Full wwPDB EM Validation Report

Apr 23, 2025 – 02:48 PM EDT

PDB ID	:	9C1L / pdb_00009c1l
EMDB ID	:	EMD-45123
Title	:	Rhesus rotavirus (VP1 structure at 2.65 Angstrom resolution)
Authors	:	Jenni, S.; Herrmann, T.; De Sautu, M.; Harrison, S.C.
Deposited on	:	2024-05-29
Resolution	:	2.65 Å(reported)

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:

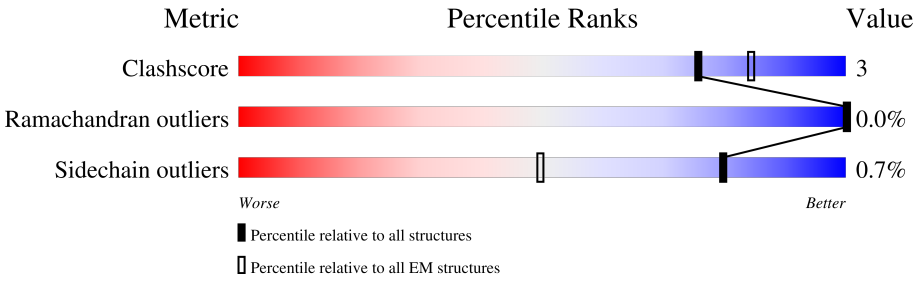
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	887	80% 8% 12%
1	B	887	81% 7% 12%
1	C	887	82% 8% 9%
1	D	887	84% 9% 7%
1	E	887	82% 8% 10%
1	F	887	84% 7% 9%
1	G	887	83% 7% 9%
1	H	887	85% 6% 9%
1	I	887	83% 7% 10%

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Mol	Chain	Length	Quality of chain
1	J	887	
2	P	1088	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 149101 atoms, of which 74750 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	782	Total	C	H	N	O	S	0	0
			12800	4057	6413	1102	1192	36		
1	B	781	Total	C	H	N	O	S	0	0
			12786	4052	6408	1101	1189	36		
1	C	803	Total	C	H	N	O	S	0	0
			13164	4174	6595	1131	1228	36		
1	D	827	Total	C	H	N	O	S	0	0
			13573	4297	6809	1163	1268	36		
1	E	795	Total	C	H	N	O	S	0	0
			13027	4132	6529	1118	1212	36		
1	F	805	Total	C	H	N	O	S	0	0
			13205	4186	6619	1134	1230	36		
1	G	804	Total	C	H	N	O	S	0	0
			13186	4180	6608	1133	1229	36		
1	H	805	Total	C	H	N	O	S	0	0
			13205	4186	6619	1134	1230	36		
1	I	799	Total	C	H	N	O	S	0	0
			13098	4154	6563	1126	1219	36		
1	J	816	Total	C	H	N	O	S	0	0
			13390	4242	6713	1149	1250	36		

- Molecule 2 is a protein called RNA-directed RNA polymerase.

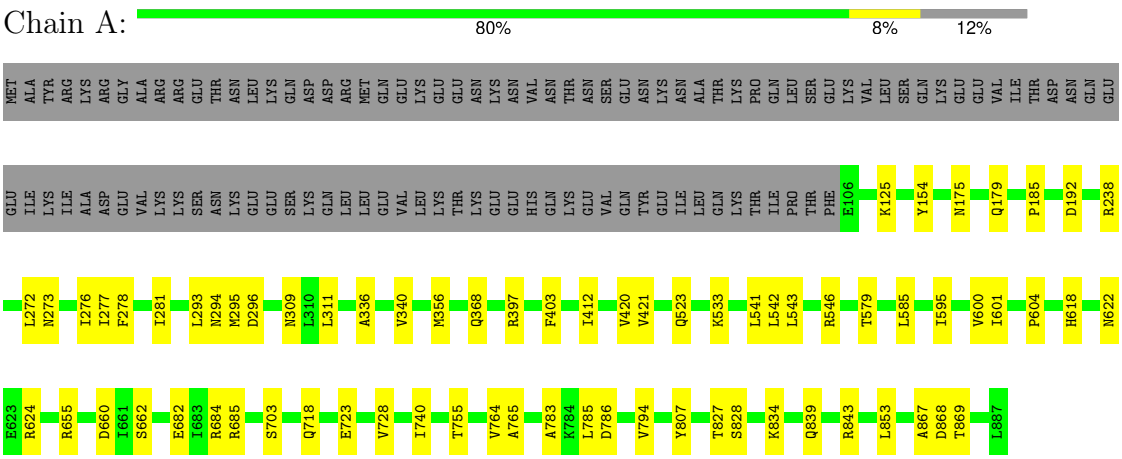
Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	1086	Total	C	H	N	O	S	0	0
			17667	5636	8874	1456	1662	39		

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.

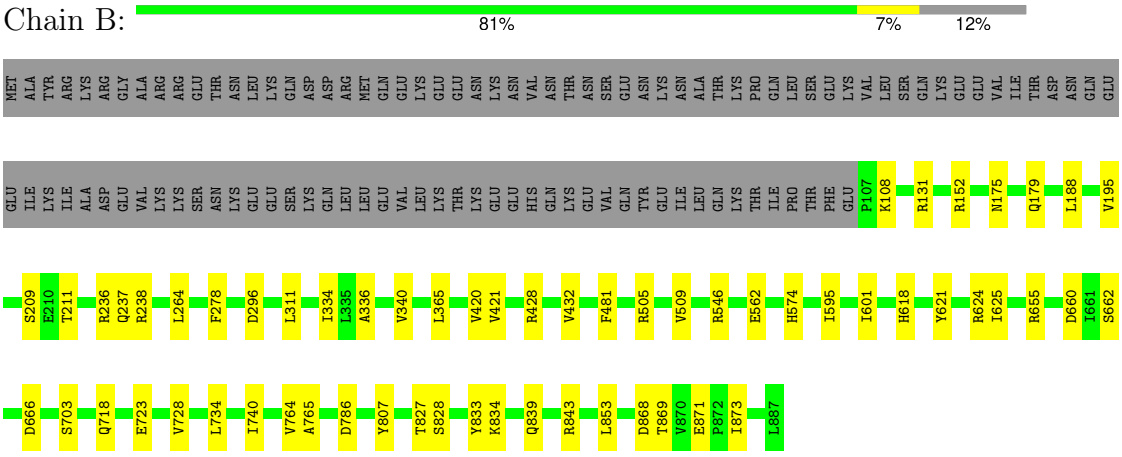
• Molecule 1: Inner capsid protein VP2

Chain A:



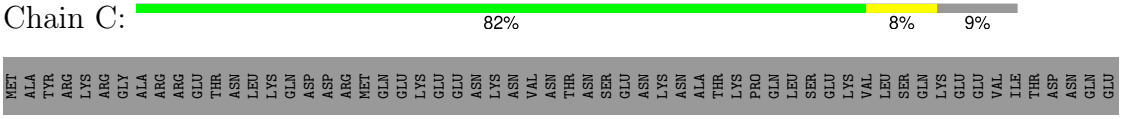
• Molecule 1: Inner capsid protein VP2

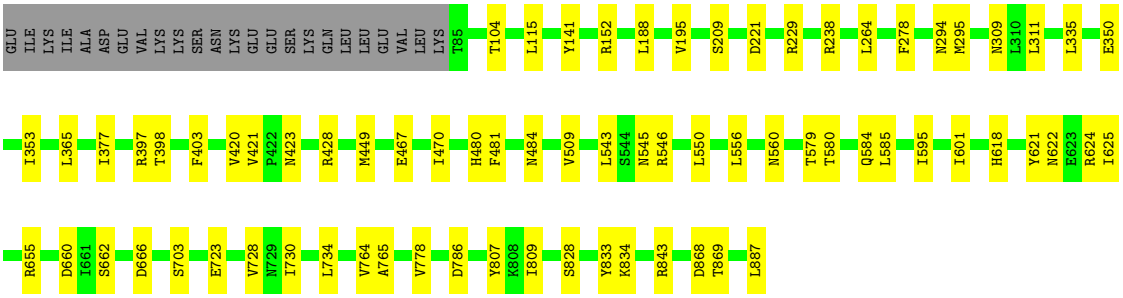
Chain B:



