



Full wwPDB EM Validation Report ⓘ

Nov 16, 2025 – 01:28 AM JST

PDB ID : 9VEL / pdb_00009vel
EMDB ID : EMD-65011
Title : The composite cryo-EM structure of bacteriophage SPO1 capsid
Authors : Zhao, X.; Wang, A.; Wang, Y.; Kang, Y.; Shao, Q.; Li, L.; Zheng, Y.; Hu, H.;
Li, X.; Fan, H.; Cai, C.; Liu, B.; Fang, Q.
Deposited on : 2025-06-09
Resolution : 3.00 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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

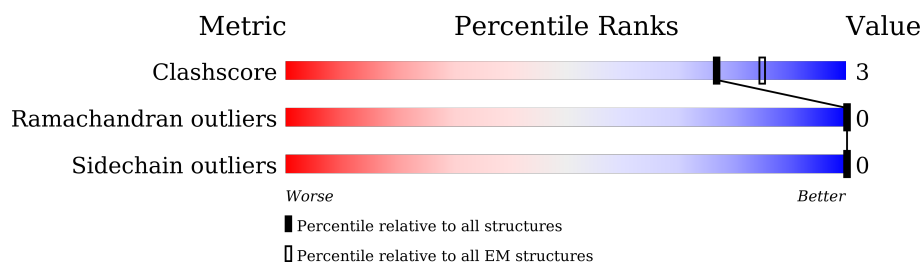
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	468	87% 6% 7%
1	B	468	89% 6% 5%
1	C	468	90% . 5%
1	D	468	86% 8% 6%
1	E	468	87% 8% 6%
1	F	468	87% 7% 5%
1	G	468	89% 6% 5%
1	H	468	88% 6% 6%
1	I	468	87% 9% 5%

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Mol	Chain	Length	Quality of chain
1	J	468	 85% 9% 6%
1	K	468	 85% 9% 6%
1	L	468	 88% 7% 5%
1	M	468	 87% 8% 5%
1	N	468	 88% 6% 6%
1	O	468	 85% 9% 6%
1	P	468	 88% 7% 5%
2	q	171	 93% 7%
2	r	171	 92% 8%
2	s	171	 86% 14%
2	v	171	 93% 7%
3	t	57	 95% 5%
4	w	96	 63% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 61498 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 Gp6.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	444	Total	C	N	O	S	0	0
			3447	2201	571	657	18		
1	F	444	Total	C	N	O	S	0	0
			3447	2201	571	657	18		
1	G	445	Total	C	N	O	S	0	0
			3455	2205	573	659	18		
1	D	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	I	445	Total	C	N	O	S	0	0
			3455	2205	573	659	18		
1	J	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	O	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	N	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	M	445	Total	C	N	O	S	0	0
			3455	2205	573	659	18		
1	H	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	K	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	L	445	Total	C	N	O	S	0	0
			3455	2205	573	659	18		
1	B	445	Total	C	N	O	S	0	0
			3455	2205	573	659	18		
1	E	441	Total	C	N	O	S	0	0
			3423	2184	568	653	18		
1	P	444	Total	C	N	O	S	0	0
			3447	2201	571	657	18		
1	A	434	Total	C	N	O	S	0	0
			3370	2153	559	640	18		

- Molecule 2 is a protein called Gp29.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	r	171	Total	C	N	O	S	0	0
			1401	886	234	280	1		
2	q	171	Total	C	N	O	S	0	0
			1401	886	234	280	1		
2	s	171	Total	C	N	O	S	0	0
			1401	886	234	280	1		
2	v	171	Total	C	N	O	S	0	0
			1401	886	234	280	1		

- Molecule 3 is a protein called Gp2.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	t	57	Total	C	N	O	S	0	0
			446	284	71	89	2		

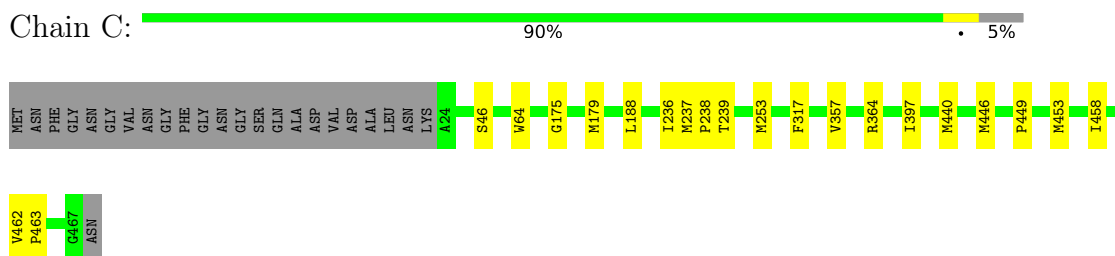
- Molecule 4 is a protein called Gp36.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	w	64	Total	C	N	O	S	0	0
			501	316	78	106	1		

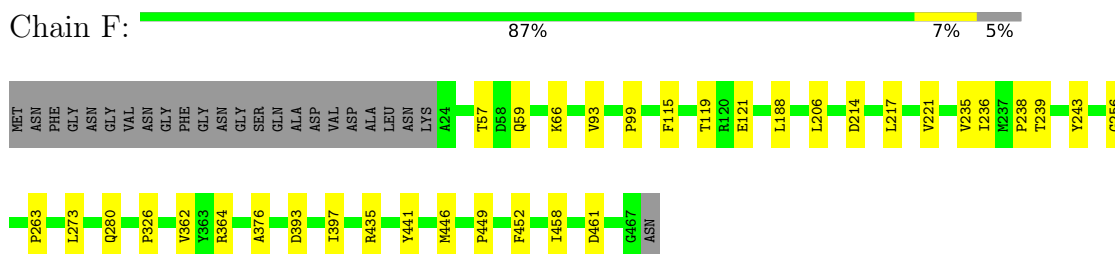
3 Residue-property plots [i](#)

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.

