54	0.44
1:A:163:VAL:HG13	1:A:163:VAL:O	2.18	0.43
1:B:576:TYR:CD1	1:B:576:TYR:O	2.70	0.43
1:C:219:ARG:N	1:C:314:GLU:O	2.51	0.43
1:A:360:THR:O	1:A:642:PHE:CE1	2.72	0.43
1:C:541:ILE:HD12	1:C:583:VAL:HG22	2.01	0.43
1:B:625:ASP:OD1	1:B:626:SER:N	2.51	0.43
1:C:545:ARG:NH1	1:C:556:GLU:OE2	2.50	0.42
1:C:355:HIS:CD2	1:C:357:THR:HG23	2.54	0.42
1:A:222:ILE:HG12	1:A:311:VAL:HG22	2.01	0.41
1:C:625:ASP:OD1	1:C:626:SER:N	2.53	0.41
1:C:236:VAL:HG12	1:C:288:LEU:HD13	2.02	0.41
1:A:303:ASP:OD1	1:A:304:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASP:OD1	1:C:457:VAL:N	2.53	0.41
1:C:474:GLN:CD	1:C:474:GLN:O	2.59	0.41
1:B:470:CYS:HB2	1:B:528:LEU:HD12	2.03	0.41
1:A:616:ASN:OD1	1:A:641:GLU:CG	2.67	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	531/669 (79%)	484 (91%)	45 (8%)	2 (0%)	36	76
1	B	528/669 (79%)	478 (90%)	49 (9%)	1 (0%)	49	85
1	C	532/669 (80%)	480 (90%)	50 (9%)	2 (0%)	36	76
All	All	1591/2007 (79%)	1442 (91%)	144 (9%)	5 (0%)	47	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	B	642	PHE
1	A	642	PHE
1	C	516	HIS
1	C	471	GLY

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	453/572 (79%)	449 (99%)	4 (1%)	81 93
1	B	451/572 (79%)	447 (99%)	4 (1%)	81 93
1	C	454/572 (79%)	448 (99%)	6 (1%)	71 91
All	All	1358/1716 (79%)	1344 (99%)	14 (1%)	80 93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	A	220	PHE
1	A	550	ARG
1	A	642	PHE
1	B	460	ASN
1	B	516	HIS
1	B	550	ARG
1	B	642	PHE
1	C	388	ARG
1	C	440	ASN
1	C	489	THR
1	C	550	ARG
1	C	641	GLU
1	C	642	PHE

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

Mol	Chain	Res	Type
1	B	400	ASN
1	C	616	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.