• Molecule 1: Inner capsid protein VP2

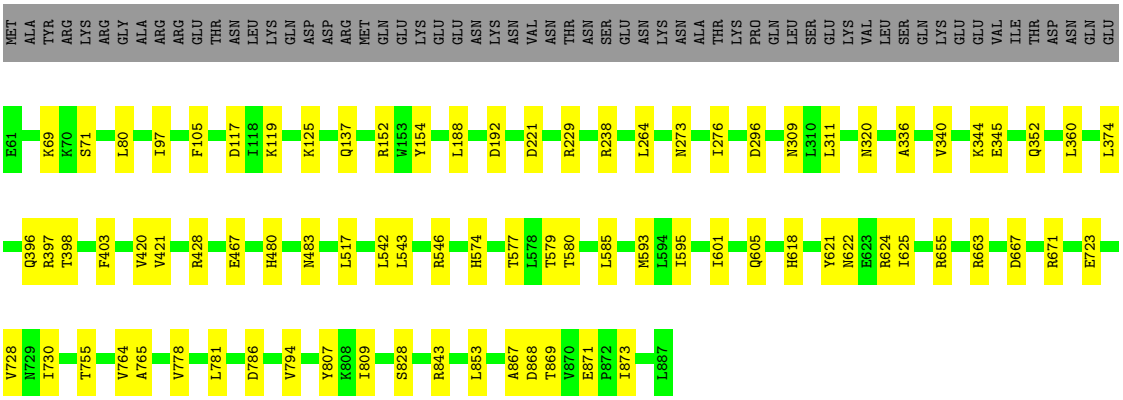
Chain C:





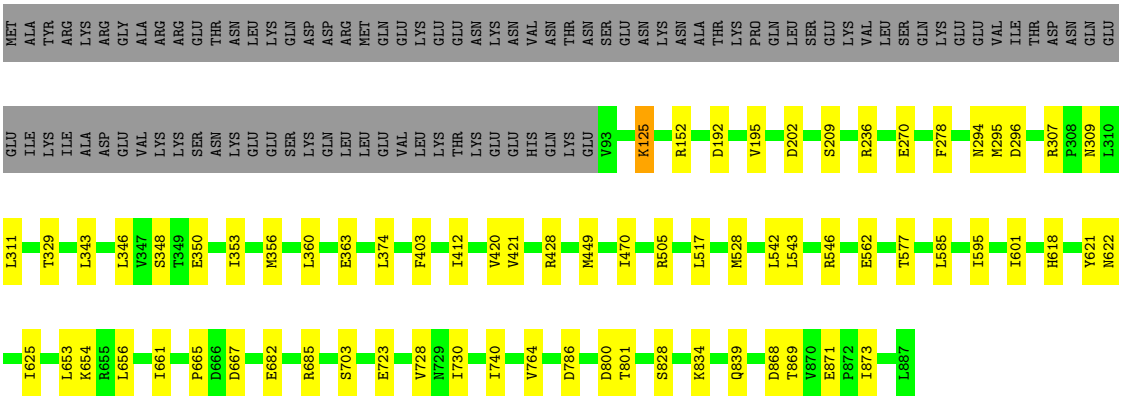
• Molecule 1: Inner capsid protein VP2

Chain D:



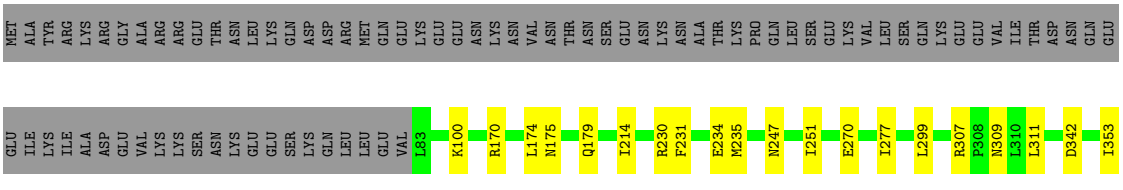
• Molecule 1: Inner capsid protein VP2

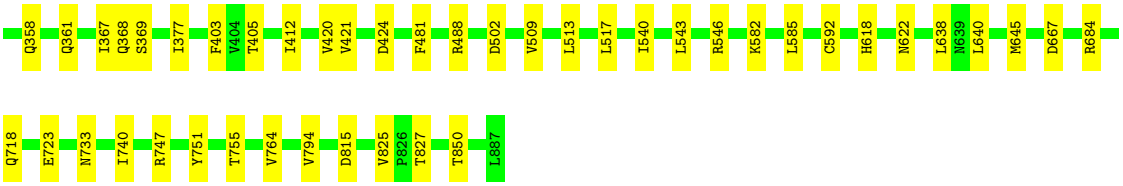
Chain E:



• Molecule 1: Inner capsid protein VP2

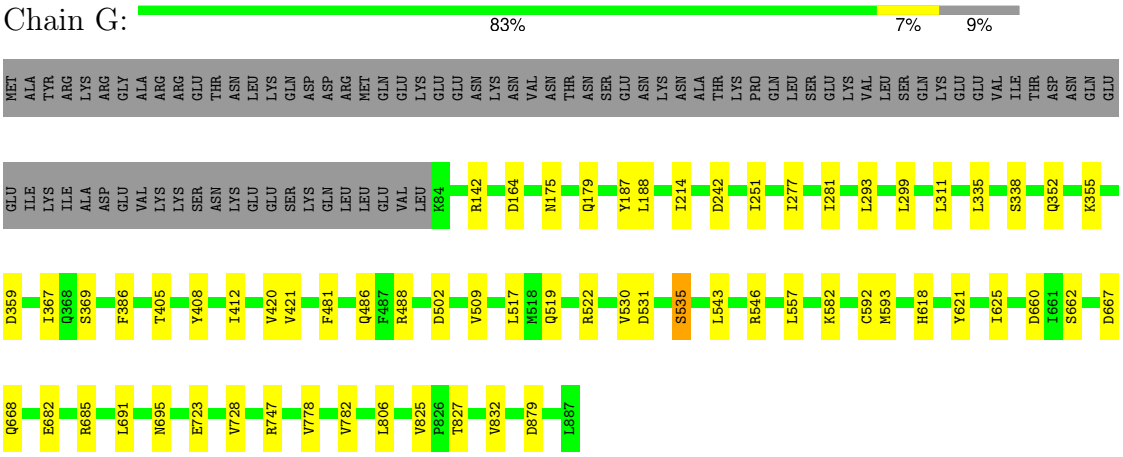
Chain F:





