



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 24, 2017 – 05:09 AM EDT

PDB ID : 5WLN
EMDB ID: : EMD-8860
Title : Cryo-EM structure of the T2SS secretin XcpQ from *Pseudomonas aeruginosa*
Authors : Hay, I.D.; Belousoff, M.J.; Lithgow, T.J.
Deposited on : unknown
Resolution : 3.57 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

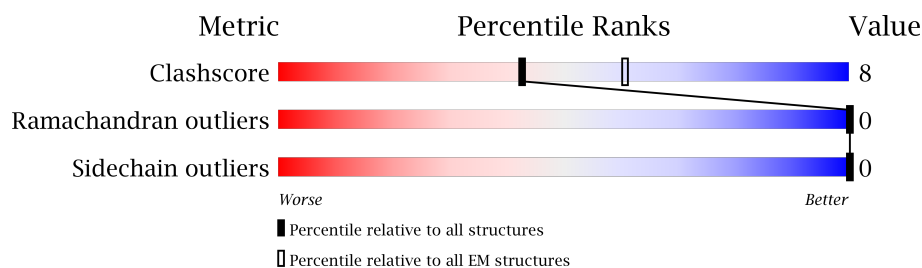
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	624	52% 12% 37%
1	B	624	51% 13% 37%
1	C	624	49% 14% 37%
1	D	624	49% 15% 37%
1	E	624	51% 13% 37%
1	F	624	51% 12% 37%
1	G	624	51% 12% 37%
1	H	624	52% 12% 37%
1	I	624	52% 11% 37%

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Mol	Chain	Length	Quality of chain
1	J	624	 52% 11% 37%
1	K	624	 52% 11% 37%
1	L	624	 53% 11% 37%
1	M	624	 53% 11% 37%
1	N	624	 52% 12% 37%
1	O	624	 52% 12% 37%

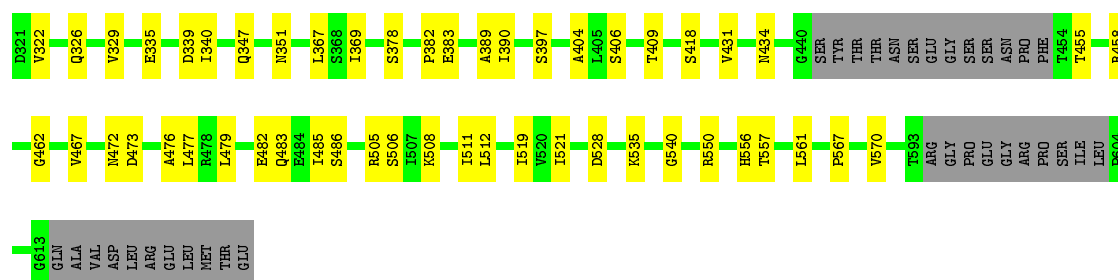
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 44415 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.

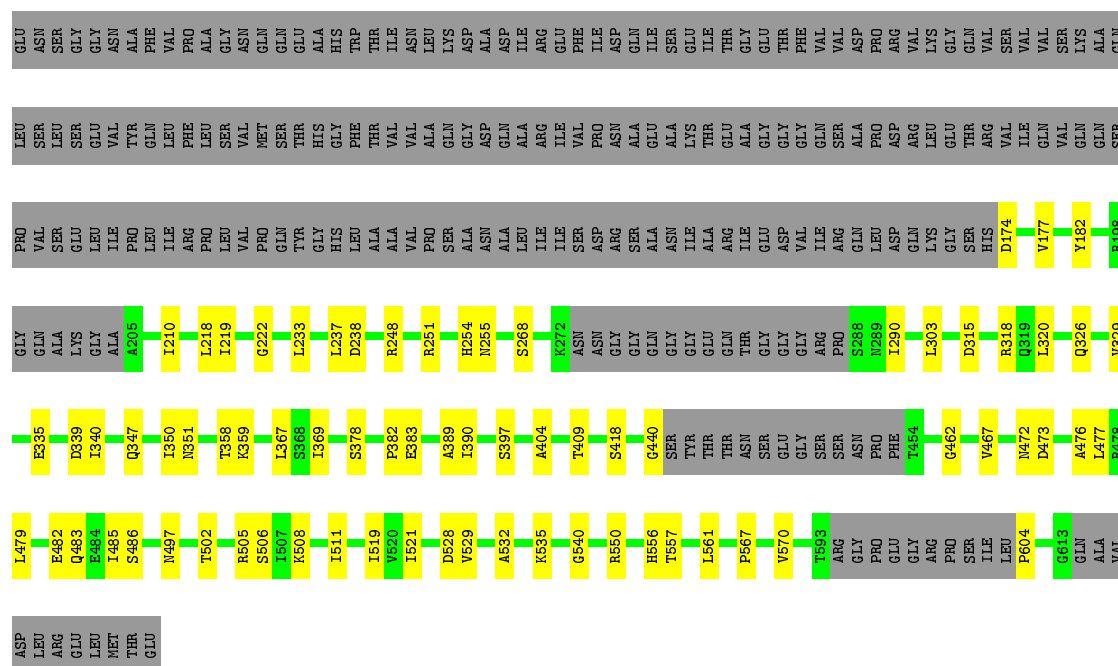
- Molecule 1 is a protein called Type II secretion system protein D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	O	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	A	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	B	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	C	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	D	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	E	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	F	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	H	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	I	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	J	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	K	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	L	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	M	396	Total 2961	C 1839	N 532	O 585	S 5	0	0
1	N	396	Total 2961	C 1839	N 532	O 585	S 5	0	0



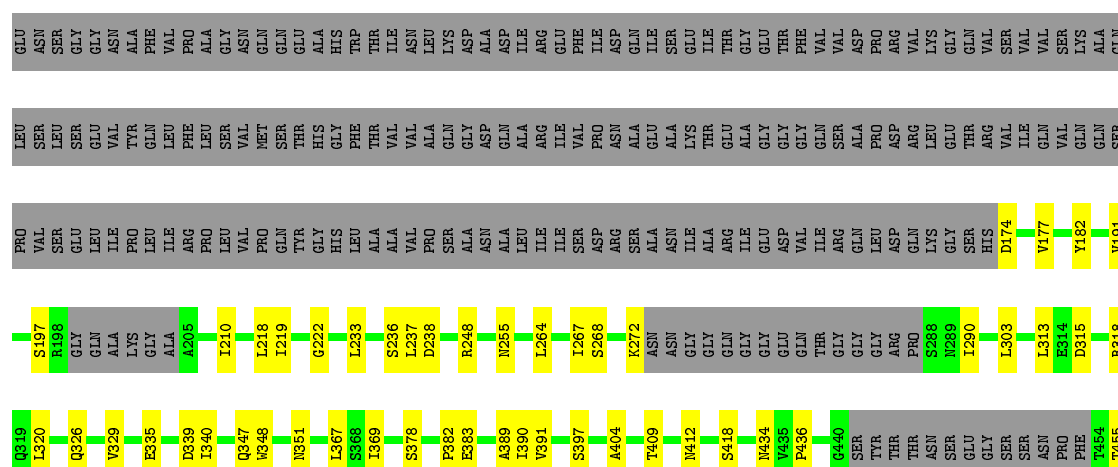
• Molecule 1: Type II secretion system protein D