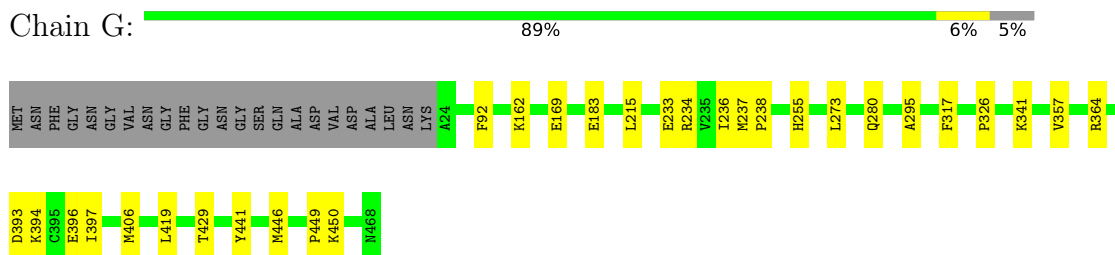
- Molecule 1: Gp6.1



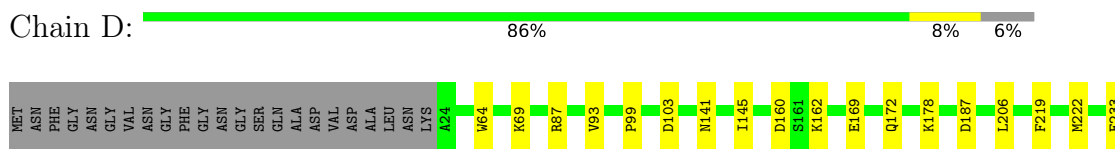
- Molecule 1: Gp6.1

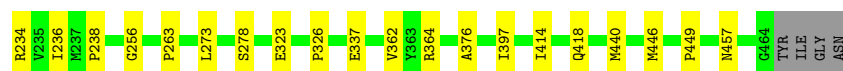


- Molecule 1: Gp6.1



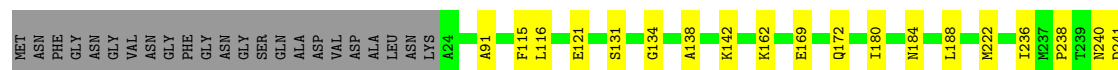
- Molecule 1: Gp6.1





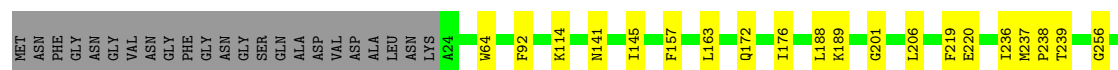
• Molecule 1: Gp6.1

Chain I: 87% 9% 5%



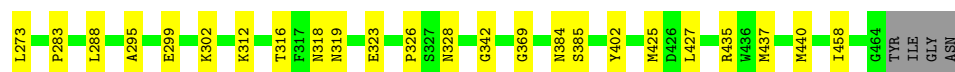
• Molecule 1: Gp6.1

Chain J: 85% 9% 6%



• Molecule 1: Gp6.1

Chain O: 85% 9% 6%



• Molecule 1: Gp6.1

Chain N: 88% 6% 6%



• Molecule 1: Gp6.1

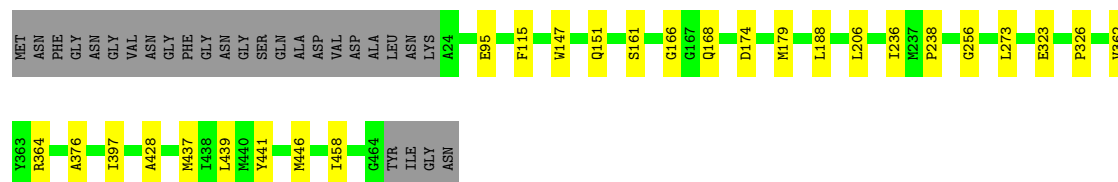
Chain M: 87% 8% 5%





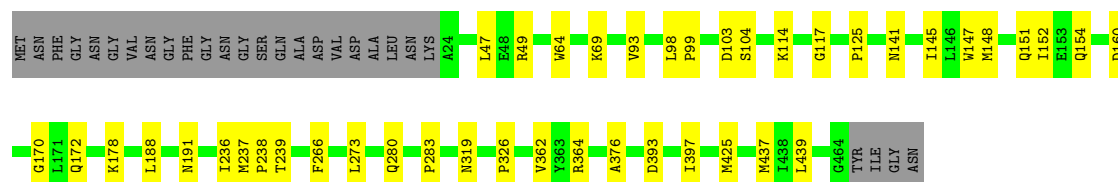
• Molecule 1: Gp6.1

Chain H: 88% 6% 6%



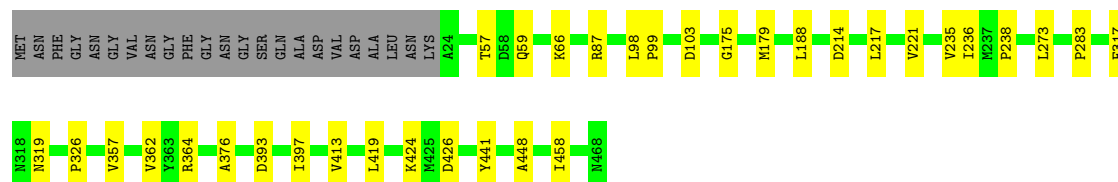
• Molecule 1: Gp6.1

Chain K: 85% 9% 6%



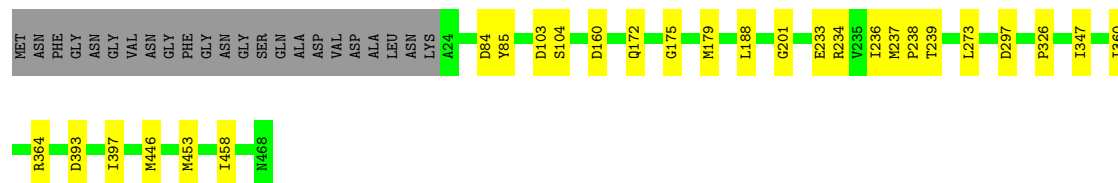
• Molecule 1: Gp6.1

Chain L: 88% 7% 5%



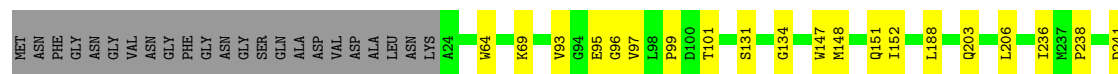
• Molecule 1: Gp6.1

Chain B: 89% 6% 5%



• Molecule 1: Gp6.1

Chain E: 87% 8% 6%





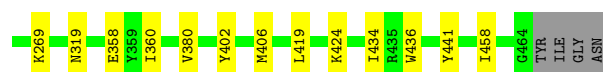
- Molecule 1: Gp6.1

Chain P: 88% 7% 5%



- Molecule 1: Gp6.1

Chain A: 87% 6% 7%



- Molecule 2: Gp29.2

Chain r: 92% 8%



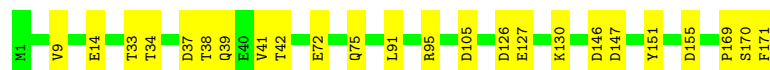
- Molecule 2: Gp29.2

Chain q: 93% 7%



- Molecule 2: Gp29.2

Chain s: 86% 14%



- Molecule 2: Gp29.2

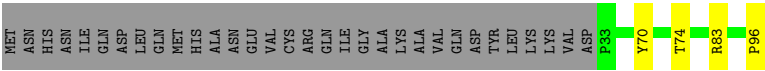
Chain v: 93% 7%



● Molecule 3: Gp2.7



● Molecule 4: Gp36.3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	626340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/3446	0.23	0/4667
1	B	0.10	0/3534	0.24	0/4789
1	C	0.10	0/3526	0.24	0/4778
1	D	0.10	0/3501	0.25	0/4744
1	E	0.11	0/3501	0.26	0/4744
1	F	0.10	0/3526	0.25	0/4778
1	G	0.10	0/3534	0.24	0/4789
1	H	0.10	0/3501	0.24	0/4744
1	I	0.11	0/3534	0.25	0/4789
1	J	0.11	0/3501	0.29	1/4744 (0.0%)
1	K	0.10	0/3501	0.24	0/4744
1	L	0.10	0/3534	0.23	0/4789
1	M	0.10	0/3534	0.24	0/4789
1	N	0.10	0/3501	0.25	0/4744
1	O	0.10	0/3501	0.25	0/4744
1	P	0.10	0/3526	0.24	0/4778
2	q	0.09	0/1436	0.26	0/1958
2	r	0.09	0/1436	0.23	0/1958
2	s	0.11	0/1436	0.26	0/1958
2	v	0.10	0/1436	0.26	0/1958
3	t	0.10	0/451	0.27	0/609
4	w	0.11	0/515	0.28	0/703
All	All	0.10	0/62911	0.25	1/85298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	319	ASN	N-CA-C	-6.70	99.67	109.18