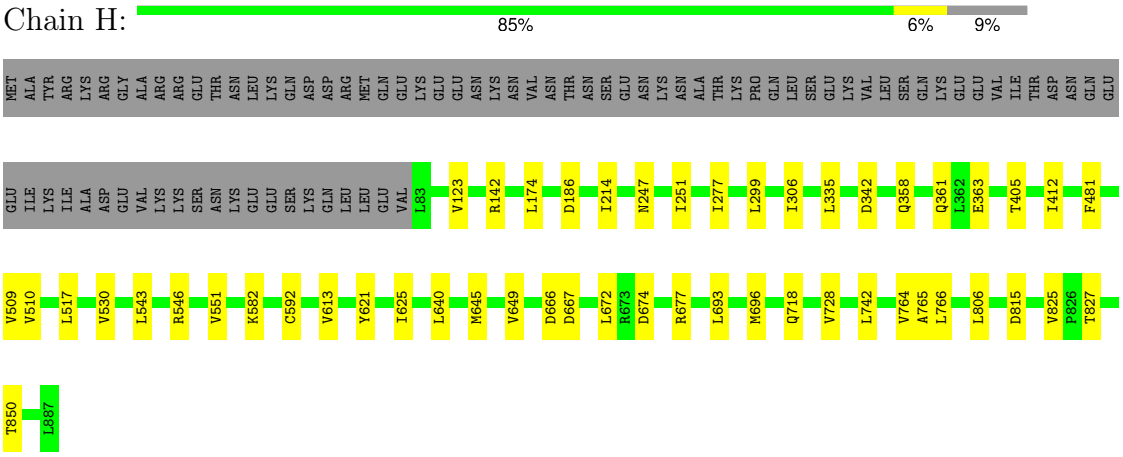
• Molecule 1: Inner capsid protein VP2

Chain G:



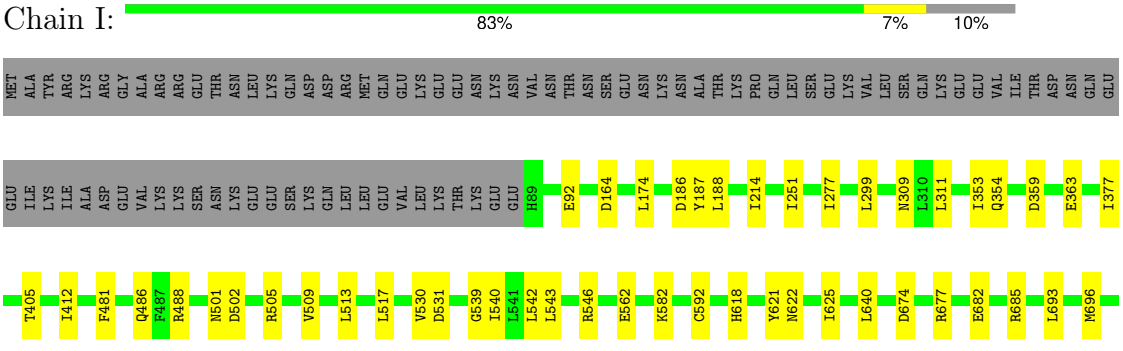
• Molecule 1: Inner capsid protein VP2

Chain H:



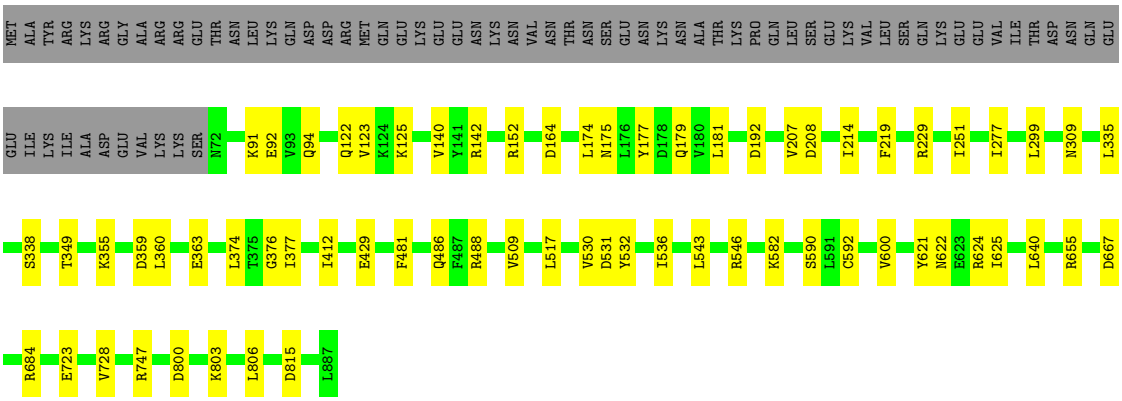
• Molecule 1: Inner capsid protein VP2

Chain I:



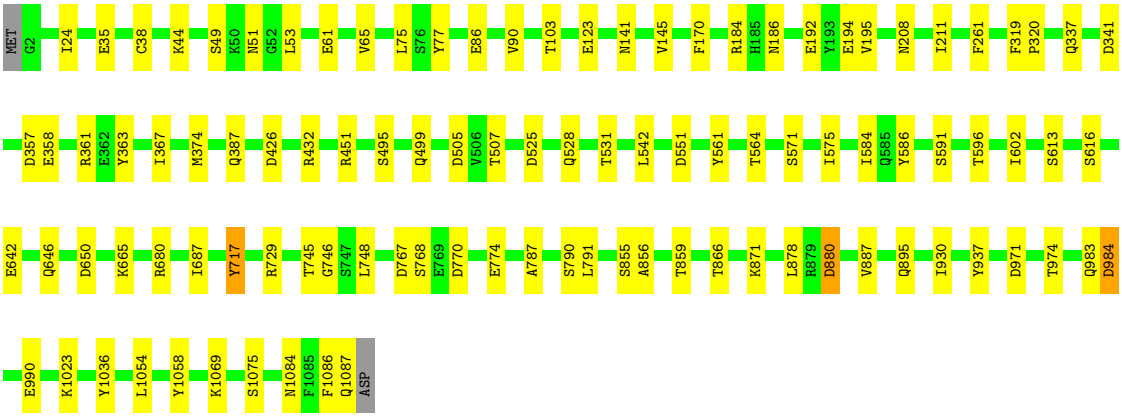
• Molecule 1: Inner capsid protein VP2

Chain J:



• Molecule 2: RNA-directed RNA polymerase

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	469892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	0.26	0/6503	0.50	0/8823
1	B	0.26	0/6494	0.49	0/8810
1	C	0.26	0/6689	0.50	0/9074
1	D	0.26	0/6884	0.49	0/9332
1	E	0.26	0/6617	0.50	0/8979
1	F	0.26	0/6706	0.49	0/9096
1	G	0.26	0/6698	0.49	0/9085
1	H	0.26	0/6706	0.49	0/9096
1	I	0.26	0/6655	0.49	0/9029
1	J	0.26	0/6797	0.49	0/9217
2	P	0.26	0/8967	0.48	0/12124
All	All	0.26	0/75716	0.49	0/102665