Chain A: 52% 12% 37%



• Molecule 1: Type II secretion system protein D

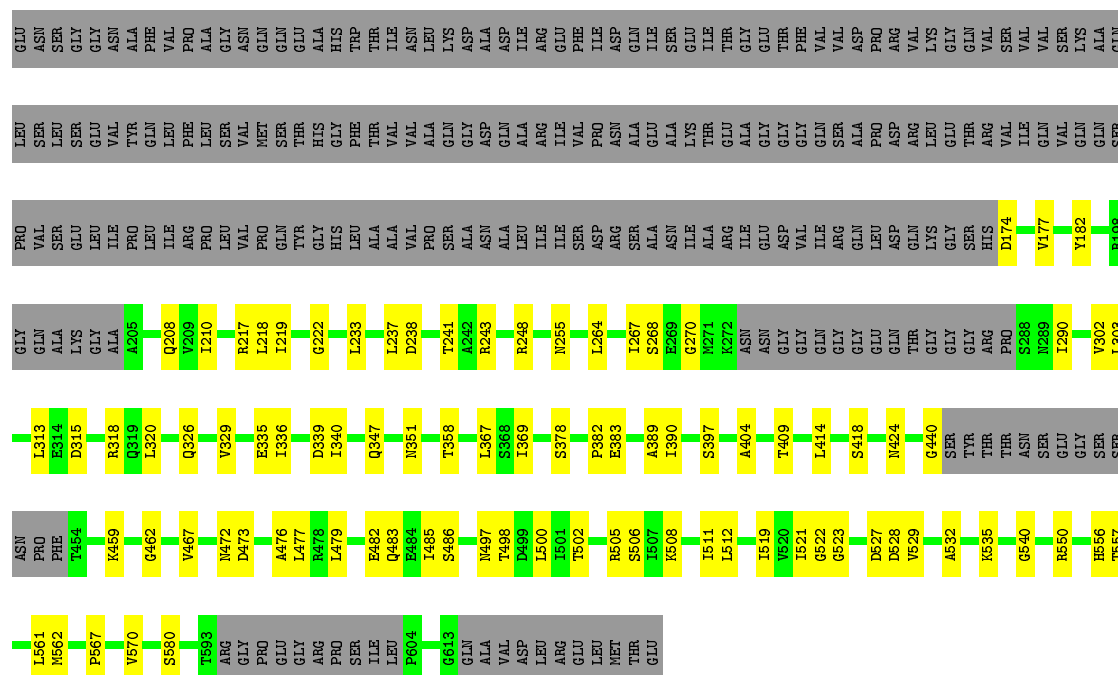
Chain B: 51% 13% 37%





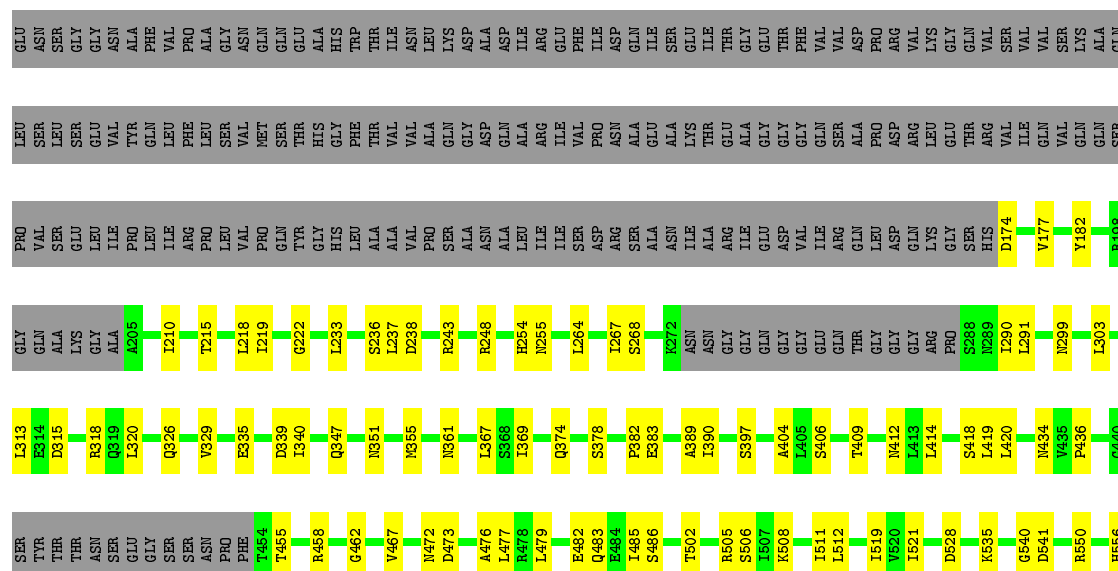
• Molecule 1: Type II secretion system protein D

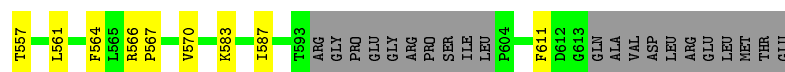
Chain C:



• Molecule 1: Type II secretion system protein D

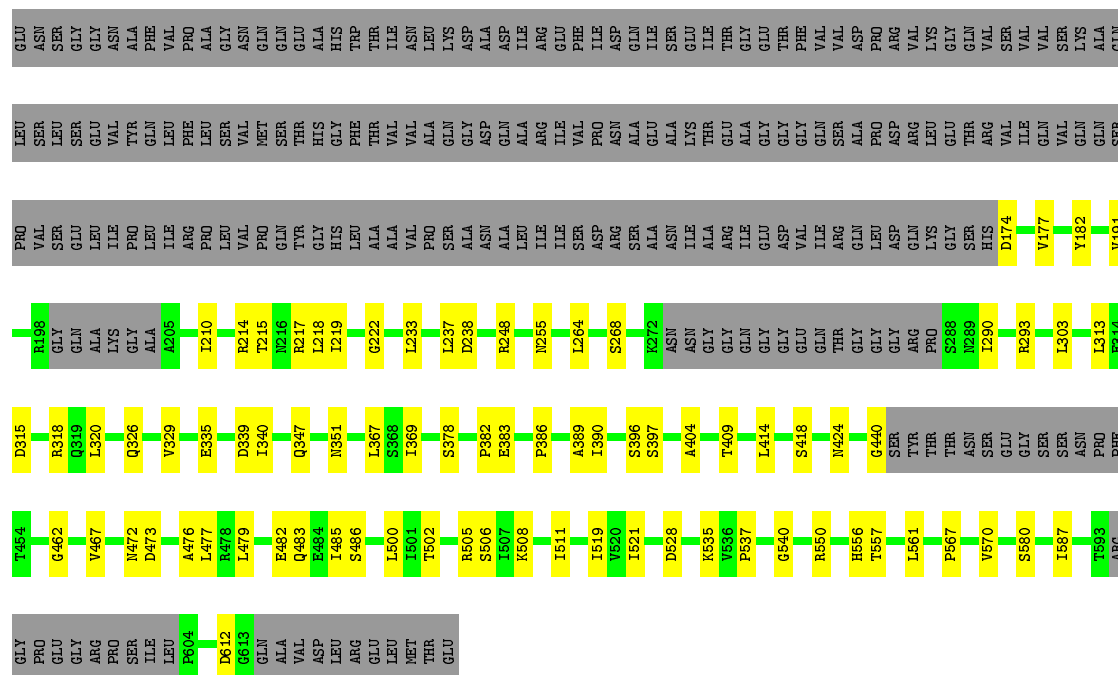
Chain D:





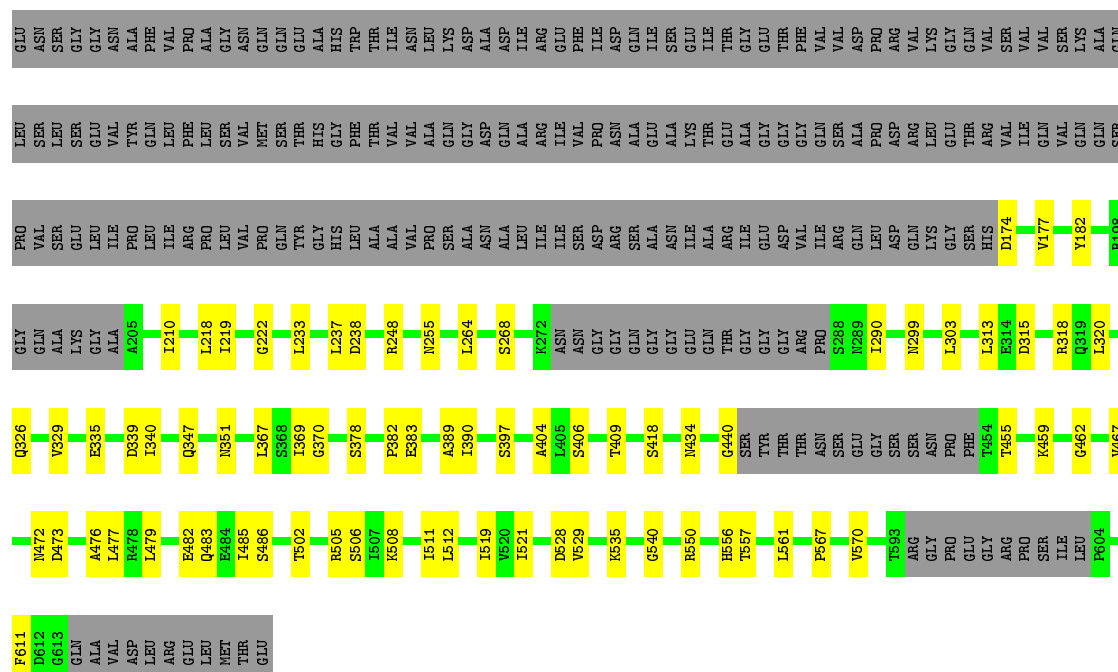
• Molecule 1: Type II secretion system protein D

Chain E: 51% 13% 37%



• Molecule 1: Type II secretion system protein D

Chain F: 51% 12% 37%



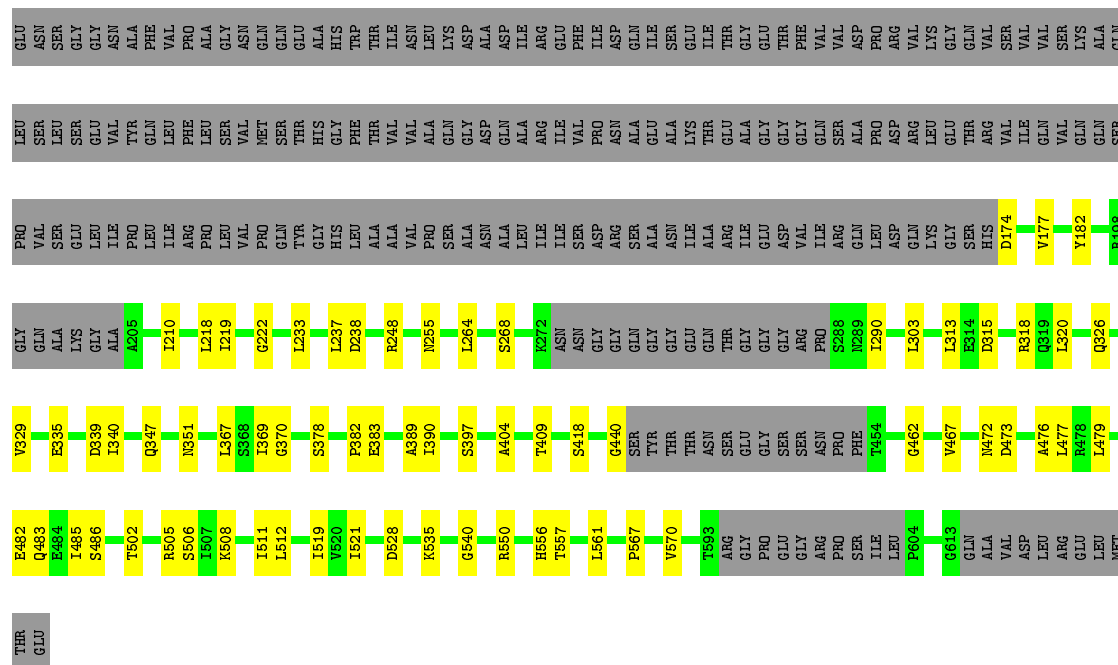
Frequency	Percentage
Daily	52%
Weekly	11%
Not at all	37%