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	3370	0	3330	13	0
1	B	3455	0	3402	15	0
1	C	3447	0	3396	14	0
1	D	3423	0	3373	24	0
1	E	3423	0	3373	23	0
1	F	3447	0	3396	23	0
1	G	3455	0	3402	18	0
1	H	3423	0	3373	15	0
1	I	3455	0	3402	23	0
1	J	3423	0	3373	27	0
1	K	3423	0	3373	26	0
1	L	3455	0	3402	19	0
1	M	3455	0	3402	22	0
1	N	3423	0	3373	18	0
1	O	3423	0	3373	26	0
1	P	3447	0	3396	17	0
2	q	1401	0	1339	6	0
2	r	1401	0	1339	9	0
2	s	1401	0	1339	16	0
2	v	1401	0	1339	7	0
3	t	446	0	460	3	0
4	w	501	0	464	3	0
All	All	61498	0	60419	337	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 (337) 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:O:236:ILE:HG22	1:O:238:PRO:HD2	1.67	0.76
1:E:236:ILE:HG22	1:E:238:PRO:HD2	1.67	0.76
1:N:236:ILE:HG22	1:N:238:PRO:HD2	1.69	0.75
1:G:236:ILE:HG22	1:G:238:PRO:HD2	1.69	0.74
1:F:236:ILE:HG22	1:F:238:PRO:HD2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:295:ALA:HB3	1:O:342:GLY:H	1.54	0.73
1:P:236:ILE:HG22	1:P:238:PRO:HD2	1.70	0.73
2:s:38:THR:HG22	2:s:39:GLN:H	1.56	0.71
1:I:446:MET:HE2	1:I:449:PRO:HA	1.73	0.70
1:I:236:ILE:HG22	1:I:238:PRO:HD2	1.73	0.70
1:O:121:GLU:HG2	1:O:435:ARG:HG2	1.75	0.69
1:D:446:MET:HE2	1:D:449:PRO:HA	1.73	0.69
1:G:183:GLU:OE2	1:G:450:LYS:NZ	2.26	0.68
1:I:240:ASN:OD1	1:I:241:ASP:N	2.22	0.68
1:A:64:TRP:O	1:A:69:LYS:NZ	2.27	0.68
1:F:364:ARG:NH2	1:F:397:ILE:O	2.27	0.67
1:J:236:ILE:HG22	1:J:238:PRO:HD2	1.76	0.67
1:P:188:LEU:HD12	1:P:458:ILE:HG12	1.76	0.67
1:I:364:ARG:NH2	1:I:397:ILE:O	2.28	0.66
1:G:446:MET:HE3	1:G:449:PRO:HA	1.78	0.66
1:C:236:ILE:HG22	1:C:238:PRO:HD2	1.78	0.66
1:J:364:ARG:NH2	1:J:397:ILE:O	2.29	0.66
1:K:236:ILE:HG22	1:K:238:PRO:HD2	1.76	0.66
2:s:130:LYS:NZ	2:s:155:ASP:OD2	2.28	0.65
3:t:15:MET:HE1	3:t:23:TYR:HE2	1.61	0.65
1:C:446:MET:HE3	1:C:449:PRO:HA	1.78	0.65
1:G:364:ARG:NH2	1:G:397:ILE:O	2.30	0.65
1:M:364:ARG:NH2	1:M:397:ILE:O	2.30	0.64
2:q:121:GLU:OE1	2:q:153:ARG:NH1	2.31	0.64
1:H:364:ARG:NH2	1:H:397:ILE:O	2.30	0.63
1:K:154:GLN:OE1	2:s:169:PRO:HA	1.98	0.63
1:P:121:GLU:HG2	1:P:435:ARG:HG2	1.82	0.62
1:C:188:LEU:HD22	1:C:458:ILE:HG12	1.81	0.62
1:B:364:ARG:NH2	1:B:397:ILE:O	2.33	0.62
1:P:212:PRO:HB3	1:P:406:MET:HE3	1.82	0.62
1:O:119:THR:HG22	1:O:437:MET:HB3	1.82	0.62
1:F:280:GLN:HB3	2:s:91:LEU:HD13	1.82	0.61
1:L:364:ARG:NH2	1:L:397:ILE:O	2.32	0.61
1:F:188:LEU:HD22	1:F:458:ILE:HG12	1.81	0.61
1:D:162:LYS:NZ	1:D:169:GLU:OE2	2.33	0.61
1:H:188:LEU:HD22	1:H:458:ILE:HG12	1.82	0.61
1:L:424:LYS:NZ	1:L:426:ASP:OD1	2.34	0.61
1:A:222:MET:HG2	1:A:263:PRO:HG3	1.82	0.61
1:O:299:GLU:OE1	1:O:302:LYS:NZ	2.35	0.60
1:O:188:LEU:HD22	1:O:458:ILE:HG12	1.84	0.60
1:M:364:ARG:NH1	1:M:393:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HG22	1:B:238:PRO:HD2	1.84	0.60
1:D:160:ASP:OD1	1:D:178:LYS:NZ	2.33	0.59
1:O:312:LYS:NZ	1:O:369:GLY:O	2.34	0.59
1:A:234:ARG:HE	1:A:236:ILE:HD11	1.67	0.59
1:D:362:VAL:HB	1:D:376:ALA:HB3	1.84	0.59
1:I:138:ALA:O	1:I:142:LYS:HG3	2.02	0.59
1:E:364:ARG:NH2	1:E:397:ILE:O	2.36	0.59
1:I:344:LYS:NZ	1:I:390:GLU:OE1	2.30	0.59
1:N:364:ARG:NH2	1:N:397:ILE:O	2.36	0.58