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	6387	6413	6413	43	0
1	B	6378	6408	6408	36	0
1	C	6569	6595	6595	41	0
1	D	6764	6809	6809	46	0
1	E	6498	6529	6529	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	6586	6619	6619	34	0
1	G	6578	6608	6608	37	0
1	H	6586	6619	6619	33	0
1	I	6535	6563	6563	34	0
1	J	6677	6713	6713	42	0
2	P	8793	8874	8872	62	0
All	All	74351	74750	74748	427	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 (427) 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)
2:P:937:TYR:OH	2:P:971:ASP:OD2	1.97	0.83
1:A:546:ARG:NH2	1:A:595:ILE:O	2.12	0.82
1:E:868:ASP:OD2	1:I:405:THR:OG1	1.99	0.80
1:J:91:LYS:NZ	2:P:642:GLU:OE2	2.15	0.80
2:P:768:SER:OG	2:P:774:GLU:OE2	2.00	0.80
1:A:368:GLN:NE2	2:P:990:GLU:OE2	2.18	0.77
1:E:270:GLU:OE1	1:E:307:ARG:NH1	2.18	0.76
1:H:247:ASN:OD1	1:H:850:THR:OG1	2.01	0.76
1:C:546:ARG:NH2	1:C:595:ILE:O	2.20	0.75
1:I:674:ASP:OD1	1:I:677:ARG:NH2	2.20	0.75
1:B:868:ASP:OD2	1:F:405:THR:OG1	2.02	0.75
1:A:523:GLN:O	1:A:533:LYS:NZ	2.18	0.74
1:B:546:ARG:NH2	1:B:595:ILE:O	2.21	0.74
1:E:546:ARG:NH2	1:E:595:ILE:O	2.20	0.74
2:P:880:ASP:OD2	2:P:1069:LYS:NZ	2.19	0.73
1:I:486:GLN:O	1:I:488:ARG:NH1	2.21	0.73
2:P:729:ARG:NH2	2:P:767:ASP:O	2.23	0.72
1:E:348:SER:OG	1:E:350:GLU:OE1	2.06	0.71
2:P:528:GLN:O	2:P:531:THR:OG1	2.08	0.71
2:P:44:LYS:NZ	2:P:61:GLU:OE2	2.23	0.71
1:I:786:ASP:OD2	1:I:830:THR:OG1	2.08	0.70
1:J:175:ASN:OD1	1:J:179:GLN:NE2	2.25	0.70
1:G:682:GLU:OE1	1:G:685:ARG:NH1	2.25	0.70
1:E:152:ARG:NH1	1:E:723:GLU:OE1	2.25	0.70
1:F:247:ASN:OD1	1:F:850:THR:OG1	2.05	0.69
1:G:486:GLN:O	1:G:488:ARG:NH1	2.25	0.69
1:H:412:ILE:HG22	1:H:543:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ASP:OD2	1:H:582:LYS:NZ	2.26	0.68
1:B:152:ARG:NH1	1:B:723:GLU:OE1	2.26	0.68
1:H:674:ASP:OD1	1:H:677:ARG:NH2	2.27	0.67
1:I:682:GLU:OE1	1:I:685:ARG:NH1	2.27	0.67
1:C:152:ARG:NH1	1:C:723:GLU:OE1	2.26	0.67
1:D:221:ASP:O	1:D:229:ARG:NH2	2.28	0.67
1:C:868:ASP:OD2	1:G:405:THR:OG1	2.09	0.67
1:E:723:GLU:OE2	1:E:839:GLN:NE2	2.28	0.67
2:P:571:SER:OG	2:P:586:TYR:O	2.14	0.66
1:A:175:ASN:OD1	1:A:179:GLN:NE2	2.29	0.66
1:D:546:ARG:NH2	1:D:595:ILE:O	2.29	0.65
1:F:353:ILE:HD11	1:F:377:ILE:HB	1.78	0.65
1:J:481:PHE:CE1	1:J:509:VAL:HG21	2.31	0.65
1:F:546:ARG:NH1	1:F:592:CYS:O	2.30	0.65
1:A:412:ILE:CG2	1:A:543:LEU:HD22	2.27	0.65
1:F:412:ILE:HG22	1:F:543:LEU:HD22	1.77	0.65
1:G:412:ILE:HG22	1:G:543:LEU:HD22	1.77	0.65
1:B:188:LEU:HD11	1:B:264:LEU:HD21	1.79	0.65
1:C:309:ASN:O	1:C:622:ASN:ND2	2.30	0.64
1:G:355:LYS:NZ	1:G:359:ASP:OD2	2.31	0.64
1:J:376:GLY:O	1:J:590:SER:OG	2.16	0.64
1:B:188:LEU:HD11	1:B:264:LEU:CD2	2.28	0.64
1:D:69:LYS:HA	1:D:80:LEU:HD11	1.79	0.64
1:C:556:LEU:O	1:C:560:ASN:ND2	2.31	0.63
1:E:296:ASP:OD2	1:I:582:LYS:NZ	2.31	0.63
1:C:104:THR:OG1	1:C:584:GLN:OE1	2.17	0.62
1:C:703:SER:O	1:C:834:LYS:NZ	2.31	0.61
1:E:412:ILE:CG2	1:E:543:LEU:HD22	2.31	0.61
1:A:311:LEU:O	1:A:618:HIS:NE2	2.33	0.61
1:I:481:PHE:CE1	1:I:509:VAL:HG21	2.35	0.61
1:J:486:GLN:O	1:J:488:ARG:NH1	2.33	0.61
1:J:723:GLU:N	1:J:723:GLU:OE1	2.32	0.61
2:P:791:LEU:HD22	2:P:856:ALA:HB1	1.82	0.61
1:E:311:LEU:O	1:E:618:HIS:NE2	2.33	0.61
1:B:723:GLU:OE2	1:B:839:GLN:NE2	2.33	0.60
1:A:125:LYS:NZ	1:A:192:ASP:OD2	2.33	0.60
1:G:660:ASP:OD1	1:G:662:SER:OG	2.19	0.60
1:E:601:ILE:HD11	1:E:869:THR:CG2	2.31	0.60
2:P:77:TYR:CZ	2:P:748:LEU:HD13	2.37	0.60
1:H:693:LEU:HD12	1:H:696:MET:SD	2.42	0.60
1:D:311:LEU:O	1:D:618:HIS:NE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:ILE:HD11	1:C:869:THR:HG21	1.84	0.59
1:G:175:ASN:ND2	1:G:179:GLN:OE1	2.35	0.59
1:H:174:LEU:HD22	1:H:640:LEU:HD12	1.84	0.59
2:P:261:PHE:O	2:P:507:THR:OG1	2.11	0.59
1:B:601:ILE:HD11	1:B:869:THR:CG2	2.33	0.59
2:P:680:ARG:HD3	2:P:687:ILE:HD11	1.84	0.59
1:A:154:TYR:OH	1:A:723:GLU:OE2	2.20	0.59
2:P:24:ILE:HD11	2:P:49:SER:OG	2.02	0.58
1:B:195:VAL:HG21	1:B:209:SER:HA	1.86	0.58
1:C:428:ARG:HG2	1:H:530:VAL:HG11	1.85	0.58
1:D:97:ILE:HD11	1:D:374:LEU:HB2	1.86	0.58
1:G:481:PHE:CD1	1:G:509:VAL:HG21	2.39	0.58
1:F:175:ASN:OD1	1:F:179:GLN:NE2	2.36	0.58
1:A:412:ILE:HG22	1:A:543:LEU:HD22	1.86	0.58
1:G:481:PHE:CE1	1:G:509:VAL:HG21	2.38	0.58
2:P:495:SER:OG	2:P:499:GLN:O	2.12	0.58
1:A:660:ASP:OD2	1:A:662:SER:OG	2.22	0.57
1:C:601:ILE:HD11	1:C:869:THR:CG2	2.35	0.57
1:D:137:GLN:NE2	1:D:221:ASP:OD2	2.35	0.57
1:D:663:ARG:NE	1:I:354:GLN:OE1	2.37	0.57
1:F:309:ASN:O	1:F:622:ASN:ND2	2.36	0.57
1:F:481:PHE:CE1	1:F:509:VAL:HG21	2.39	0.57
1:H:481:PHE:CE1	1:H:509:VAL:HG21	2.38	0.57
1:H:546:ARG:NH1	1:H:592:CYS:O	2.36	0.57
1:A:703:SER:O	1:A:834:LYS:NZ	2.34	0.57
1:H:517:LEU:HD11	1:H:543:LEU:HD23	1.87	0.57
1:J:309:ASN:O	1:J:622:ASN:ND2	2.38	0.56
1:C:480:HIS:O	1:C:484:ASN:ND2	2.37	0.56
1:G:311:LEU:O	1:G:618:HIS:NE2	2.36	0.56
1:J:355:LYS:NZ	1:J:359:ASP:OD2	2.37	0.56
1:F:270:GLU:OE1	1:F:307:ARG:NH1	2.38	0.56
2:P:363:TYR:CZ	2:P:367:ILE:HD11	2.40	0.56
2:P:729:ARG:NE	2:P:770:ASP:OD1	2.38	0.56
1:H:825:VAL:O	1:H:827:THR:HG23	2.06	0.56
1:H:363:GLU:OE1	1:H:363:GLU:N	2.37	0.56