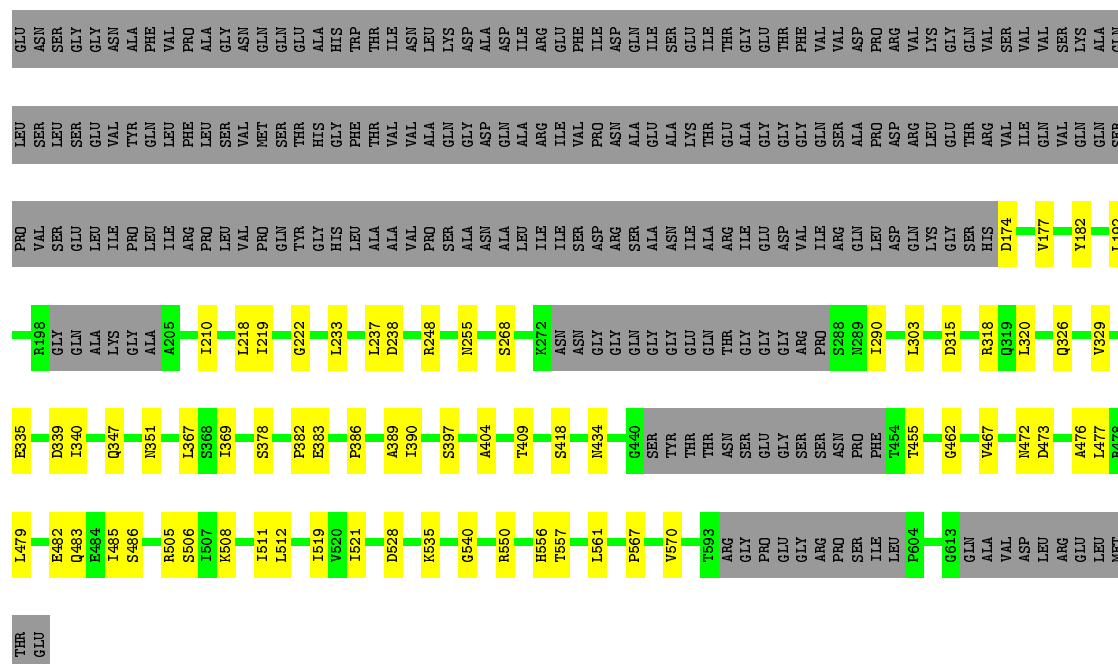
Frequency	Percentage
Daily	52%
Weekly	11%
Not at all	37%



Device Type	Percentage
Smartphones	53%
Tablets	11%
Other mobile devices	37%



- Molecule 1: Type II secretion system protein D



- Molecule 1: Type II secretion system protein D





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	18005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/2987	0.67	0/4050
1	B	0.44	0/2987	0.67	0/4050
1	C	0.44	0/2987	0.67	0/4050
1	D	0.44	0/2987	0.67	0/4050
1	E	0.44	0/2987	0.67	0/4050
1	F	0.44	0/2987	0.67	0/4050
1	G	0.44	0/2987	0.67	0/4050
1	H	0.44	0/2987	0.67	0/4050
1	I	0.44	0/2987	0.67	0/4050
1	J	0.44	0/2987	0.67	0/4050
1	K	0.44	0/2987	0.67	0/4050
1	L	0.44	0/2987	0.67	0/4050
1	M	0.44	0/2987	0.67	0/4050
1	N	0.44	0/2987	0.67	0/4050
1	O	0.44	0/2987	0.67	0/4050
All	All	0.44	0/44805	0.67	0/60750

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 [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	2961	0	3052	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2961	0	3052	60	0
1	C	2961	0	3052	74	0
1	D	2961	0	3052	79	0
1	E	2961	0	3052	63	0
1	F	2961	0	3052	55	0
1	G	2961	0	3052	55	0
1	H	2961	0	3052	53	0
1	I	2961	0	3052	50	0
1	J	2961	0	3052	48	0
1	K	2961	0	3052	48	0
1	L	2961	0	3052	47	0
1	M	2961	0	3052	46	0
1	N	2961	0	3052	56	0
1	O	2961	0	3052	56	0
All	All	44415	0	45780	738	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 8.