1:H:236:ILE:HG22	1:H:238:PRO:HD2	1.86	0.58
2:r:31:GLU:OE2	2:r:47:ARG:NE	2.34	0.57
1:A:419:LEU:HB3	1:A:441:TYR:HB2	1.86	0.57
1:C:253:MET:HE3	1:E:241:ASP:HB3	1.85	0.57
1:I:188:LEU:HD22	1:I:458:ILE:HG12	1.87	0.57
1:N:224:GLN:NE2	1:N:461:ASP:OD1	2.37	0.57
1:D:278:SER:HG	1:D:323:GLU:H	1.52	0.57
1:K:64:TRP:O	1:K:69:LYS:NZ	2.36	0.57
1:A:127:THR:HG21	1:A:434:ILE:HD12	1.87	0.56
1:B:273:LEU:HD11	1:B:326:PRO:HG3	1.86	0.56
1:P:84:ASP:OD1	1:P:85:TYR:N	2.37	0.56
1:J:220:GLU:OE2	1:O:203:GLN:NE2	2.39	0.56
1:L:236:ILE:HG22	1:L:238:PRO:HD2	1.87	0.56
1:J:189:LYS:HG2	1:J:302:LYS:HB2	1.88	0.56
1:O:220:GLU:OE2	1:N:203:GLN:NE2	2.38	0.56
1:O:93:VAL:HG11	1:O:99:PRO:HB3	1.88	0.55
1:M:236:ILE:HG22	1:M:238:PRO:HD2	1.87	0.55
1:H:166:GLY:O	1:H:168:GLN:NE2	2.40	0.55
1:F:93:VAL:HG11	1:F:99:PRO:HB3	1.87	0.55
1:K:280:GLN:HG3	2:s:151:TYR:O	2.06	0.55
1:A:188:LEU:HD22	1:A:458:ILE:HG12	1.89	0.55
1:L:273:LEU:HD11	1:L:326:PRO:HG3	1.89	0.55
1:K:364:ARG:NH2	1:K:397:ILE:O	2.39	0.54
1:L:87:ARG:NH1	1:L:103:ASP:OD1	2.40	0.54
1:N:121:GLU:HG2	1:N:435:ARG:HG2	1.89	0.54
1:A:252:PHE:HB2	1:A:261:PHE:HE1	1.73	0.54
1:D:273:LEU:HD11	1:D:326:PRO:HG3	1.90	0.54
1:H:206:LEU:HD11	1:H:256:GLY:HA3	1.90	0.54
2:v:121:GLU:OE1	2:v:153:ARG:NH1	2.39	0.54
1:F:119:THR:HB	1:E:101:THR:HG22	1.90	0.54
1:D:206:LEU:HD11	1:D:256:GLY:HA3	1.90	0.54
1:D:64:TRP:CH2	1:D:440:MET:HE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASN:O	1:D:145:ILE:HG12	2.07	0.53
1:E:148:MET:O	1:E:152:ILE:HG13	2.08	0.53
1:O:384:ASN:OD1	1:O:385:SER:N	2.41	0.53
1:G:317:PHE:HD2	1:G:357:VAL:HG21	1.74	0.53
1:N:312:LYS:NZ	1:N:331:ASP:OD1	2.40	0.53
1:K:364:ARG:NH1	1:K:393:ASP:OD2	2.41	0.53
1:E:362:VAL:HB	1:E:376:ALA:HB3	1.91	0.53
1:I:312:LYS:HB2	1:I:365:SER:HB3	1.91	0.53
1:J:188:LEU:HD22	1:J:458:ILE:HG12	1.89	0.53
1:L:66:LYS:NZ	1:L:214:ASP:OD2	2.33	0.53
1:I:91:ALA:N	2:r:171:PHE:O	2.42	0.53
1:K:98:LEU:HD12	1:K:99:PRO:HD2	1.91	0.53
1:O:288:LEU:N	1:O:328:ASN:OD1	2.39	0.52
1:O:427:LEU:HD21	1:O:437:MET:HE3	1.90	0.52
1:O:217:LEU:HD12	1:O:221:VAL:HG12	1.91	0.52
2:r:121:GLU:OE1	2:r:153:ARG:NH1	2.39	0.52
1:F:446:MET:HE2	1:F:449:PRO:HA	1.91	0.52
1:I:364:ARG:NH1	1:I:393:ASP:OD2	2.43	0.52
1:D:236:ILE:HG22	1:D:238:PRO:HD2	1.90	0.52
1:M:219:PHE:HE2	1:M:265:LEU:HB2	1.74	0.52
1:F:235:VAL:HG22	1:G:237:MET:HB2	1.91	0.52
1:O:64:TRP:O	1:O:69:LYS:NZ	2.42	0.52
1:D:222:MET:SD	1:D:263:PRO:HG3	2.50	0.51
1:M:362:VAL:HB	1:M:376:ALA:HB3	1.92	0.51
1:H:323:GLU:OE2	2:r:158:ARG:NH2	2.34	0.51
1:H:147:TRP:O	1:H:151:GLN:HG2	2.10	0.51
1:C:64:TRP:CH2	1:C:440:MET:HE1	2.45	0.51
1:M:273:LEU:HD11	1:M:326:PRO:HG3	1.91	0.51
1:K:103:ASP:OD1	1:K:104:SER:N	2.43	0.51
1:B:364:ARG:NH1	1:B:393:ASP:OD2	2.42	0.51
1:P:364:ARG:NH2	1:P:397:ILE:O	2.43	0.51
1:N:364:ARG:NH1	1:N:393:ASP:OD2	2.43	0.51
2:q:141:GLN:HE22	2:q:150:HIS:HB2	1.76	0.51
1:E:364:ARG:NH1	1:E:393:ASP:OD2	2.40	0.51
1:B:297:ASP:OD1	1:B:297:ASP:N	2.43	0.51
2:v:31:GLU:OE1	2:v:47:ARG:NH2	2.43	0.51
1:P:205:ILE:HD12	1:P:406:MET:HE2	1.93	0.51
1:N:381:THR:HG23	1:N:389:THR:HG23	1.93	0.51
1:K:147:TRP:O	1:K:151:GLN:HG2	2.11	0.51