1:D:398:THR:HB	1:D:580:THR:HG22	1.87	0.56
1:E:786:ASP:OD2	1:E:828:SER:OG	2.24	0.56
1:G:517:LEU:HD11	1:G:543:LEU:HD23	1.88	0.56
1:D:601:ILE:HD11	1:D:869:THR:OG1	2.05	0.55
2:P:887:VAL:HG22	2:P:1054:LEU:CD2	2.35	0.55
1:D:396:GLN:OE1	1:D:574:HIS:ND1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:PHE:CD1	1:F:509:VAL:HG21	2.41	0.55
1:E:309:ASN:O	1:E:622:ASN:ND2	2.37	0.55
1:C:397:ARG:NH2	1:C:579:THR:OG1	2.40	0.55
1:D:403:PHE:HB3	1:D:585:LEU:HD12	1.89	0.55
1:H:742:LEU:HD21	1:H:766:LEU:HB3	1.89	0.55
2:P:1084:ASN:O	2:P:1087:GLN:NE2	2.36	0.55
1:B:311:LEU:O	1:B:618:HIS:NE2	2.37	0.55
1:D:868:ASP:OD2	1:H:405:THR:OG1	2.14	0.55
1:H:481:PHE:CD1	1:H:509:VAL:HG21	2.42	0.55
1:E:412:ILE:HG22	1:E:543:LEU:HD22	1.88	0.55
1:D:336:ALA:O	1:D:340:VAL:HG23	2.06	0.55
2:P:103:THR:HG22	2:P:103:THR:O	2.06	0.55
1:A:868:ASP:OD1	1:A:869:THR:N	2.40	0.55
1:D:152:ARG:NH1	1:D:723:GLU:OE1	2.40	0.55
1:I:546:ARG:NH1	1:I:592:CYS:O	2.40	0.54
1:I:621:TYR:CZ	1:I:625:ILE:HD11	2.41	0.54
1:J:377:ILE:O	1:J:377:ILE:HG22	2.07	0.54
1:A:718:GLN:HA	1:A:827:THR:HG22	1.90	0.54
1:E:125:LYS:NZ	1:E:192:ASP:OD2	2.41	0.54
1:I:481:PHE:CD1	1:I:509:VAL:HG21	2.42	0.54
1:J:125:LYS:NZ	1:J:192:ASP:OD2	2.33	0.54
1:D:352:GLN:NE2	1:D:593:MET:O	2.41	0.54
1:G:667:ASP:OD1	1:G:668:GLN:N	2.41	0.54
2:P:855:SER:O	2:P:859:THR:HG23	2.07	0.54
2:P:787:ALA:O	2:P:790:SER:OG	2.18	0.54
1:I:164:ASP:N	1:I:164:ASP:OD1	2.40	0.54
1:J:546:ARG:NH1	1:J:592:CYS:O	2.40	0.54
2:P:505:ASP:OD1	2:P:505:ASP:N	2.41	0.54
2:P:561:TYR:O	2:P:564:THR:OG1	2.22	0.53
1:C:350:GLU:OE2	1:D:71:SER:OG	2.08	0.53
1:D:344:LYS:NZ	1:D:345:GLU:OE2	2.41	0.53
1:E:601:ILE:HD11	1:E:869:THR:HG21	1.89	0.53
1:F:277:ILE:HD11	1:F:299:LEU:HD11	1.90	0.53
1:H:815:ASP:OD1	1:H:815:ASP:N	2.39	0.53
1:B:601:ILE:HD11	1:B:869:THR:HG21	1.90	0.53
1:C:311:LEU:O	1:C:618:HIS:NE2	2.37	0.53
1:J:363:GLU:N	1:J:363:GLU:OE1	2.41	0.53
2:P:186:ASN:ND2	2:P:192:GLU:OE2	2.40	0.53
1:A:336:ALA:O	1:A:340:VAL:HG23	2.09	0.53
1:B:420:VAL:HG23	1:B:421:VAL:HG23	1.91	0.53
1:D:320:ASN:O	1:D:671:ARG:NH2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:THR:HB	1:C:580:THR:HG22	1.91	0.53
1:D:397:ARG:NH2	1:D:579:THR:OG1	2.40	0.53
2:P:24:ILE:HD12	2:P:77:TYR:HE1	1.73	0.53
2:P:141:ASN:ND2	2:P:208:ASN:OD1	2.41	0.53
1:E:195:VAL:HG21	1:E:209:SER:HA	1.91	0.52
1:B:621:TYR:CZ	1:B:625:ILE:HD11	2.43	0.52
1:D:117:ASP:O	1:D:119:LYS:NZ	2.39	0.52
1:J:728:VAL:CG2	1:J:806:LEU:HD11	2.40	0.52
2:P:24:ILE:HD12	2:P:77:TYR:CE1	2.44	0.52
1:A:541:LEU:HD13	1:E:528:MET:CE	2.40	0.52
1:E:420:VAL:HG23	1:E:421:VAL:HG23	1.90	0.52
1:C:221:ASP:O	1:C:229:ARG:NH2	2.42	0.52
1:B:718:GLN:HA	1:B:827:THR:HG22	1.92	0.52
1:C:543:LEU:HG	1:C:550:LEU:HD11	1.91	0.52
2:P:887:VAL:HG22	2:P:1054:LEU:HD21	1.91	0.51
1:J:349:THR:OG1	2:P:358:GLU:OE2	2.11	0.51
2:P:51:ASN:OD1	2:P:53:LEU:HD13	2.10	0.51
1:E:800:ASP:OD1	1:E:801:THR:N	2.44	0.51
1:J:481:PHE:CD1	1:J:509:VAL:HG21	2.45	0.51
1:D:125:LYS:NZ	1:D:192:ASP:OD2	2.41	0.51
1:F:815:ASP:OD1	1:F:815:ASP:N	2.44	0.51
1:G:621:TYR:CZ	1:G:625:ILE:HD11	2.46	0.51
1:I:309:ASN:O	1:I:622:ASN:ND2	2.39	0.51
2:P:357:ASP:OD2	2:P:361:ARG:NE	2.43	0.51
1:G:367:ILE:HG22	1:G:369:SER:H	1.76	0.51
1:E:682:GLU:OE1	1:E:685:ARG:NH1	2.44	0.51
1:B:432:VAL:HG12	1:C:887:LEU:HD22	1.91	0.51
1:C:728:VAL:HG23	1:C:807:TYR:O	2.10	0.51
1:D:517:LEU:CD1	1:D:543:LEU:HD23	2.41	0.51
1:J:92:GLU:OE2	1:J:94:GLN:NE2	2.40	0.50
1:H:277:ILE:HD11	1:H:299:LEU:HD11	1.94	0.50
1:E:202:ASP:OD2	1:E:236:ARG:NH1	2.44	0.50
1:A:601:ILE:HD11	1:A:869:THR:CG2	2.41	0.50
1:B:336:ALA:O	1:B:340:VAL:HG23	2.11	0.50
1:F:358:GLN:O	1:F:361:GLN:NE2	2.38	0.50
1:G:352:GLN:NE2	1:G:593:MET:O	2.40	0.50
1:H:621:TYR:CZ	1:H:625:ILE:HD11	2.47	0.50
1:J:621:TYR:CZ	1:J:625:ILE:HD11	2.46	0.50
1:J:815:ASP:OD1	1:J:815:ASP:N	2.44	0.49
1:A:397:ARG:NH2	1:A:579:THR:OG1	2.44	0.49
1:B:660:ASP:OD2	1:B:662:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:GLU:HG3	1:B:873:ILE:HG22	1.94	0.49
1:A:356:MET:HG2	1:A:542:LEU:HD22	1.94	0.49
1:J:360:LEU:HD12	1:J:374:LEU:HD21	1.95	0.49
2:P:194:GLU:N	2:P:194:GLU:OE1	2.46	0.49
1:E:740:ILE:HD12	1:E:764:VAL:HG21	1.93	0.49
1:I:723:GLU:OE1	1:I:723:GLU:N	2.42	0.49
1:F:718:GLN:HA	1:F:827:THR:HG22	1.95	0.49
1:A:420:VAL:HG23	1:A:421:VAL:HG23	1.94	0.49
1:J:140:VAL:HG11	1:J:152:ARG:HD2	1.94	0.49
1:A:786:ASP:OD2	1:A:828:SER:OG	2.31	0.49
1:G:214:ILE:HG21	1:G:251:ILE:HG21	1.95	0.49
2:P:717:TYR:OH	2:P:770:ASP:OD2	2.21	0.49
2:P:1023:LYS:NZ	2:P:1058:TYR:O	2.37	0.49
1:C:188:LEU:HD23	1:C:264:LEU:CD2	2.42	0.48
1:E:505:ARG:NH2	1:E:562:GLU:OE1	2.45	0.48
1:G:546:ARG:NH1	1:G:592:CYS:O	2.46	0.48
1:B:728:VAL:HG23	1:B:807:TYR:O	2.13	0.48
1:D:309:ASN:O	1:D:622:ASN:ND2	2.43	0.48
1:F:230:ARG:NH1	1:F:234:GLU:OE2	2.47	0.48
1:I:174:LEU:HD22	1:I:640:LEU:CD1	2.43	0.48
1:I:728:VAL:CG2	1:I:806:LEU:HD11	2.42	0.48
1:E:621:TYR:CZ	1:E:625:ILE:HD11	2.49	0.48
1:F:517:LEU:HB2	1:F:540:ILE:HG23	1.94	0.48
1:G:335:LEU:O	1:G:338:SER:OG	2.30	0.48
1:D:403:PHE:CB	1:D:585:LEU:HD12	2.43	0.48