All (738) 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:D:512:LEU:HB3	1:E:326:GLN:HE21	1.22	1.04
1:G:440:GLY:HA2	1:H:455:THR:HA	1.51	0.90
1:D:233:LEU:O	1:D:237:LEU:HB2	1.77	0.85
1:F:233:LEU:O	1:F:237:LEU:HB2	1.77	0.85
1:I:233:LEU:O	1:I:237:LEU:HB2	1.77	0.85
1:K:233:LEU:O	1:K:237:LEU:HB2	1.77	0.85
1:A:233:LEU:O	1:A:237:LEU:HB2	1.77	0.85
1:M:233:LEU:O	1:M:237:LEU:HB2	1.77	0.85
1:B:233:LEU:O	1:B:237:LEU:HB2	1.77	0.84
1:C:233:LEU:O	1:C:237:LEU:HB2	1.77	0.84
1:H:233:LEU:O	1:H:237:LEU:HB2	1.77	0.84
1:N:233:LEU:O	1:N:237:LEU:HB2	1.77	0.84
1:O:233:LEU:O	1:O:237:LEU:HB2	1.77	0.84
1:G:233:LEU:O	1:G:237:LEU:HB2	1.77	0.84
1:E:233:LEU:O	1:E:237:LEU:HB2	1.77	0.83
1:J:233:LEU:O	1:J:237:LEU:HB2	1.77	0.83
1:L:233:LEU:O	1:L:237:LEU:HB2	1.77	0.83
1:G:502:THR:HB	1:H:434:ASN:HD22	1.44	0.81
1:C:440:GLY:HA2	1:D:455:THR:HA	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:HB3	1:C:326:GLN:HE21	1.48	0.77
1:C:500:LEU:O	1:D:434:ASN:HB3	1.88	0.73
1:D:512:LEU:HB3	1:E:326:GLN:NE2	2.00	0.73
1:G:434:ASN:HD22	1:F:502:THR:HB	1.54	0.73
1:D:374:GLN:NE2	1:E:383:GLU:O	2.22	0.72
1:C:424:ASN:HD21	1:D:299:ASN:HD21	1.39	0.71
1:C:498:THR:O	1:D:458:ARG:NH2	2.21	0.70
1:A:182:TYR:H	1:A:238:ASP:HB2	1.57	0.69
1:H:182:TYR:H	1:H:238:ASP:HB2	1.57	0.69
1:B:182:TYR:H	1:B:238:ASP:HB2	1.57	0.69
1:E:182:TYR:H	1:E:238:ASP:HB2	1.57	0.69
1:D:182:TYR:H	1:D:238:ASP:HB2	1.57	0.69
1:K:182:TYR:H	1:K:238:ASP:HB2	1.57	0.69
1:N:182:TYR:H	1:N:238:ASP:HB2	1.57	0.69
1:I:440:GLY:HA2	1:J:455:THR:HA	1.74	0.69
1:G:182:TYR:H	1:G:238:ASP:HB2	1.57	0.69
1:O:291:LEU:HD13	1:N:267:ILE:HA	1.75	0.68
1:I:182:TYR:H	1:I:238:ASP:HB2	1.57	0.68
1:O:210:ILE:HG21	1:N:191:VAL:HG13	1.75	0.68
1:F:182:TYR:H	1:F:238:ASP:HB2	1.57	0.68
1:M:182:TYR:H	1:M:238:ASP:HB2	1.57	0.68
1:D:566:ARG:NH1	1:E:612:ASP:O	2.26	0.68
1:O:182:TYR:H	1:O:238:ASP:HB2	1.57	0.68
1:O:458:ARG:NH2	1:N:498:THR:O	2.21	0.68
1:C:182:TYR:H	1:C:238:ASP:HB2	1.57	0.68
1:J:182:TYR:H	1:J:238:ASP:HB2	1.57	0.67
1:L:182:TYR:H	1:L:238:ASP:HB2	1.57	0.67
1:D:237:LEU:HD12	1:E:215:THR:HG21	1.76	0.66
1:A:440:GLY:HA2	1:B:455:THR:HA	1.78	0.64
1:O:406:SER:HB2	1:N:537:PRO:HB3	1.80	0.64
1:I:502:THR:HB	1:J:434:ASN:HD22	1.63	0.64
1:J:512:LEU:O	1:K:326:GLN:NE2	2.31	0.64
1:B:248:ARG:HB3	1:B:303:LEU:HB2	1.81	0.63
1:C:248:ARG:HB3	1:C:303:LEU:HB2	1.81	0.63
1:L:248:ARG:HB3	1:L:303:LEU:HB2	1.81	0.63
1:A:358:THR:HA	1:B:391:VAL:HA	1.80	0.63
1:M:248:ARG:HB3	1:M:303:LEU:HB2	1.81	0.63
1:D:248:ARG:HB3	1:D:303:LEU:HB2	1.81	0.63
1:K:248:ARG:HB3	1:K:303:LEU:HB2	1.81	0.63
1:A:248:ARG:HB3	1:A:303:LEU:HB2	1.81	0.63
1:D:512:LEU:O	1:E:326:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:248:ARG:HB3	1:J:303:LEU:HB2	1.81	0.63
1:O:210:ILE:HD13	1:N:191:VAL:HG13	1.79	0.63
1:N:248:ARG:HB3	1:N:303:LEU:HB2	1.81	0.63
1:O:248:ARG:HB3	1:O:303:LEU:HB2	1.81	0.63
1:E:248:ARG:HB3	1:E:303:LEU:HB2	1.81	0.63
1:I:248:ARG:HB3	1:I:303:LEU:HB2	1.81	0.63
1:F:248:ARG:HB3	1:F:303:LEU:HB2	1.81	0.62
1:C:414:LEU:HD21	1:D:611:PHE:HZ	1.65	0.62
1:G:248:ARG:HB3	1:G:303:LEU:HB2	1.81	0.62
1:H:248:ARG:HB3	1:H:303:LEU:HB2	1.81	0.62
1:G:326:GLN:NE2	1:F:512:LEU:O	2.33	0.62
1:O:512:LEU:O	1:A:326:GLN:NE2	2.34	0.61
1:B:540:GLY:O	1:B:550:ARG:NH1	2.34	0.60
1:O:540:GLY:O	1:O:550:ARG:NH1	2.34	0.60
1:L:502:THR:HB	1:M:434:ASN:HD22	1.65	0.60
1:A:540:GLY:O	1:A:550:ARG:NH1	2.34	0.60
1:C:540:GLY:O	1:C:550:ARG:NH1	2.34	0.60
1:M:540:GLY:O	1:M:550:ARG:NH1	2.34	0.60
1:O:431:VAL:HG21	1:N:524:LEU:HD22	1.84	0.60
1:N:540:GLY:O	1:N:550:ARG:NH1	2.34	0.60
1:D:540:GLY:O	1:D:550:ARG:NH1	2.34	0.60
1:L:540:GLY:O	1:L:550:ARG:NH1	2.34	0.60
1:O:217:ARG:HH12	1:N:236:SER:HB2	1.66	0.59
1:I:540:GLY:O	1:I:550:ARG:NH1	2.34	0.59
1:H:540:GLY:O	1:H:550:ARG:NH1	2.34	0.59
1:E:424:ASN:HD21	1:F:299:ASN:HD21	1.49	0.59
1:C:270:GLY:O	1:D:243:ARG:NH2	2.36	0.59
1:J:540:GLY:O	1:J:550:ARG:NH1	2.34	0.59
1:K:540:GLY:O	1:K:550:ARG:NH1	2.34	0.59
1:G:540:GLY:O	1:G:550:ARG:NH1	2.34	0.59
1:O:299:ASN:HD21	1:N:424:ASN:HD21	1.51	0.59
1:A:502:THR:HB	1:B:434:ASN:HD22	1.67	0.59
1:G:255:ASN:ND2	1:G:320:LEU:O	2.36	0.59
1:L:255:ASN:ND2	1:L:320:LEU:O	2.36	0.59
1:F:506:SER:OG	1:F:508:LYS:NZ	2.35	0.58
1:K:255:ASN:ND2	1:K:320:LEU:O	2.36	0.58
1:J:255:ASN:ND2	1:J:320:LEU:O	2.36	0.58
1:M:255:ASN:ND2	1:M:320:LEU:O	2.36	0.58
1:N:255:ASN:ND2	1:N:320:LEU:O	2.36	0.58
1:C:506:SER:OG	1:C:508:LYS:NZ	2.35	0.58
1:D:477:LEU:HD21	1:D:567:PRO:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:SER:OG	1:E:508:LYS:NZ	2.35	0.58
1:E:540:GLY:O	1:E:550:ARG:NH1	2.34	0.58
1:E:477:LEU:HD21	1:E:567:PRO:HB2	1.86	0.58
1:H:255:ASN:ND2	1:H:320:LEU:O	2.36	0.58
1:I:255:ASN:ND2	1:I:320:LEU:O	2.36	0.58
1:A:482:GLU:HG3	1:A:508:LYS:HG2	1.85	0.58
1:A:359:LYS:HE2	1:B:390:ILE:HD11	1.84	0.58
1:H:477:LEU:HD21	1:H:567:PRO:HB2	1.86	0.58
1:I:477:LEU:HD21	1:I:567:PRO:HB2	1.86	0.58
1:J:477:LEU:HD21	1:J:567:PRO:HB2	1.86	0.58
1:C:502:THR:HB	1:D:434:ASN:HD22	1.67	0.58
1:E:255:ASN:ND2	1:E:320:LEU:O	2.36	0.58
1:G:506:SER:OG	1:G:508:LYS:NZ	2.35	0.58
1:M:477:LEU:HD21	1:M:567:PRO:HB2	1.86	0.58
1:F:255:ASN:ND2	1:F:320:LEU:O	2.36	0.58
1:F:540:GLY:O	1:F:550:ARG:NH1	2.34	0.58
1:G:477:LEU:HD21	1:G:567:PRO:HB2	1.86	0.58
1:J:482:GLU:HG3	1:J:508:LYS:HG2	1.86	0.58
1:K:477:LEU:HD21	1:K:567:PRO:HB2	1.86	0.58
1:K:482:GLU:HG3	1:K:508:LYS:HG2	1.85	0.58
1:N:477:LEU:HD21	1:N:567:PRO:HB2	1.86	0.58
1:O:255:ASN:ND2	1:O:320:LEU:O	2.36	0.58
1:B:267:ILE:HD13	1:C:302:VAL:HG11	1.85	0.58
1:D:339:ASP:OD1	1:D:409:THR:OG1	2.22	0.58
1:E:339:ASP:OD1	1:E:409:THR:OG1	2.22	0.58
1:F:477:LEU:HD21	1:F:567:PRO:HB2	1.86	0.58
1:I:482:GLU:HG3	1:I:508:LYS:HG2	1.85	0.58
1:A:255:ASN:ND2	1:A:320:LEU:O	2.36	0.58
1:B:482:GLU:HG3	1:B:508:LYS:HG2	1.85	0.58
1:C:477:LEU:HD21	1:C:567:PRO:HB2	1.86	0.58
1:L:477:LEU:HD21	1:L:567:PRO:HB2	1.86	0.58
1:O:482:GLU:HG3	1:O:508:LYS:HG2	1.86	0.58
1:B:477:LEU:HD21	1:B:567:PRO:HB2	1.86	0.57
1:D:255:ASN:ND2	1:D:320:LEU:O	2.36	0.57