1:D:233:GLU:O	1:D:234:ARG:NH1	2.44	0.50
1:F:362:VAL:HB	1:F:376:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ILE:HG21	1:E:360:ILE:HD13	1.94	0.50
1:I:131:SER:OG	1:I:134:GLY:O	2.26	0.50
1:F:206:LEU:HD11	1:F:256:GLY:HA3	1.93	0.50
1:N:297:ASP:OD1	1:N:297:ASP:N	2.43	0.50
1:D:87:ARG:NH1	1:D:103:ASP:OD1	2.44	0.49
1:M:217:LEU:O	1:M:263:PRO:HA	2.12	0.49
1:M:432:PRO:HG2	1:E:96:GLY:HA2	1.93	0.49
1:J:297:ASP:OD1	1:J:297:ASP:N	2.45	0.49
1:B:201:GLY:HA2	1:B:453:MET:HE3	1.94	0.49
2:s:37:ASP:OD1	2:s:38:THR:N	2.45	0.49
1:G:233:GLU:O	1:G:234:ARG:NH1	2.44	0.49
1:J:427:LEU:HD21	1:J:437:MET:HE2	1.93	0.49
1:L:364:ARG:NH1	1:L:393:ASP:OD2	2.44	0.49
1:F:121:GLU:HG2	1:F:435:ARG:HG2	1.94	0.49
1:B:103:ASP:OD1	1:B:104:SER:N	2.46	0.49
1:N:147:TRP:O	1:N:151:GLN:HG2	2.12	0.49
1:M:91:ALA:N	2:v:171:PHE:O	2.43	0.49
1:P:317:PHE:HD2	1:P:357:VAL:HG21	1.77	0.49
1:C:462:VAL:HB	1:C:463:PRO:HD3	1.95	0.49
1:E:455:TYR:HB2	1:E:458:ILE:HD11	1.94	0.49
1:I:362:VAL:HB	1:I:376:ALA:HB3	1.95	0.49
1:J:157:PHE:HA	1:J:176:ILE:HG22	1.95	0.49
1:I:162:LYS:NZ	1:I:169:GLU:OE1	2.34	0.49
1:O:269:LYS:HB3	1:O:402:TYR:CE2	2.48	0.49
1:C:364:ARG:NH2	1:C:397:ILE:O	2.45	0.48
1:M:188:LEU:HD12	1:M:458:ILE:HG12	1.93	0.48
1:E:147:TRP:O	1:E:151:GLN:HG2	2.13	0.48
1:L:283:PRO:HD3	1:L:319:ASN:ND2	2.28	0.48
1:E:64:TRP:O	1:E:69:LYS:NZ	2.44	0.48
1:I:121:GLU:HG2	1:I:435:ARG:HG2	1.96	0.48
1:I:222:MET:HE1	1:I:263:PRO:HD3	1.95	0.48
2:s:126:ASP:O	2:s:127:GLU:HG2	2.14	0.48
1:D:414:ILE:HA	1:D:446:MET:HA	1.96	0.48
2:s:34:THR:HG22	2:s:41:VAL:HG12	1.95	0.48
1:H:95:GLU:HG3	1:K:125:PRO:HG2	1.95	0.48
1:I:116:LEU:HD21	1:I:440:MET:HE2	1.96	0.47
1:J:201:GLY:HA2	1:J:453:MET:HE3	1.96	0.47
1:M:365:SER:HB3	1:M:372:LEU:HD23	1.96	0.47
1:K:114:LYS:NZ	1:K:170:GLY:O	2.47	0.47
1:B:237:MET:O	1:B:239:THR:N	2.46	0.47
2:s:33:THR:HG1	2:s:42:THR:HG1	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:w:70:TYR:O	4:w:74:THR:HG22	2.14	0.47
1:G:255:HIS:HD2	1:D:219:PHE:HD1	1.62	0.47
1:G:364:ARG:NH1	1:G:393:ASP:OD2	2.47	0.47
1:O:318:ASN:HD22	1:O:323:GLU:CD	2.22	0.47
1:H:362:VAL:HB	1:H:376:ALA:HB3	1.95	0.47
1:K:141:ASN:O	1:K:145:ILE:HG12	2.14	0.47
2:q:91:LEU:HD11	2:q:108:TRP:HB3	1.96	0.47
1:M:398:LEU:O	1:M:401:THR:OG1	2.30	0.47
1:M:402:TYR:HB2	1:M:458:ILE:HB	1.95	0.47
1:H:161:SER:OG	1:H:174:ASP:OD2	2.26	0.47
1:J:141:ASN:O	1:J:145:ILE:HG12	2.15	0.47
1:K:188:LEU:O	1:K:191:ASN:ND2	2.45	0.47
2:v:29:ASP:OD1	2:v:30:LYS:N	2.48	0.47
1:D:160:ASP:O	1:D:172:GLN:HB2	2.16	0.46
1:E:419:LEU:HB3	1:E:441:TYR:HB2	1.96	0.46
1:C:175:GLY:O	1:C:179:MET:HG3	2.14	0.46
1:K:237:MET:HB2	1:L:235:VAL:HG22	1.96	0.46
1:K:362:VAL:HB	1:K:376:ALA:HB3	1.96	0.46
1:J:64:TRP:CH2	1:J:440:MET:HE1	2.51	0.46
1:J:237:MET:HB2	1:O:235:VAL:HG22	1.96	0.46
2:q:53:VAL:HB	2:q:82:TYR:HB3	1.98	0.46
1:D:364:ARG:NH2	1:D:397:ILE:O	2.45	0.46
1:E:131:SER:OG	1:E:134:GLY:O	2.26	0.46
1:A:269:LYS:HB3	1:A:402:TYR:CE2	2.50	0.46
1:F:239:THR:HG21	1:E:246:GLY:O	2.16	0.46
1:L:175:GLY:O	1:L:179:MET:HG3	2.16	0.46
1:P:164:ALA:HB3	1:P:168:GLN:HB2	1.96	0.46
1:E:203:GLN:HA	1:E:206:LEU:HG	1.96	0.46