1:A:294:ASN:OD1	1:A:295:MET:N	2.46	0.48
1:A:723:GLU:OE2	1:A:839:GLN:NE2	2.46	0.48
1:B:786:ASP:OD2	1:B:828:SER:OG	2.31	0.48
1:C:195:VAL:HG21	1:C:209:SER:HA	1.96	0.48
1:C:188:LEU:HD23	1:C:264:LEU:HG	1.96	0.48
1:G:281:ILE:HD13	1:G:293:LEU:HD13	1.96	0.47
2:P:930:ILE:N	2:P:984:ASP:OD2	2.45	0.47
1:C:778:VAL:HG22	1:C:809:ILE:HG23	1.96	0.47
2:P:591:SER:HA	2:P:596:THR:HG21	1.96	0.47
1:H:718:GLN:HA	1:H:827:THR:HG22	1.95	0.47
1:C:621:TYR:CZ	1:C:625:ILE:HD11	2.50	0.47
1:C:786:ASP:OD2	1:C:828:SER:OG	2.32	0.47
1:J:122:GLN:OE1	1:J:123:VAL:N	2.47	0.47
1:A:541:LEU:HD13	1:E:528:MET:HE1	1.96	0.47
1:C:728:VAL:HG22	1:C:730:ILE:HG12	1.95	0.47
1:D:621:TYR:CZ	1:D:625:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:311:LEU:O	1:I:618:HIS:NE2	2.41	0.47
1:I:353:ILE:HD11	1:I:377:ILE:HB	1.96	0.47
2:P:145:VAL:HG11	2:P:170:PHE:CD1	2.49	0.47
1:E:403:PHE:HB3	1:E:585:LEU:HD12	1.97	0.47
1:J:412:ILE:HG22	1:J:543:LEU:HD22	1.96	0.47
2:P:646:GLN:NE2	2:P:650:ASP:OD1	2.47	0.47
1:E:363:GLU:O	2:P:983:GLN:NE2	2.48	0.46
1:C:420:VAL:HG23	1:C:421:VAL:HG23	1.97	0.46
1:C:660:ASP:OD2	1:C:662:SER:OG	2.34	0.46
1:C:403:PHE:CB	1:C:585:LEU:HD12	2.46	0.46
1:D:786:ASP:OD2	1:D:828:SER:OG	2.33	0.46
1:C:467:GLU:OE2	1:C:480:HIS:ND1	2.40	0.46
1:F:367:ILE:HG22	1:F:369:SER:H	1.81	0.46
1:D:428:ARG:HG2	1:I:530:VAL:HG11	1.97	0.46
1:I:746:MET:SD	1:I:747:ARG:NH1	2.89	0.46
1:D:154:TYR:OH	1:D:723:GLU:OE2	2.33	0.46
2:P:745:THR:HG22	2:P:746:GLY:H	1.81	0.46
1:A:853:LEU:HD23	1:J:667:ASP:HA	1.98	0.45
1:F:751:TYR:O	1:F:755:THR:OG1	2.22	0.45
1:G:519:GLN:OE1	1:G:522:ARG:NH2	2.47	0.45
1:D:577:THR:OG1	1:D:579:THR:O	2.29	0.45
1:H:174:LEU:HD22	1:H:640:LEU:CD1	2.47	0.45
1:D:778:VAL:HG22	1:D:809:ILE:HG23	1.97	0.45
1:A:296:ASP:OD2	1:J:582:LYS:NZ	2.49	0.45
1:A:403:PHE:HB3	1:A:585:LEU:HD12	1.99	0.45
2:P:387:GLN:NE2	2:P:551:ASP:OD2	2.46	0.45
2:P:575:ILE:HD12	2:P:584:ILE:HD12	1.97	0.45
1:A:728:VAL:HG23	1:A:807:TYR:O	2.17	0.45
1:F:311:LEU:O	1:F:618:HIS:NE2	2.47	0.45
1:F:755:THR:HG23	1:F:794:VAL:HG13	1.97	0.45
2:P:542:LEU:HD11	2:P:561:TYR:HD1	1.82	0.45
1:B:703:SER:O	1:B:834:LYS:NZ	2.45	0.45
1:D:764:VAL:HG22	1:D:765:ALA:N	2.31	0.45
1:I:187:TYR:C	1:I:188:LEU:HD12	2.37	0.45
1:J:177:TYR:CZ	1:J:181:LEU:HD11	2.51	0.45
2:P:75:LEU:HD22	2:P:748:LEU:HD11	1.97	0.45
1:D:467:GLU:OE1	1:D:483:ASN:ND2	2.45	0.45
1:C:481:PHE:CZ	1:C:509:VAL:HG11	2.52	0.44
1:A:185:PRO:O	1:A:684:ARG:NH2	2.50	0.44
1:I:214:ILE:HG21	1:I:251:ILE:HG21	1.99	0.44
1:D:360:LEU:HD21	1:D:542:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:SER:O	1:E:834:LYS:NZ	2.51	0.44
1:H:728:VAL:CG2	1:H:806:LEU:HD11	2.48	0.44
2:P:86:GLU:O	2:P:90:VAL:HG13	2.17	0.44
1:E:517:LEU:CD1	1:E:543:LEU:HD23	2.47	0.44
1:F:718:GLN:HG2	1:F:825:VAL:HG11	1.99	0.44
1:G:187:TYR:C	1:G:188:LEU:HD12	2.38	0.44
1:H:277:ILE:CD1	1:H:299:LEU:HD11	2.47	0.44
1:A:403:PHE:CB	1:A:585:LEU:HD12	2.47	0.44
1:C:353:ILE:HD11	1:C:377:ILE:HB	1.99	0.44
1:E:428:ARG:HG2	1:J:530:VAL:HG21	2.00	0.44
1:G:825:VAL:O	1:G:827:THR:HG23	2.17	0.44
1:I:531:ASP:N	1:I:531:ASP:OD1	2.51	0.44
1:J:800:ASP:N	1:J:800:ASP:OD1	2.50	0.44
1:B:740:ILE:HD12	1:B:764:VAL:HG21	2.00	0.44
1:G:408:TYR:OH	1:G:535:SER:OG	2.35	0.44
1:F:174:LEU:HD22	1:F:640:LEU:HD12	2.00	0.44
1:D:853:LEU:HD23	1:H:667:ASP:HA	2.00	0.43
1:J:214:ILE:HG21	1:J:251:ILE:HG21	2.00	0.43
1:A:309:ASN:O	1:A:622:ASN:ND2	2.46	0.43
1:D:624:ARG:HD2	1:D:655:ARG:HB3	2.00	0.43
1:E:871:GLU:HG3	1:E:873:ILE:HG22	1.99	0.43
1:G:386:PHE:CE1	1:G:557:LEU:HD12	2.54	0.43
1:H:649:VAL:HG13	1:H:672:LEU:HD23	2.00	0.43
1:I:517:LEU:HB2	1:I:540:ILE:HG23	1.99	0.43
1:D:755:THR:HG23	1:D:794:VAL:HG13	2.01	0.43
1:F:214:ILE:HG21	1:F:251:ILE:HG21	1.99	0.43
1:G:242:ASP:OD1	1:G:242:ASP:N	2.51	0.43
1:G:778:VAL:O	1:G:782:VAL:HG23	2.18	0.43
1:J:349:THR:HG23	1:J:377:ILE:O	2.18	0.43
1:A:755:THR:HG23	1:A:794:VAL:HG13	2.01	0.43
1:B:505:ARG:NH2	1:B:562:GLU:OE1	2.47	0.43
2:P:613:SER:O	2:P:616:SER:OG	2.35	0.43
1:E:353:ILE:HG13	2:P:974:THR:HG23	2.00	0.43
1:E:517:LEU:HD13	1:E:543:LEU:HD23	2.01	0.43
1:I:412:ILE:HG22	1:I:543:LEU:HD22	1.99	0.43
1:I:513:LEU:O	1:I:517:LEU:HG	2.19	0.43
1:J:174:LEU:HD22	1:J:640:LEU:CD1	2.48	0.43
2:P:374:MET:SD	2:P:602:ILE:HD11	2.58	0.43
1:A:272:LEU:HD11	1:A:277:ILE:HG13	2.01	0.43
1:B:734:LEU:HD21	1:B:833:TYR:CG	2.53	0.43
1:I:764:VAL:HG22	1:I:765:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:145:VAL:CG2	2:P:211:ILE:HG23	2.49	0.43
1:F:420:VAL:HG23	1:F:421:VAL:HG23	2.00	0.43
1:G:691:LEU:O	1:G:695:ASN:ND2	2.52	0.43
2:P:184:ARG:H	2:P:195:VAL:HG21	1.83	0.43
2:P:319:PHE:N	2:P:320:PRO:HD2	2.33	0.43
1:F:277:ILE:CD1	1:F:299:LEU:HD11	2.49	0.43
1:G:420:VAL:HG23	1:G:421:VAL:HG23	2.00	0.43
1:H:510:VAL:HB	1:H:551:VAL:HG22	2.01	0.43
1:I:825:VAL:O	1:I:827:THR:HG23	2.19	0.43
1:J:621:TYR:CE2	1:J:625:ILE:HD11	2.54	0.43
1:A:764:VAL:HG22	1:A:765:ALA:H	1.84	0.42
1:G:723:GLU:OE1	1:G:723:GLU:N	2.50	0.42
2:P:337:GLN:O	2:P:451:ARG:NH1	2.46	0.42
1:A:604:PRO:HB2	1:A:867:ALA:HB3	2.01	0.42
1:A:624:ARG:HD2	1:A:655:ARG:HB3	2.01	0.42