1:D:506:SER:OG	1:D:508:LYS:NZ	2.35	0.57
1:N:339:ASP:OD1	1:N:409:THR:OG1	2.22	0.57
1:M:339:ASP:OD1	1:M:409:THR:OG1	2.22	0.57
1:C:482:GLU:HG3	1:C:508:LYS:HG2	1.85	0.57
1:L:482:GLU:HG3	1:L:508:LYS:HG2	1.85	0.57
1:M:506:SER:OG	1:M:508:LYS:NZ	2.35	0.57
1:A:477:LEU:HD21	1:A:567:PRO:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ASP:OD1	1:C:409:THR:OG1	2.22	0.57
1:K:339:ASP:OD1	1:K:409:THR:OG1	2.22	0.57
1:O:477:LEU:HD21	1:O:567:PRO:HB2	1.86	0.57
1:H:482:GLU:HG3	1:H:508:LYS:HG2	1.85	0.57
1:B:255:ASN:ND2	1:B:320:LEU:O	2.36	0.57
1:E:440:GLY:HA2	1:F:455:THR:HA	1.87	0.57
1:O:339:ASP:OD1	1:O:409:THR:OG1	2.22	0.57
1:F:339:ASP:OD1	1:F:409:THR:OG1	2.22	0.57
1:H:506:SER:OG	1:H:508:LYS:NZ	2.35	0.57
1:N:482:GLU:HG3	1:N:508:LYS:HG2	1.85	0.57
1:B:506:SER:OG	1:B:508:LYS:NZ	2.35	0.57
1:J:502:THR:HB	1:K:434:ASN:HD22	1.70	0.57
1:C:529:VAL:HG13	1:D:412:ASN:HB3	1.87	0.57
1:D:482:GLU:HG3	1:D:508:LYS:HG2	1.85	0.57
1:E:389:ALA:HB3	1:E:404:ALA:O	2.05	0.57
1:I:389:ALA:HB3	1:I:404:ALA:O	2.05	0.57
1:C:255:ASN:ND2	1:C:320:LEU:O	2.36	0.56
1:G:389:ALA:HB3	1:G:404:ALA:O	2.05	0.56
1:I:506:SER:OG	1:I:508:LYS:NZ	2.35	0.56
1:K:389:ALA:HB3	1:K:404:ALA:O	2.05	0.56
1:G:482:GLU:HG3	1:G:508:LYS:HG2	1.85	0.56
1:L:339:ASP:OD1	1:L:409:THR:OG1	2.22	0.56
1:C:389:ALA:HB3	1:C:404:ALA:O	2.05	0.56
1:E:482:GLU:HG3	1:E:508:LYS:HG2	1.85	0.56
1:L:440:GLY:HA2	1:M:455:THR:HA	1.87	0.56
1:N:389:ALA:HB3	1:N:404:ALA:O	2.05	0.56
1:A:339:ASP:OD1	1:A:409:THR:OG1	2.22	0.56
1:B:339:ASP:OD1	1:B:409:THR:OG1	2.22	0.56
1:J:506:SER:OG	1:J:508:LYS:NZ	2.35	0.56
1:M:482:GLU:HG3	1:M:508:LYS:HG2	1.85	0.56
1:O:215:THR:HA	1:N:241:THR:HB	1.87	0.56
1:M:389:ALA:HB3	1:M:404:ALA:O	2.05	0.56
1:N:477:LEU:HD13	1:N:479:LEU:HG	1.88	0.56
1:F:482:GLU:HG3	1:F:508:LYS:HG2	1.85	0.56
1:A:506:SER:OG	1:A:508:LYS:NZ	2.35	0.56
1:B:477:LEU:HD13	1:B:479:LEU:HG	1.88	0.56
1:J:477:LEU:CD1	1:J:479:LEU:HG	2.36	0.56
1:M:477:LEU:HD13	1:M:479:LEU:HG	1.88	0.56
1:O:477:LEU:HD13	1:O:479:LEU:HG	1.88	0.56
1:O:477:LEU:CD1	1:O:479:LEU:HG	2.36	0.56
1:A:477:LEU:CD1	1:A:479:LEU:HG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:477:LEU:CD1	1:L:479:LEU:HG	2.36	0.56
1:M:477:LEU:CD1	1:M:479:LEU:HG	2.36	0.56
1:G:339:ASP:OD1	1:G:409:THR:OG1	2.22	0.56
1:L:477:LEU:HD13	1:L:479:LEU:HG	1.88	0.56
1:O:389:ALA:HB3	1:O:404:ALA:O	2.05	0.56
1:C:477:LEU:CD1	1:C:479:LEU:HG	2.36	0.56
1:I:477:LEU:CD1	1:I:479:LEU:HG	2.36	0.56
1:A:389:ALA:HB3	1:A:404:ALA:O	2.05	0.56
1:A:477:LEU:HD13	1:A:479:LEU:HG	1.88	0.56
1:C:477:LEU:HD13	1:C:479:LEU:HG	1.88	0.56
1:D:389:ALA:HB3	1:D:404:ALA:O	2.05	0.56
1:C:527:ASP:HB3	1:D:414:LEU:HD23	1.87	0.56
1:J:477:LEU:HD13	1:J:479:LEU:HG	1.88	0.56
1:K:477:LEU:HD13	1:K:479:LEU:HG	1.88	0.56
1:K:506:SER:OG	1:K:508:LYS:NZ	2.35	0.56
1:F:389:ALA:HB3	1:F:404:ALA:O	2.05	0.55
1:L:389:ALA:HB3	1:L:404:ALA:O	2.05	0.55
1:B:477:LEU:CD1	1:B:479:LEU:HG	2.36	0.55
1:N:477:LEU:CD1	1:N:479:LEU:HG	2.36	0.55
1:C:523:GLY:N	1:D:418:SER:O	2.38	0.55
1:F:477:LEU:CD1	1:F:479:LEU:HG	2.36	0.55
1:G:477:LEU:CD1	1:G:479:LEU:HG	2.36	0.55
1:O:506:SER:OG	1:O:508:LYS:NZ	2.35	0.55
1:B:236:SER:O	1:C:217:ARG:NH2	2.40	0.55
1:H:389:ALA:HB3	1:H:404:ALA:O	2.05	0.55
1:B:389:ALA:HB3	1:B:404:ALA:O	2.05	0.55
1:J:389:ALA:HB3	1:J:404:ALA:O	2.05	0.55
1:K:477:LEU:CD1	1:K:479:LEU:HG	2.36	0.55
1:G:455:THR:HA	1:F:440:GLY:HA2	1.88	0.55
1:G:315:ASP:OD1	1:G:318:ARG:NH2	2.40	0.55
1:I:477:LEU:HD13	1:I:479:LEU:HG	1.88	0.55
1:O:455:THR:HA	1:N:440:GLY:HA2	1.89	0.55
1:D:477:LEU:CD1	1:D:479:LEU:HG	2.36	0.55
1:H:315:ASP:OD1	1:H:318:ARG:NH2	2.40	0.55
1:A:532:ALA:HA	1:B:409:THR:HA	1.89	0.55
1:E:477:LEU:HD13	1:E:479:LEU:HG	1.88	0.55
1:K:315:ASP:OD1	1:K:318:ARG:NH2	2.40	0.55
1:M:315:ASP:OD1	1:M:318:ARG:NH2	2.40	0.55
1:N:315:ASP:OD1	1:N:318:ARG:NH2	2.40	0.55
1:C:315:ASP:OD1	1:C:318:ARG:NH2	2.40	0.55
1:D:477:LEU:HD13	1:D:479:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:477:LEU:CD1	1:H:479:LEU:HG	2.36	0.55
1:O:315:ASP:OD1	1:O:318:ARG:NH2	2.40	0.55
1:A:315:ASP:OD1	1:A:318:ARG:NH2	2.40	0.55
1:B:315:ASP:OD1	1:B:318:ARG:NH2	2.40	0.55
1:E:414:LEU:HD21	1:F:611:PHE:HZ	1.72	0.55
1:E:477:LEU:CD1	1:E:479:LEU:HG	2.36	0.55
1:E:315:ASP:OD1	1:E:318:ARG:NH2	2.40	0.54
1:F:477:LEU:HD13	1:F:479:LEU:HG	1.88	0.54
1:L:315:ASP:OD1	1:L:318:ARG:NH2	2.40	0.54
1:L:506:SER:OG	1:L:508:LYS:NZ	2.35	0.54
1:G:477:LEU:HD13	1:G:479:LEU:HG	1.88	0.54
1:H:477:LEU:HD13	1:H:479:LEU:HG	1.88	0.54
1:J:315:ASP:OD1	1:J:318:ARG:NH2	2.40	0.54
1:D:315:ASP:OD1	1:D:318:ARG:NH2	2.40	0.54
1:F:315:ASP:OD1	1:F:318:ARG:NH2	2.40	0.54
1:O:329:VAL:O	1:O:418:SER:HA	2.08	0.54
1:G:329:VAL:O	1:G:418:SER:HA	2.08	0.54
1:I:315:ASP:OD1	1:I:318:ARG:NH2	2.40	0.54
1:A:329:VAL:O	1:A:418:SER:HA	2.08	0.54
1:F:329:VAL:O	1:F:418:SER:HA	2.08	0.54
1:L:512:LEU:O	1:M:326:GLN:NE2	2.40	0.54
1:G:512:LEU:O	1:H:326:GLN:NE2	2.40	0.54
1:H:329:VAL:O	1:H:418:SER:HA	2.08	0.54
1:B:329:VAL:O	1:B:418:SER:HA	2.08	0.54
1:E:329:VAL:O	1:E:418:SER:HA	2.08	0.54
1:N:329:VAL:O	1:N:418:SER:HA	2.08	0.54
1:N:506:SER:OG	1:N:508:LYS:NZ	2.35	0.54
1:K:329:VAL:O	1:K:418:SER:HA	2.08	0.53
1:B:272:LYS:O	1:C:243:ARG:NH2	2.42	0.53
1:L:329:VAL:O	1:L:418:SER:HA	2.08	0.53
1:C:329:VAL:O	1:C:418:SER:HA	2.08	0.53
1:C:336:ILE:HD13	1:D:587:ILE:HD11	1.91	0.53
1:D:329:VAL:O	1:D:418:SER:HA	2.08	0.53
1:H:339:ASP:OD1	1:H:409:THR:OG1	2.22	0.53
1:J:329:VAL:O	1:J:418:SER:HA	2.08	0.53
1:E:477:LEU:HD12	1:E:477:LEU:O	2.09	0.53
1:N:528:ASP:HB3	1:N:557:THR:HB	1.91	0.53
1:C:267:ILE:HA	1:D:291:LEU:HD13	1.91	0.53
1:D:528:ASP:HB3	1:D:557:THR:HB	1.91	0.53
1:F:528:ASP:HB3	1:F:557:THR:HB	1.91	0.53
1:M:329:VAL:O	1:M:418:SER:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:528:ASP:HB3	1:M:557:THR:HB	1.91	0.53
1:C:528:ASP:HB3	1:C:557:THR:HB	1.91	0.53
1:G:528:ASP:HB3	1:G:557:THR:HB	1.91	0.53
1:I:339:ASP:OD1	1:I:409:THR:OG1	2.22	0.53
1:K:528:ASP:HB3	1:K:557:THR:HB	1.91	0.53
1:L:528:ASP:HB3	1:L:557:THR:HB	1.91	0.53