1:J:394:LYS:HB2	1:J:396:GLU:OE2	2.15	0.46
1:L:188:LEU:HD22	1:L:458:ILE:HG12	1.97	0.46
1:F:239:THR:HG23	1:F:243:TYR:HE2	1.81	0.45
1:J:364:ARG:NH1	1:J:393:ASP:OD2	2.48	0.45
1:O:316:THR:HG22	1:O:326:PRO:HA	1.97	0.45
1:N:154:GLN:OE1	2:v:169:PRO:HA	2.16	0.45
1:P:362:VAL:HB	1:P:376:ALA:HB3	1.98	0.45
1:K:425:MET:HE3	1:K:437:MET:HE3	1.98	0.45
1:J:64:TRP:CZ2	1:J:440:MET:HE1	2.51	0.45
2:s:9:VAL:HG23	2:s:14:GLU:HG3	1.98	0.45
1:C:64:TRP:CZ2	1:C:440:MET:HE1	2.50	0.45
1:F:364:ARG:NH1	1:F:393:ASP:OD2	2.50	0.45
1:J:219:PHE:HD1	1:O:255:HIS:HD2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:170:SER:O	2:s:171:PHE:C	2.60	0.45
1:B:179:MET:HB2	1:B:446:MET:HE2	1.97	0.45
1:E:381:THR:HG23	1:E:389:THR:HG23	1.98	0.45
1:A:206:LEU:HD11	1:A:256:GLY:HA3	1.98	0.45
1:D:187:ASP:OD1	1:D:457:ASN:ND2	2.44	0.45
1:I:222:MET:HE2	1:I:261:PHE:HB3	1.99	0.45
1:A:360:ILE:HD11	1:A:380:VAL:HG12	1.99	0.45
1:F:280:GLN:HB3	2:s:91:LEU:CD1	2.47	0.45
1:L:419:LEU:HB3	1:L:441:TYR:HB2	1.99	0.45
1:B:347:ILE:HG21	1:B:360:ILE:HD13	1.98	0.45
1:E:283:PRO:HD3	1:E:319:ASN:ND2	2.31	0.45
1:E:148:MET:HE3	1:E:148:MET:HB3	1.84	0.45
1:N:455:TYR:HB2	1:N:458:ILE:HD11	1.98	0.45
2:v:9:VAL:HG23	2:v:14:GLU:HG3	1.98	0.44
1:F:461:ASP:OD1	1:F:461:ASP:N	2.49	0.44
1:O:273:LEU:HD11	1:O:326:PRO:HG3	1.99	0.44
1:N:432:PRO:HG2	1:P:96:GLY:HA2	1.99	0.44
2:q:66:VAL:HG23	2:q:68:PRO:HD2	1.98	0.44
1:P:222:MET:SD	1:P:263:PRO:HG3	2.58	0.44
1:G:429:THR:H	1:H:428:ALA:HB2	1.82	0.44
1:B:84:ASP:OD1	1:B:85:TYR:N	2.51	0.44
1:P:179:MET:HE3	1:P:446:MET:HE3	1.99	0.44
1:K:47:LEU:HB3	1:K:49:ARG:HH12	1.82	0.44
1:K:160:ASP:O	1:K:172:GLN:HB2	2.17	0.44
1:L:98:LEU:HD12	1:L:99:PRO:HD2	1.99	0.44
1:H:437:MET:HE3	1:H:439:LEU:HD11	2.00	0.44
2:s:95:ARG:NH2	2:s:105:ASP:OD2	2.51	0.44
1:F:66:LYS:NZ	1:F:214:ASP:OD2	2.50	0.44
1:M:57:THR:HG23	1:M:59:GLN:H	1.82	0.44
1:H:273:LEU:HD11	1:H:326:PRO:HG3	1.99	0.44
1:K:160:ASP:OD1	1:K:178:LYS:NZ	2.36	0.44
1:G:273:LEU:HD11	1:G:326:PRO:HG3	2.00	0.43
1:J:163:LEU:HD23	1:J:359:TYR:CE1	2.54	0.43
1:M:253:MET:SD	1:M:258:GLU:HG2	2.58	0.43
1:L:103:ASP:OD1	1:L:103:ASP:N	2.50	0.43
1:L:413:VAL:HG13	1:L:448:ALA:HB3	1.99	0.43
1:M:121:GLU:HB2	1:M:435:ARG:HG2	1.98	0.43
1:K:273:LEU:HD11	1:K:326:PRO:HG3	2.00	0.43
1:I:184:ASN:HB3	1:I:453:MET:HB3	2.00	0.43
1:I:180:ILE:HG12	1:I:446:MET:HE1	2.00	0.43
1:P:461:ASP:OD1	1:P:461:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:PHE:HD2	1:C:357:VAL:HG11	1.83	0.43
1:M:297:ASP:N	1:M:297:ASP:OD1	2.51	0.43
1:E:93:VAL:HG12	1:E:97:VAL:HB	1.99	0.43
1:M:283:PRO:HD3	1:M:319:ASN:ND2	2.34	0.43
1:I:466:ILE:HG13	1:I:466:ILE:O	2.19	0.43
1:J:206:LEU:HD11	1:J:256:GLY:HA3	2.01	0.43
1:F:217:LEU:HD12	1:F:221:VAL:HG12	2.00	0.43
1:N:317:PHE:HD2	1:N:357:VAL:HG11	1.84	0.43
1:K:154:GLN:HE21	1:K:266:PHE:HB3	1.84	0.43
1:L:362:VAL:HB	1:L:376:ALA:HB3	2.00	0.43
1:B:233:GLU:O	1:B:234:ARG:NH1	2.47	0.43
1:G:394:LYS:HB2	1:G:396:GLU:OE2	2.19	0.43
1:N:114:LYS:HE3	1:N:172:GLN:O	2.19	0.43
2:r:121:GLU:HG3	2:r:134:TYR:CE2	2.53	0.43
1:D:93:VAL:HG11	1:D:99:PRO:HB3	2.01	0.42
1:M:125:PRO:HG2	1:E:95:GLU:HG3	2.01	0.42