1:A:682:GLU:OE1	1:A:685:ARG:NH1	2.52	0.42
1:B:108:LYS:HG3	1:B:334:ILE:HD12	2.01	0.42
1:D:728:VAL:HG23	1:D:807:TYR:O	2.19	0.42
1:F:740:ILE:HD12	1:F:764:VAL:HG21	2.01	0.42
1:H:186:ASP:OD2	1:H:186:ASP:N	2.51	0.42
1:E:621:TYR:CE2	1:E:625:ILE:HD11	2.54	0.42
1:F:424:ASP:OD1	1:F:424:ASP:N	2.52	0.42
1:E:329:THR:HG21	1:E:577:THR:HG21	2.01	0.42
1:E:449:MET:SD	1:E:470:ILE:HD13	2.59	0.42
1:E:353:ILE:HG23	1:E:374:LEU:HD23	2.02	0.42
1:H:214:ILE:HG21	1:H:251:ILE:HG21	2.01	0.42
1:H:517:LEU:CD1	1:H:543:LEU:HD23	2.49	0.42
2:P:426:ASP:OD2	2:P:432:ARG:NH2	2.51	0.42
1:B:764:VAL:HG22	1:B:765:ALA:H	1.84	0.42
1:J:531:ASP:OD1	1:J:531:ASP:N	2.52	0.42
2:P:531:THR:H	2:P:531:THR:HG1	1.62	0.42
1:D:605:GLN:NE2	1:D:867:ALA:O	2.50	0.42
1:I:539:GLY:HA2	1:I:542:LEU:HD12	2.02	0.42
1:B:624:ARG:HD2	1:B:655:ARG:HB3	2.02	0.42
1:F:170:ARG:NE	1:F:638:LEU:O	2.52	0.42
1:H:123:VAL:HG22	1:H:306:ILE:HD12	2.01	0.42
1:I:277:ILE:CD1	1:I:299:LEU:HD11	2.50	0.42
1:I:501:ASN:OD1	1:I:502:ASP:N	2.53	0.42
1:A:740:ILE:HD12	1:A:764:VAL:HG21	2.01	0.42
1:C:294:ASN:OD1	1:C:295:MET:N	2.52	0.42
1:D:781:LEU:HD13	1:D:807:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:871:GLU:HG3	1:D:873:ILE:HG22	2.01	0.42
1:G:879:ASP:OD1	1:G:879:ASP:N	2.51	0.42
1:J:164:ASP:OD1	1:J:164:ASP:N	2.42	0.42
1:B:175:ASN:OD1	1:B:179:GLN:NE2	2.49	0.42
1:D:728:VAL:HG22	1:D:730:ILE:HG13	2.02	0.42
1:F:645:MET:SD	1:F:645:MET:N	2.93	0.42
2:P:35:GLU:OE2	2:P:866:THR:HG22	2.19	0.42
1:A:601:ILE:HD11	1:A:869:THR:HG21	2.01	0.41
1:B:365:LEU:HD13	1:C:365:LEU:HG	2.00	0.41
1:J:600:VAL:O	1:J:600:VAL:HG23	2.20	0.41
2:P:878:LEU:HD22	2:P:1036:TYR:CD1	2.55	0.41
1:A:281:ILE:HD13	1:A:293:LEU:HD13	2.02	0.41
1:C:624:ARG:HD2	1:C:655:ARG:HB3	2.02	0.41
1:D:420:VAL:HG23	1:D:421:VAL:HG23	2.02	0.41
1:E:654:LYS:HG3	1:E:661:ILE:HD13	2.03	0.41
1:G:531:ASP:OD1	1:G:531:ASP:N	2.50	0.41
2:P:38:CYS:SG	2:P:65:VAL:HG13	2.60	0.41
1:A:783:ALA:HB3	1:A:785:LEU:HD13	2.02	0.41
1:B:131:ARG:NH2	1:B:211:THR:OG1	2.52	0.41
1:B:188:LEU:HD11	1:B:264:LEU:HD23	2.02	0.41
1:D:467:GLU:OE2	1:D:480:HIS:ND1	2.42	0.41
1:E:343:LEU:HB3	1:E:346:LEU:HD21	2.00	0.41
1:G:164:ASP:OD1	1:G:164:ASP:N	2.53	0.41
1:J:207:VAL:HA	1:J:208:ASP:HA	1.88	0.41
1:D:188:LEU:HD22	1:D:264:LEU:HD21	2.02	0.41
1:D:273:ASN:ND2	1:D:276:ILE:HD12	2.35	0.41
1:H:335:LEU:CD1	1:H:613:VAL:HG11	2.51	0.41
1:I:693:LEU:HD12	1:I:696:MET:SD	2.61	0.41
1:C:141:TYR:N	1:C:723:GLU:O	2.51	0.41
1:J:219:PHE:O	1:J:229:ARG:NH1	2.51	0.41
1:B:296:ASP:OD1	1:B:296:ASP:N	2.48	0.41
1:H:764:VAL:HG22	1:H:765:ALA:N	2.35	0.41
1:J:429:GLU:OE1	1:J:429:GLU:N	2.53	0.41
1:A:600:VAL:HG23	1:A:600:VAL:O	2.21	0.41
1:A:764:VAL:HG22	1:A:765:ALA:N	2.36	0.41
1:E:356:MET:HG2	1:E:542:LEU:HD22	2.03	0.41
1:G:806:LEU:HD13	1:G:832:VAL:HB	2.02	0.41
1:I:505:ARG:NH2	1:I:562:GLU:OE1	2.46	0.41
1:F:403:PHE:HB3	1:F:585:LEU:HD12	2.01	0.41
1:J:532:TYR:CE2	1:J:536:ILE:HD11	2.56	0.41
1:C:449:MET:SD	1:C:470:ILE:HD13	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:LEU:HD12	1:G:188:LEU:N	2.36	0.41
1:I:186:ASP:N	1:I:186:ASP:OD1	2.53	0.41
1:J:517:LEU:HD11	1:J:543:LEU:HD23	2.03	0.41
1:C:764:VAL:HG22	1:C:765:ALA:N	2.35	0.41
1:B:428:ARG:HG2	1:G:530:VAL:HG11	2.02	0.40
1:B:853:LEU:HD23	1:F:667:ASP:HA	2.01	0.40
1:E:653:LEU:HD23	1:E:656:LEU:HD12	2.03	0.40
1:F:513:LEU:O	1:F:517:LEU:HG	2.20	0.40
1:F:723:GLU:OE1	1:F:723:GLU:N	2.49	0.40
1:G:728:VAL:CG2	1:G:806:LEU:HD11	2.50	0.40
2:P:77:TYR:CE1	2:P:748:LEU:HD13	2.56	0.40
2:P:123:GLU:OE1	2:P:123:GLU:N	2.48	0.40
1:A:273:ASN:OD1	1:A:276:ILE:HD12	2.21	0.40
1:B:621:TYR:CE2	1:B:625:ILE:HD11	2.57	0.40
1:C:115:LEU:HD23	1:C:335:LEU:HB2	2.01	0.40
1:C:403:PHE:HB3	1:C:585:LEU:HD12	2.04	0.40
1:E:728:VAL:HG22	1:E:730:ILE:HG13	2.02	0.40
1:J:277:ILE:CD1	1:J:299:LEU:HD11	2.50	0.40
1:J:335:LEU:O	1:J:338:SER:OG	2.33	0.40
2:P:1084:ASN:ND2	2:P:1086:PHE:O	2.54	0.40
1:B:236:ARG:NH2	1:B:237:GLN:O	2.53	0.40
2:P:542:LEU:HD11	2:P:561:TYR:CD1	2.56	0.40
1:B:481:PHE:CZ	1:B:509:VAL:HG11	2.56	0.40
1:C:734:LEU:HD21	1:C:833:TYR:CG	2.56	0.40
1:E:294:ASN:OD1	1:E:295:MET:N	2.55	0.40
1:E:360:LEU:HD21	1:E:542:LEU:HD11	2.02	0.40
1:J:624:ARG:HD2	1:J:655:ARG:HB3	2.04	0.40
1:F:231:PHE:O	1:F:235:MET:N	2.51	0.40
1:G:277:ILE:HD11	1:G:299:LEU:HD11	2.03	0.40
1:H:358:GLN:O	1:H:361:GLN:NE2	2.54	0.40
1:H:412:ILE:CG2	1:H:543:LEU:HD22	2.47	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	780/887 (88%)	767 (98%)	13 (2%)	0	100	100
1	B	779/887 (88%)	767 (98%)	12 (2%)	0	100	100
1	C	801/887 (90%)	787 (98%)	14 (2%)	0	100	100
1	D	825/887 (93%)	811 (98%)	13 (2%)	1 (0%)	48	67
1	E	793/887 (89%)	782 (99%)	11 (1%)	0	100	100
1	F	803/887 (90%)	789 (98%)	14 (2%)	0	100	100
1	G	802/887 (90%)	789 (98%)	13 (2%)	0	100	100
1	H	803/887 (90%)	790 (98%)	13 (2%)	0	100	100
1	I	797/887 (90%)	787 (99%)	10 (1%)	0	100	100
1	J	814/887 (92%)	800 (98%)	14 (2%)	0	100	100
2	P	1084/1088 (100%)	1054 (97%)	30 (3%)	0	100	100
All	All	9081/9958 (91%)	8923 (98%)	157 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	PHE