1:N:477:LEU:HD12	1:N:477:LEU:O	2.09	0.53
1:O:477:LEU:O	1:O:477:LEU:HD12	2.09	0.53
1:A:528:ASP:HB3	1:A:557:THR:HB	1.91	0.52
1:B:528:ASP:HB3	1:B:557:THR:HB	1.91	0.52
1:D:477:LEU:O	1:D:477:LEU:HD12	2.09	0.52
1:E:528:ASP:HB3	1:E:557:THR:HB	1.91	0.52
1:F:477:LEU:HD12	1:F:477:LEU:O	2.09	0.52
1:I:329:VAL:O	1:I:418:SER:HA	2.08	0.52
1:J:528:ASP:HB3	1:J:557:THR:HB	1.91	0.52
1:M:477:LEU:HD12	1:M:477:LEU:O	2.09	0.52
1:C:477:LEU:O	1:C:477:LEU:HD12	2.09	0.52
1:D:483:GLN:HE22	1:D:485:ILE:HG13	1.75	0.52
1:F:483:GLN:HE22	1:F:485:ILE:HG13	1.75	0.52
1:K:483:GLN:HE22	1:K:485:ILE:HG13	1.75	0.52
1:N:483:GLN:HE22	1:N:485:ILE:HG13	1.75	0.52
1:B:483:GLN:HE22	1:B:485:ILE:HG13	1.75	0.52
1:D:355:MET:HB3	1:E:396:SER:HA	1.90	0.52
1:G:497:ASN:OD1	1:H:436:PRO:HG3	2.09	0.52
1:H:483:GLN:HE22	1:H:485:ILE:HG13	1.75	0.52
1:I:528:ASP:HB3	1:I:557:THR:HB	1.91	0.52
1:O:528:ASP:HB3	1:O:557:THR:HB	1.91	0.52
1:A:477:LEU:O	1:A:477:LEU:HD12	2.09	0.52
1:G:477:LEU:O	1:G:477:LEU:HD12	2.09	0.52
1:H:528:ASP:HB3	1:H:557:THR:HB	1.91	0.52
1:O:175:TYR:HB2	1:N:229:LYS:NZ	2.25	0.52
1:B:477:LEU:O	1:B:477:LEU:HD12	2.09	0.52
1:C:497:ASN:OD1	1:D:436:PRO:HG3	2.10	0.52
1:H:477:LEU:O	1:H:477:LEU:HD12	2.09	0.52
1:I:483:GLN:HE22	1:I:485:ILE:HG13	1.75	0.52
1:J:477:LEU:HD12	1:J:477:LEU:O	2.09	0.52
1:L:477:LEU:O	1:L:477:LEU:HD12	2.09	0.52
1:A:483:GLN:HE22	1:A:485:ILE:HG13	1.75	0.52
1:K:378:SER:HA	1:K:382:PRO:HD2	1.92	0.52
1:L:378:SER:HA	1:L:382:PRO:HD2	1.92	0.52
1:O:483:GLN:HE22	1:O:485:ILE:HG13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:477:LEU:O	1:I:477:LEU:HD12	2.09	0.51
1:O:434:ASN:HD22	1:N:502:THR:HB	1.75	0.51
1:J:339:ASP:OD1	1:J:409:THR:OG1	2.22	0.51
1:J:483:GLN:HE22	1:J:485:ILE:HG13	1.75	0.51
1:K:477:LEU:HD12	1:K:477:LEU:O	2.09	0.51
1:L:483:GLN:HE22	1:L:485:ILE:HG13	1.75	0.51
1:M:483:GLN:HE22	1:M:485:ILE:HG13	1.75	0.51
1:I:477:LEU:C	1:I:477:LEU:HD12	2.31	0.51
1:J:378:SER:HA	1:J:382:PRO:HD2	1.92	0.51
1:L:329:VAL:HG21	1:L:467:VAL:HG11	1.93	0.51
1:C:477:LEU:C	1:C:477:LEU:HD12	2.31	0.51
1:C:532:ALA:HA	1:D:409:THR:HA	1.92	0.51
1:G:412:ASN:HB3	1:F:529:VAL:HG13	1.92	0.51
1:M:329:VAL:HG21	1:M:467:VAL:HG11	1.93	0.51
1:F:477:LEU:HD12	1:F:477:LEU:C	2.31	0.51
1:G:483:GLN:HE22	1:G:485:ILE:HG13	1.75	0.51
1:L:477:LEU:HD12	1:L:477:LEU:C	2.31	0.51
1:E:477:LEU:HD12	1:E:477:LEU:C	2.31	0.51
1:H:477:LEU:C	1:H:477:LEU:HD12	2.31	0.51
1:K:329:VAL:HG21	1:K:467:VAL:HG11	1.93	0.51
1:K:477:LEU:C	1:K:477:LEU:HD12	2.31	0.51
1:M:378:SER:HA	1:M:382:PRO:HD2	1.93	0.51
1:C:483:GLN:HE22	1:C:485:ILE:HG13	1.75	0.51
1:I:378:SER:HA	1:I:382:PRO:HD2	1.92	0.51
1:K:174:ASP:N	1:K:222:GLY:O	2.44	0.51
1:N:477:LEU:C	1:N:477:LEU:HD12	2.31	0.51
1:C:174:ASP:N	1:C:222:GLY:O	2.44	0.50
1:E:483:GLN:HE22	1:E:485:ILE:HG13	1.75	0.50
1:F:329:VAL:HG21	1:F:467:VAL:HG11	1.93	0.50
1:J:477:LEU:C	1:J:477:LEU:HD12	2.31	0.50
1:N:233:LEU:O	1:N:237:LEU:CB	2.57	0.50
1:N:329:VAL:HG21	1:N:467:VAL:HG11	1.92	0.50
1:E:329:VAL:HG21	1:E:467:VAL:HG11	1.93	0.50
1:G:386:PRO:HG3	1:F:370:GLY:HA3	1.93	0.50
1:G:477:LEU:C	1:G:477:LEU:HD12	2.31	0.50
1:J:329:VAL:HG21	1:J:467:VAL:HG11	1.93	0.50
1:B:174:ASP:N	1:B:222:GLY:O	2.45	0.50
1:B:378:SER:HA	1:B:382:PRO:HD2	1.92	0.50
1:B:477:LEU:HD12	1:B:477:LEU:C	2.31	0.50
1:E:378:SER:HA	1:E:382:PRO:HD2	1.92	0.50
1:O:477:LEU:C	1:O:477:LEU:HD12	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:O	1:D:237:LEU:CB	2.57	0.50
1:D:361:ASN:HD22	1:E:386:PRO:HB2	1.77	0.50
1:F:378:SER:HA	1:F:382:PRO:HD2	1.93	0.50
1:G:378:SER:HA	1:G:382:PRO:HD2	1.92	0.50
1:J:174:ASP:N	1:J:222:GLY:O	2.44	0.50
1:A:378:SER:HA	1:A:382:PRO:HD2	1.92	0.50
1:C:378:SER:HA	1:C:382:PRO:HD2	1.92	0.50
1:N:174:ASP:N	1:N:222:GLY:O	2.44	0.50
1:A:174:ASP:N	1:A:222:GLY:O	2.44	0.50
1:A:477:LEU:C	1:A:477:LEU:HD12	2.31	0.50
1:D:329:VAL:HG21	1:D:467:VAL:HG11	1.93	0.50
1:G:329:VAL:HG21	1:G:467:VAL:HG11	1.93	0.50
1:H:378:SER:HA	1:H:382:PRO:HD2	1.92	0.50
1:N:378:SER:HA	1:N:382:PRO:HD2	1.92	0.50
1:D:174:ASP:N	1:D:222:GLY:O	2.45	0.50
1:H:174:ASP:N	1:H:222:GLY:O	2.45	0.50
1:M:477:LEU:HD12	1:M:477:LEU:C	2.31	0.50
1:D:378:SER:HA	1:D:382:PRO:HD2	1.93	0.50
1:D:477:LEU:C	1:D:477:LEU:HD12	2.31	0.50
1:L:174:ASP:N	1:L:222:GLY:O	2.44	0.50
1:C:329:VAL:HG21	1:C:467:VAL:HG11	1.93	0.50
1:G:174:ASP:N	1:G:222:GLY:O	2.44	0.50
1:H:329:VAL:HG21	1:H:467:VAL:HG11	1.93	0.50
1:I:329:VAL:HG21	1:I:467:VAL:HG11	1.93	0.50
1:M:233:LEU:O	1:M:237:LEU:CB	2.57	0.50
1:I:174:ASP:N	1:I:222:GLY:O	2.45	0.49
1:K:512:LEU:O	1:L:326:GLN:NE2	2.45	0.49
1:O:329:VAL:HG21	1:O:467:VAL:HG11	1.93	0.49
1:O:505:ARG:HE	1:O:561:LEU:HD22	1.77	0.49
1:D:505:ARG:HE	1:D:561:LEU:HD22	1.77	0.49
1:E:174:ASP:N	1:E:222:GLY:O	2.44	0.49
1:F:174:ASP:N	1:F:222:GLY:O	2.44	0.49
1:G:505:ARG:HE	1:G:561:LEU:HD22	1.77	0.49
1:M:174:ASP:N	1:M:222:GLY:O	2.44	0.49
1:O:378:SER:HA	1:O:382:PRO:HD2	1.93	0.49
1:F:511:ILE:HG21	1:F:521:ILE:HD12	1.95	0.49
1:B:329:VAL:HG21	1:B:467:VAL:HG11	1.93	0.49
1:G:191:VAL:HG13	1:H:210:ILE:HG21	1.95	0.49
1:H:511:ILE:HG21	1:H:521:ILE:HD12	1.95	0.49
1:I:511:ILE:HG21	1:I:521:ILE:HD12	1.94	0.49
1:O:174:ASP:N	1:O:222:GLY:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:HE	1:A:561:LEU:HD22	1.77	0.49
1:M:505:ARG:HE	1:M:561:LEU:HD22	1.77	0.49
1:A:329:VAL:HG21	1:A:467:VAL:HG11	1.93	0.49
1:B:505:ARG:HE	1:B:561:LEU:HD22	1.77	0.49
1:C:473:ASP:N	1:C:473:ASP:OD1	2.46	0.49
1:D:511:ILE:HG21	1:D:521:ILE:HD12	1.95	0.49
1:J:505:ARG:HE	1:J:561:LEU:HD22	1.77	0.49
1:L:473:ASP:N	1:L:473:ASP:OD1	2.46	0.49
1:L:505:ARG:HE	1:L:561:LEU:HD22	1.77	0.49
1:B:473:ASP:OD1	1:B:473:ASP:N	2.46	0.49
1:C:505:ARG:HE	1:C:561:LEU:HD22	1.78	0.49
1:F:505:ARG:HE	1:F:561:LEU:HD22	1.77	0.49
1:H:473:ASP:N	1:H:473:ASP:OD1	2.46	0.49
1:K:511:ILE:HG21	1:K:521:ILE:HD12	1.95	0.49
1:A:473:ASP:OD1	1:A:473:ASP:N	2.46	0.49
1:G:233:LEU:O	1:G:237:LEU:CB	2.57	0.49
1:G:511:ILE:HG21	1:G:521:ILE:HD12	1.95	0.49
1:L:233:LEU:O	1:L:237:LEU:CB	2.57	0.48