1:G:280:GLN:HB3	2:r:91:LEU:HB2	2.00	0.42
1:N:419:LEU:HB3	1:N:441:TYR:HB2	2.00	0.42
1:M:237:MET:O	1:M:239:THR:N	2.51	0.42
1:N:172:GLN:HG2	1:M:92:PHE:CD2	2.53	0.42
1:K:283:PRO:HD3	1:K:319:ASN:ND2	2.34	0.42
1:L:217:LEU:HD12	1:L:221:VAL:HG12	2.01	0.42
2:s:127:GLU:HB2	2:s:130:LYS:HG3	2.02	0.42
1:F:115:PHE:HD1	1:F:441:TYR:CD1	2.37	0.42
1:O:425:MET:HB3	1:O:437:MET:HG3	2.00	0.42
1:J:409:MET:HE3	1:J:409:MET:HB3	1.95	0.42
1:J:347:ILE:HD13	1:J:360:ILE:HD13	2.02	0.42
2:r:21:SER:OG	2:r:22:ASP:N	2.52	0.42
1:D:69:LYS:HE2	4:w:96:PRO:HA	2.01	0.42
1:L:317:PHE:HD2	1:L:357:VAL:HG11	1.85	0.42
1:C:237:MET:O	1:C:239:THR:HG23	2.20	0.42
1:J:413:VAL:HG13	1:J:448:ALA:HB3	2.01	0.42
1:K:148:MET:O	1:K:152:ILE:HG13	2.19	0.42
1:K:93:VAL:HG11	1:K:99:PRO:HB3	2.01	0.42
2:v:37:ASP:OD1	2:v:38:THR:N	2.53	0.42
2:q:60:GLU:HG2	2:q:78:THR:HG22	2.01	0.42
1:P:230:PHE:O	1:P:233:GLU:HG3	2.20	0.42
1:F:57:THR:HG23	1:F:59:GLN:HG2	2.02	0.41
1:I:172:GLN:HG2	1:J:92:PHE:CD2	2.55	0.41
1:O:283:PRO:HD3	1:O:319:ASN:ND2	2.35	0.41
1:E:188:LEU:HD12	1:E:458:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:MET:HE1	1:F:452:PHE:HB2	2.02	0.41
1:O:116:LEU:HD11	1:O:440:MET:HB3	2.02	0.41
1:K:117:GLY:HA3	1:K:439:LEU:HD23	2.02	0.41
1:I:317:PHE:HD2	1:I:357:VAL:HG11	1.85	0.41
1:J:237:MET:O	1:J:239:THR:N	2.53	0.41
1:B:160:ASP:O	1:B:172:GLN:HB2	2.21	0.41
1:A:319:ASN:HA	1:A:358:GLU:HG3	2.01	0.41
1:C:46:SER:OG	4:w:83:ARG:NH1	2.53	0.41
1:P:117:GLY:HA2	1:P:438:ILE:O	2.20	0.41
3:t:15:MET:HE2	3:t:19:GLU:HB3	2.02	0.41
1:J:172:GLN:HG2	1:O:92:PHE:CD2	2.56	0.41
1:L:57:THR:HG23	1:L:59:GLN:H	1.85	0.41
1:E:93:VAL:HG21	1:E:99:PRO:HB3	2.01	0.41
1:A:215:LEU:HD13	1:A:406:MET:HB2	2.01	0.41
1:I:115:PHE:HD1	1:I:441:TYR:CD1	2.38	0.41
1:B:188:LEU:HD22	1:B:458:ILE:HG12	2.02	0.41
1:G:162:LYS:NZ	1:G:169:GLU:OE1	2.50	0.41
1:D:103:ASP:OD1	1:D:103:ASP:N	2.53	0.41
1:D:418:GLN:HE21	1:D:440:MET:HE3	1.85	0.41
1:M:317:PHE:HD2	1:M:357:VAL:HG11	1.86	0.41
1:P:115:PHE:HD1	1:P:441:TYR:CD1	2.38	0.41
1:C:237:MET:O	1:C:239:THR:N	2.54	0.41
1:C:453:MET:HE2	1:C:453:MET:HB2	1.96	0.41
1:F:217:LEU:O	1:F:263:PRO:HA	2.19	0.41
1:G:92:PHE:CD2	1:D:172:GLN:HG2	2.56	0.41
1:D:337:GLU:OE2	1:D:337:GLU:N	2.53	0.41
1:A:424:LYS:HG3	1:A:436:TRP:CD1	2.56	0.41
1:G:419:LEU:HB3	1:G:441:TYR:HB2	2.01	0.41
1:O:203:GLN:HA	1:O:206:LEU:HG	2.01	0.41
1:H:115:PHE:HD1	1:H:441:TYR:CD1	2.39	0.41
1:H:179:MET:HE3	1:H:446:MET:HE3	2.02	0.41
2:s:146:ASP:OD1	2:s:147:ASP:N	2.49	0.41
2:s:72:GLU:HB2	2:s:75:GLN:HB2	2.02	0.41
1:J:114:LYS:HE3	1:J:172:GLN:O	2.21	0.40
1:J:287:THR:HG22	1:J:348:THR:HB	2.03	0.40
3:t:15:MET:HE1	3:t:23:TYR:CE2	2.50	0.40
1:N:93:VAL:HG23	1:N:94:GLY:N	2.36	0.40
1:J:273:LEU:HD11	1:J:326:PRO:HG3	2.03	0.40
1:K:237:MET:O	1:K:239:THR:N	2.54	0.40
1:G:215:LEU:HD13	1:G:406:MET:HB2	2.04	0.40
1:G:295:ALA:O	1:G:341:LYS:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:28:LEU:HD12	2:r:48:VAL:HG22	2.03	0.40
2:r:66:VAL:HG23	2:r:68:PRO:HD2	2.04	0.40
1:F:273:LEU:HD11	1:F:326:PRO:HG3	2.04	0.40
1:B:175:GLY:O	1:B:179:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	430/468 (92%)	425 (99%)	5 (1%)	0	100	100