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	718/818 (88%)	715 (100%)	3 (0%)	89	95
1	B	717/818 (88%)	712 (99%)	5 (1%)	81	90
1	C	739/818 (90%)	733 (99%)	6 (1%)	79	89
1	D	762/818 (93%)	759 (100%)	3 (0%)	89	95
1	E	731/818 (89%)	727 (100%)	4 (0%)	86	94
1	F	741/818 (91%)	732 (99%)	9 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	740/818 (90%)	735 (99%)	5 (1%)	81 90
1	H	741/818 (91%)	737 (100%)	4 (0%)	86 94
1	I	735/818 (90%)	731 (100%)	4 (0%)	86 94
1	J	752/818 (92%)	748 (100%)	4 (0%)	86 94
2	P	987/989 (100%)	978 (99%)	9 (1%)	75 87
All	All	8363/9169 (91%)	8307 (99%)	56 (1%)	80 90

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ARG
1	A	278	PHE
1	A	843	ARG
1	B	238	ARG
1	B	278	PHE
1	B	574	HIS
1	B	666	ASP
1	B	843	ARG
1	C	238	ARG
1	C	278	PHE
1	C	423	ASN
1	C	545	ASN
1	C	666	ASP
1	C	843	ARG
1	D	238	ARG
1	D	667	ASP
1	D	843	ARG
1	E	125	LYS
1	E	278	PHE
1	E	665	PRO
1	E	667	ASP
1	F	100	LYS
1	F	342	ASP
1	F	368	GLN
1	F	488	ARG
1	F	502	ASP
1	F	582	LYS
1	F	684	ARG
1	F	733	ASN
1	F	747	ARG

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Mol	Chain	Res	Type
1	G	142	ARG
1	G	502	ASP
1	G	535	SER
1	G	582	LYS
1	G	747	ARG
1	H	142	ARG
1	H	342	ASP
1	H	645	MET
1	H	666	ASP
1	I	92	GLU
1	I	359	ASP
1	I	363	GLU
1	I	815	ASP
1	J	142	ARG
1	J	684	ARG
1	J	747	ARG
1	J	803	LYS
2	P	341	ASP
2	P	525	ASP
2	P	665	LYS
2	P	717	TYR
2	P	871	LYS
2	P	880	ASP
2	P	895	GLN
2	P	984	ASP
2	P	1075	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45123. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.