1:I:505:ARG:HE	1:I:561:LEU:HD22	1.77	0.48
1:E:505:ARG:HE	1:E:561:LEU:HD22	1.77	0.48
1:H:505:ARG:HE	1:H:561:LEU:HD22	1.77	0.48
1:J:511:ILE:HG21	1:J:521:ILE:HD12	1.94	0.48
1:B:511:ILE:HG21	1:B:521:ILE:HD12	1.95	0.48
1:D:367:LEU:HD12	1:D:390:ILE:HG21	1.96	0.48
1:N:505:ARG:HE	1:N:561:LEU:HD22	1.77	0.48
1:O:473:ASP:N	1:O:473:ASP:OD1	2.46	0.48
1:G:473:ASP:OD1	1:G:473:ASP:N	2.46	0.48
1:B:477:LEU:HD21	1:B:567:PRO:CB	2.44	0.48
1:C:367:LEU:HD12	1:C:390:ILE:HG21	1.96	0.48
1:C:521:ILE:O	1:D:420:LEU:N	2.45	0.48
1:E:367:LEU:HD12	1:E:390:ILE:HG21	1.96	0.48
1:G:351:ASN:HD21	1:G:397:SER:HB2	1.79	0.48
1:K:505:ARG:HE	1:K:561:LEU:HD22	1.77	0.48
1:M:511:ILE:HG21	1:M:521:ILE:HD12	1.94	0.48
1:C:511:ILE:HG21	1:C:521:ILE:HD12	1.94	0.48
1:D:351:ASN:HD21	1:D:397:SER:HB2	1.79	0.48
1:D:477:LEU:HD21	1:D:567:PRO:CB	2.44	0.48
1:E:351:ASN:HD21	1:E:397:SER:HB2	1.79	0.48
1:F:351:ASN:HD21	1:F:397:SER:HB2	1.79	0.48
1:G:367:LEU:HD12	1:G:390:ILE:HG21	1.96	0.48
1:H:502:THR:HB	1:I:434:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:473:ASP:N	1:K:473:ASP:OD1	2.46	0.48
1:N:511:ILE:HG21	1:N:521:ILE:HD12	1.94	0.48
1:O:477:LEU:HD21	1:O:567:PRO:CB	2.44	0.48
1:B:367:LEU:HD12	1:B:390:ILE:HG21	1.96	0.48
1:C:233:LEU:O	1:C:237:LEU:CB	2.57	0.48
1:F:367:LEU:HD12	1:F:390:ILE:HG21	1.96	0.48
1:H:367:LEU:HD12	1:H:390:ILE:HG21	1.96	0.48
1:H:351:ASN:HD21	1:H:397:SER:HB2	1.79	0.48
1:I:367:LEU:HD12	1:I:390:ILE:HG21	1.96	0.48
1:A:511:ILE:HG21	1:A:521:ILE:HD12	1.95	0.48
1:E:511:ILE:HG21	1:E:521:ILE:HD12	1.95	0.48
1:J:367:LEU:HD12	1:J:390:ILE:HG21	1.96	0.48
1:J:473:ASP:OD1	1:J:473:ASP:N	2.46	0.48
1:K:477:LEU:HD21	1:K:567:PRO:CB	2.44	0.48
1:L:477:LEU:HD21	1:L:567:PRO:CB	2.44	0.48
1:M:477:LEU:HD21	1:M:567:PRO:CB	2.44	0.48
1:C:351:ASN:HD21	1:C:397:SER:HB2	1.79	0.47
1:I:473:ASP:N	1:I:473:ASP:OD1	2.46	0.47
1:O:511:ILE:HG21	1:O:521:ILE:HD12	1.94	0.47
1:D:237:LEU:HG	1:E:214:ARG:NH2	2.28	0.47
1:K:233:LEU:O	1:K:237:LEU:CB	2.57	0.47
1:O:347:GLN:HB3	1:O:369:ILE:HD11	1.96	0.47
1:A:367:LEU:HD12	1:A:390:ILE:HG21	1.96	0.47
1:E:233:LEU:O	1:E:237:LEU:CB	2.57	0.47
1:G:477:LEU:HD21	1:G:567:PRO:CB	2.44	0.47
1:K:367:LEU:HD12	1:K:390:ILE:HG21	1.96	0.47
1:I:351:ASN:HD21	1:I:397:SER:HB2	1.79	0.47
1:J:477:LEU:HD21	1:J:567:PRO:CB	2.44	0.47
1:L:351:ASN:HD21	1:L:397:SER:HB2	1.79	0.47
1:M:351:ASN:HD21	1:M:397:SER:HB2	1.79	0.47
1:G:347:GLN:HB3	1:G:369:ILE:HD11	1.96	0.47
1:N:351:ASN:HD21	1:N:397:SER:HB2	1.79	0.47
1:A:477:LEU:HD21	1:A:567:PRO:CB	2.44	0.47
1:B:347:GLN:HB3	1:B:369:ILE:HD11	1.96	0.47
1:E:477:LEU:HD21	1:E:567:PRO:CB	2.44	0.47
1:N:477:LEU:HD21	1:N:567:PRO:CB	2.44	0.47
1:O:367:LEU:HD12	1:O:390:ILE:HG21	1.96	0.47
1:F:347:GLN:HB3	1:F:369:ILE:HD11	1.96	0.47
1:L:367:LEU:HD12	1:L:390:ILE:HG21	1.96	0.47
1:L:511:ILE:HG21	1:L:521:ILE:HD12	1.94	0.47
1:M:347:GLN:HB3	1:M:369:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:O	1:C:326:GLN:NE2	2.46	0.47
1:C:512:LEU:HD11	1:D:254:HIS:CE1	2.50	0.47
1:F:477:LEU:HD21	1:F:567:PRO:CB	2.44	0.47
1:H:347:GLN:HB3	1:H:369:ILE:HD11	1.96	0.47
1:L:347:GLN:HB3	1:L:369:ILE:HD11	1.96	0.47
1:N:473:ASP:OD1	1:N:473:ASP:N	2.46	0.47
1:I:347:GLN:HB3	1:I:369:ILE:HD11	1.96	0.47
1:I:477:LEU:HD21	1:I:567:PRO:CB	2.44	0.47
1:K:351:ASN:HD21	1:K:397:SER:HB2	1.79	0.47
1:M:367:LEU:HD12	1:M:390:ILE:HG21	1.96	0.47
1:A:347:GLN:HB3	1:A:369:ILE:HD11	1.96	0.47
1:C:477:LEU:HD21	1:C:567:PRO:CB	2.44	0.47
1:J:233:LEU:O	1:J:237:LEU:CB	2.57	0.47
1:B:351:ASN:HD21	1:B:397:SER:HB2	1.79	0.47
1:N:347:GLN:HB3	1:N:369:ILE:HD11	1.96	0.47
1:N:367:LEU:HD12	1:N:390:ILE:HG21	1.96	0.47
1:D:378:SER:O	1:D:383:GLU:N	2.48	0.46
1:F:233:LEU:O	1:F:237:LEU:CB	2.57	0.46
1:J:351:ASN:HD21	1:J:397:SER:HB2	1.79	0.46
1:D:347:GLN:HB3	1:D:369:ILE:HD11	1.96	0.46
1:E:347:GLN:HB3	1:E:369:ILE:HD11	1.96	0.46
1:H:535:LYS:HD2	1:H:540:GLY:HA3	1.98	0.46
1:J:347:GLN:HB3	1:J:369:ILE:HD11	1.96	0.46
1:M:473:ASP:N	1:M:473:ASP:OD1	2.46	0.46
1:O:351:ASN:HD21	1:O:397:SER:HB2	1.79	0.46
1:C:347:GLN:HB3	1:C:369:ILE:HD11	1.96	0.46
1:C:535:LYS:HD2	1:C:540:GLY:HA3	1.98	0.46
1:D:473:ASP:N	1:D:473:ASP:OD1	2.46	0.46
1:D:535:LYS:HD2	1:D:540:GLY:HA3	1.98	0.46
1:E:535:LYS:HD2	1:E:540:GLY:HA3	1.98	0.46
1:F:378:SER:O	1:F:383:GLU:N	2.48	0.46
1:I:535:LYS:HD2	1:I:540:GLY:HA3	1.98	0.46
1:K:378:SER:O	1:K:383:GLU:N	2.48	0.46
1:A:351:ASN:HD21	1:A:397:SER:HB2	1.79	0.46
1:G:535:LYS:HD2	1:G:540:GLY:HA3	1.98	0.46
1:H:477:LEU:HD21	1:H:567:PRO:CB	2.44	0.46
1:B:535:LYS:HD2	1:B:540:GLY:HA3	1.98	0.46
1:D:237:LEU:HG	1:E:214:ARG:HH22	1.80	0.46
1:A:497:ASN:OD1	1:B:436:PRO:HG3	2.16	0.46
1:E:502:THR:HB	1:F:434:ASN:HD22	1.80	0.46
1:F:535:LYS:HD2	1:F:540:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:535:LYS:HD2	1:J:540:GLY:HA3	1.98	0.46
1:K:347:GLN:HB3	1:K:369:ILE:HD11	1.96	0.46
1:B:233:LEU:O	1:B:237:LEU:CB	2.57	0.46
1:H:378:SER:O	1:H:383:GLU:N	2.48	0.46
1:A:535:LYS:HD2	1:A:540:GLY:HA3	1.98	0.45
1:O:535:LYS:HD2	1:O:540:GLY:HA3	1.98	0.45
1:J:378:SER:O	1:J:383:GLU:N	2.48	0.45
1:K:535:LYS:HD2	1:K:540:GLY:HA3	1.98	0.45
1:L:535:LYS:HD2	1:L:540:GLY:HA3	1.98	0.45
1:N:535:LYS:HD2	1:N:540:GLY:HA3	1.98	0.45
1:I:378:SER:O	1:I:383:GLU:N	2.48	0.45
1:O:472:ASN:HD21	1:A:254:HIS:CE1	2.34	0.45
1:G:378:SER:O	1:G:383:GLU:N	2.48	0.45
1:J:462:GLY:H	1:J:486:SER:HB2	1.82	0.45
1:K:462:GLY:H	1:K:486:SER:HB2	1.82	0.45
1:M:535:LYS:HD2	1:M:540:GLY:HA3	1.98	0.45
1:N:378:SER:O	1:N:383:GLU:N	2.48	0.45
1:D:519:ILE:HA	1:E:580:SER:HB2	1.98	0.45
1:I:462:GLY:H	1:I:486:SER:HB2	1.82	0.45
1:C:522:GLY:HA2	1:D:419:LEU:HA	1.99	0.45
1:L:378:SER:O	1:L:383:GLU:N	2.48	0.45
1:A:472:ASN:ND2	1:A:476:ALA:O	2.50	0.45
1:G:462:GLY:H	1:G:486:SER:HB2	1.82	0.45
1:I:472:ASN:ND2	1:I:476:ALA:O	2.50	0.45
1:J:472:ASN:ND2	1:J:476:ALA:O	2.50	0.45
1:L:462:GLY:H	1:L:486:SER:HB2	1.82	0.45
1:E:472:ASN:ND2	1:E:476:ALA:O	2.51	0.44
1:B:472:ASN:ND2	1:B:476:ALA:O	2.50	0.44
1:E:500:LEU:O	1:F:434:ASN:HB3	2.17	0.44
1:F:473:ASP:OD1	1:F:473:ASP:N	2.46	0.44