1	B	443/468 (95%)	437 (99%)	6 (1%)	0	100	100
1	C	442/468 (94%)	433 (98%)	9 (2%)	0	100	100
1	D	439/468 (94%)	433 (99%)	6 (1%)	0	100	100
1	E	439/468 (94%)	433 (99%)	6 (1%)	0	100	100
1	F	442/468 (94%)	438 (99%)	4 (1%)	0	100	100
1	G	443/468 (95%)	431 (97%)	12 (3%)	0	100	100
1	H	439/468 (94%)	433 (99%)	6 (1%)	0	100	100
1	I	443/468 (95%)	429 (97%)	14 (3%)	0	100	100
1	J	439/468 (94%)	433 (99%)	6 (1%)	0	100	100
1	K	439/468 (94%)	434 (99%)	5 (1%)	0	100	100
1	L	443/468 (95%)	436 (98%)	7 (2%)	0	100	100
1	M	443/468 (95%)	437 (99%)	6 (1%)	0	100	100
1	N	439/468 (94%)	430 (98%)	9 (2%)	0	100	100
1	O	439/468 (94%)	430 (98%)	9 (2%)	0	100	100
1	P	442/468 (94%)	431 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
2	r	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
2	s	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
2	v	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
3	t	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
4	w	62/96 (65%)	60 (97%)	2 (3%)	0	100	100
All	All	7837/8325 (94%)	7698 (98%)	139 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	362/386 (94%)	362 (100%)	0	100	100
1	B	370/386 (96%)	370 (100%)	0	100	100
1	C	369/386 (96%)	369 (100%)	0	100	100
1	D	367/386 (95%)	367 (100%)	0	100	100
1	E	367/386 (95%)	367 (100%)	0	100	100
1	F	369/386 (96%)	369 (100%)	0	100	100
1	G	370/386 (96%)	370 (100%)	0	100	100
1	H	367/386 (95%)	367 (100%)	0	100	100
1	I	370/386 (96%)	370 (100%)	0	100	100
1	J	367/386 (95%)	367 (100%)	0	100	100
1	K	367/386 (95%)	367 (100%)	0	100	100
1	L	370/386 (96%)	370 (100%)	0	100	100
1	M	370/386 (96%)	370 (100%)	0	100	100
1	N	367/386 (95%)	367 (100%)	0	100	100
1	O	367/386 (95%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	369/386 (96%)	369 (100%)	0	100	100
2	q	154/154 (100%)	154 (100%)	0	100	100
2	r	154/154 (100%)	154 (100%)	0	100	100
2	s	154/154 (100%)	154 (100%)	0	100	100
2	v	154/154 (100%)	154 (100%)	0	100	100
3	t	49/49 (100%)	49 (100%)	0	100	100
4	w	56/84 (67%)	56 (100%)	0	100	100
All	All	6609/6925 (95%)	6609 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	GLN
1	C	124	HIS
1	C	177	ASN
1	F	52	HIS
1	F	244	GLN
1	G	52	HIS
1	G	78	GLN
1	G	140	GLN
1	G	418	GLN
1	D	32	ASN
1	D	70	GLN
1	D	81	GLN
1	D	124	HIS
1	D	135	ASN
1	D	140	GLN
1	D	151	GLN
1	D	224	GLN
1	D	418	GLN
1	I	70	GLN
1	I	89	GLN
1	I	336	ASN
1	J	52	HIS
1	J	244	GLN
1	J	384	ASN
1	O	29	HIS

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Mol	Chain	Res	Type
1	O	59	GLN
1	O	140	GLN
1	O	141	ASN
1	O	244	GLN
1	O	321	HIS
1	N	177	ASN
1	M	52	HIS
1	M	70	GLN
1	M	141	ASN
1	M	154	GLN
1	M	208	ASN
1	H	59	GLN
1	H	70	GLN
1	H	124	HIS
1	K	124	HIS
1	K	151	GLN
1	K	370	GLN
1	L	124	HIS
1	L	135	ASN
1	L	280	GLN
1	L	321	HIS
1	B	81	GLN
1	B	140	GLN
1	B	154	GLN
2	q	75	GLN
2	q	162	HIS
2	s	137	ASN
1	E	52	HIS
1	E	70	GLN
1	E	124	HIS
1	P	89	GLN
1	P	141	ASN
1	P	177	ASN
1	P	336	ASN
1	A	140	GLN
1	A	141	ASN
1	A	177	ASN
1	A	457	ASN
4	w	60	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 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.