1:B:462:GLY:H	1:B:486:SER:HB2	1.82	0.44
1:D:177:VAL:HA	1:D:218:LEU:O	2.18	0.44
1:E:473:ASP:N	1:E:473:ASP:OD1	2.46	0.44
1:F:462:GLY:H	1:F:486:SER:HB2	1.82	0.44
1:G:177:VAL:HA	1:G:218:LEU:O	2.18	0.44
1:H:472:ASN:ND2	1:H:476:ALA:O	2.50	0.44
1:K:177:VAL:HA	1:K:218:LEU:O	2.18	0.44
1:K:472:ASN:ND2	1:K:476:ALA:O	2.51	0.44
1:O:175:TYR:HD2	1:N:229:LYS:HD2	1.81	0.44
1:B:177:VAL:HA	1:B:218:LEU:O	2.18	0.44
1:C:177:VAL:HA	1:C:218:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:ASN:ND2	1:D:476:ALA:O	2.50	0.44
1:L:472:ASN:ND2	1:L:476:ALA:O	2.50	0.44
1:O:177:VAL:HA	1:O:218:LEU:O	2.18	0.44
1:A:177:VAL:HA	1:A:218:LEU:O	2.18	0.44
1:A:378:SER:O	1:A:383:GLU:N	2.48	0.44
1:C:462:GLY:H	1:C:486:SER:HB2	1.82	0.44
1:D:267:ILE:HG22	1:E:293:ARG:HB2	1.98	0.44
1:F:472:ASN:ND2	1:F:476:ALA:O	2.50	0.44
1:H:462:GLY:H	1:H:486:SER:HB2	1.82	0.44
1:H:529:VAL:HG13	1:I:412:ASN:HB3	2.00	0.44
1:N:462:GLY:H	1:N:486:SER:HB2	1.82	0.44
1:O:472:ASN:ND2	1:O:476:ALA:O	2.51	0.44
1:D:462:GLY:H	1:D:486:SER:HB2	1.82	0.44
1:E:177:VAL:HA	1:E:218:LEU:O	2.18	0.44
1:H:177:VAL:HA	1:H:218:LEU:O	2.18	0.44
1:J:177:VAL:HA	1:J:218:LEU:O	2.18	0.44
1:N:177:VAL:HA	1:N:218:LEU:O	2.18	0.44
1:B:197:SER:HA	1:C:208:GLN:HE22	1.83	0.44
1:F:177:VAL:HA	1:F:218:LEU:O	2.18	0.44
1:M:177:VAL:HA	1:M:218:LEU:O	2.18	0.44
1:A:462:GLY:H	1:A:486:SER:HB2	1.82	0.44
1:C:378:SER:O	1:C:383:GLU:N	2.48	0.44
1:E:191:VAL:HG13	1:F:210:ILE:HG21	1.99	0.44
1:G:268:SER:HB3	1:G:290:ILE:HG12	2.00	0.44
1:G:486:SER:OG	1:G:502:THR:O	2.29	0.44
1:M:462:GLY:H	1:M:486:SER:HB2	1.82	0.44
1:M:512:LEU:O	1:N:326:GLN:NE2	2.50	0.44
1:E:378:SER:O	1:E:383:GLU:N	2.48	0.44
1:I:268:SER:HB3	1:I:290:ILE:HG12	2.00	0.44
1:M:472:ASN:ND2	1:M:476:ALA:O	2.50	0.44
1:E:268:SER:HB3	1:E:290:ILE:HG12	2.00	0.43
1:I:535:LYS:NZ	1:I:541:ASP:OD1	2.38	0.43
1:N:472:ASN:ND2	1:N:476:ALA:O	2.50	0.43
1:C:486:SER:OG	1:C:502:THR:O	2.29	0.43
1:G:472:ASN:ND2	1:G:476:ALA:O	2.50	0.43
1:H:233:LEU:O	1:H:237:LEU:CB	2.57	0.43
1:K:268:SER:HB3	1:K:290:ILE:HG12	2.00	0.43
1:L:486:SER:OG	1:L:502:THR:O	2.29	0.43
1:D:535:LYS:NZ	1:D:541:ASP:OD1	2.38	0.43
1:J:268:SER:HB3	1:J:290:ILE:HG12	2.00	0.43
1:E:462:GLY:H	1:E:486:SER:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:268:SER:HB3	1:H:290:ILE:HG12	2.00	0.43
1:F:486:SER:OG	1:F:502:THR:O	2.29	0.43
1:L:177:VAL:HA	1:L:218:LEU:O	2.18	0.43
1:M:268:SER:HB3	1:M:290:ILE:HG12	2.00	0.43
1:O:462:GLY:H	1:O:486:SER:HB2	1.82	0.43
1:A:529:VAL:HG13	1:B:412:ASN:HB3	1.99	0.43
1:D:236:SER:HB2	1:E:217:ARG:HH22	1.84	0.43
1:I:233:LEU:O	1:I:237:LEU:CB	2.57	0.43
1:B:236:SER:HB2	1:C:217:ARG:HH22	1.84	0.43
1:C:472:ASN:ND2	1:C:476:ALA:O	2.51	0.43
1:F:268:SER:HB3	1:F:290:ILE:HG12	2.00	0.43
1:I:177:VAL:HA	1:I:218:LEU:O	2.18	0.43
1:L:268:SER:HB3	1:L:290:ILE:HG12	2.00	0.43
1:B:191:VAL:HG13	1:C:210:ILE:HG21	2.00	0.43
1:D:564:PHE:HZ	1:E:587:ILE:HG21	1.84	0.43
1:G:370:GLY:HA3	1:H:386:PRO:HG3	2.00	0.43
1:H:512:LEU:O	1:I:326:GLN:NE2	2.52	0.43
1:A:210:ILE:HB	1:A:219:ILE:HB	2.01	0.43
1:K:535:LYS:NZ	1:K:541:ASP:OD1	2.38	0.43
1:O:233:LEU:O	1:O:237:LEU:CB	2.57	0.42
1:B:210:ILE:HB	1:B:219:ILE:HB	2.01	0.42
1:B:268:SER:HB3	1:B:290:ILE:HG12	2.00	0.42
1:D:268:SER:HB3	1:D:290:ILE:HG12	2.00	0.42
1:N:486:SER:OG	1:N:502:THR:O	2.29	0.42
1:C:268:SER:HB3	1:C:290:ILE:HG12	2.00	0.42
1:D:564:PHE:CZ	1:E:587:ILE:HG21	2.55	0.42
1:I:210:ILE:HB	1:I:219:ILE:HB	2.01	0.42
1:I:512:LEU:O	1:J:326:GLN:NE2	2.53	0.42
1:O:210:ILE:HB	1:O:219:ILE:HB	2.01	0.42
1:O:268:SER:HB3	1:O:290:ILE:HG12	2.00	0.42
1:C:562:MET:HE1	1:D:583:LYS:HD2	2.00	0.42
1:H:210:ILE:HB	1:H:219:ILE:HB	2.01	0.42
1:J:210:ILE:HB	1:J:219:ILE:HB	2.01	0.42
1:A:268:SER:HB3	1:A:290:ILE:HG12	2.00	0.42
1:C:210:ILE:HB	1:C:219:ILE:HB	2.01	0.42
1:G:210:ILE:HB	1:G:219:ILE:HB	2.01	0.42
1:A:233:LEU:O	1:A:237:LEU:CB	2.57	0.42
1:A:511:ILE:HD13	1:A:519:ILE:HD11	2.02	0.42
1:D:511:ILE:HD13	1:D:519:ILE:HD11	2.02	0.42
1:F:210:ILE:HB	1:F:219:ILE:HB	2.01	0.42
1:H:511:ILE:HD13	1:H:519:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:210:ILE:HB	1:M:219:ILE:HB	2.01	0.42
1:N:210:ILE:HB	1:N:219:ILE:HB	2.01	0.42
1:E:511:ILE:HD13	1:E:519:ILE:HD11	2.02	0.42
1:O:322:VAL:HG11	1:A:251:ARG:HH22	1.84	0.42
1:C:335:GLU:OE1	1:C:505:ARG:NH1	2.53	0.42
1:E:210:ILE:HB	1:E:219:ILE:HB	2.01	0.42
1:F:335:GLU:OE1	1:F:505:ARG:NH1	2.53	0.42
1:G:335:GLU:OE1	1:G:505:ARG:NH1	2.53	0.42
1:G:511:ILE:HD13	1:G:519:ILE:HD11	2.02	0.42
1:C:511:ILE:HD13	1:C:519:ILE:HD11	2.02	0.42
1:D:210:ILE:HB	1:D:219:ILE:HB	2.01	0.42
1:D:335:GLU:OE1	1:D:505:ARG:NH1	2.53	0.42
1:E:335:GLU:OE1	1:E:505:ARG:NH1	2.53	0.42
1:H:335:GLU:OE1	1:H:505:ARG:NH1	2.53	0.42
1:I:511:ILE:HD13	1:I:519:ILE:HD11	2.02	0.42
1:K:210:ILE:HB	1:K:219:ILE:HB	2.01	0.42
1:L:210:ILE:HB	1:L:219:ILE:HB	2.01	0.42
1:M:335:GLU:OE1	1:M:505:ARG:NH1	2.53	0.42
1:N:268:SER:HB3	1:N:290:ILE:HG12	2.00	0.42
1:N:335:GLU:OE1	1:N:505:ARG:NH1	2.53	0.42
1:O:335:GLU:OE1	1:O:505:ARG:NH1	2.53	0.42
1:B:511:ILE:HD13	1:B:519:ILE:HD11	2.02	0.42
1:C:535:LYS:O	1:D:406:SER:HB3	2.20	0.42
1:E:326:GLN:HB2	1:E:570:VAL:HG23	2.02	0.42
1:F:326:GLN:HB2	1:F:570:VAL:HG23	2.02	0.42
1:F:511:ILE:HD13	1:F:519:ILE:HD11	2.02	0.42
1:I:335:GLU:OE1	1:I:505:ARG:NH1	2.53	0.42
1:K:264:LEU:O	1:K:268:SER:OG	2.30	0.42
1:O:511:ILE:HD13	1:O:519:ILE:HD11	2.02	0.42
1:B:335:GLU:OE1	1:B:505:ARG:NH1	2.53	0.41
1:J:340:ILE:HG23	1:J:556:HIS:HB3	2.02	0.41
1:J:511:ILE:HD13	1:J:519:ILE:HD11	2.02	0.41
1:K:511:ILE:HD13	1:K:519:ILE:HD11	2.02	0.41
1:K:340:ILE:HG23	1:K:556:HIS:HB3	2.02	0.41
1:E:340:ILE:HG23	1:E:556:HIS:HB3	2.03	0.41
1:F:340:ILE:HG23	1:F:556:HIS:HB3	2.02	0.41
1:I:340:ILE:HG23	1:I:556:HIS:HB3	2.02	0.41
1:L:335:GLU:OE1	1:L:505:ARG:NH1	2.53	0.41
1:L:370:GLY:HA3	1:M:386:PRO:HG3	2.02	0.41
1:N:511:ILE:HD13	1:N:519:ILE:HD11	2.02	0.41
1:D:340:ILE:HG23	1:D:556:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ILE:HG23	1:G:556:HIS:HB3	2.02	0.41
1:H:340:ILE:HG23	1:H:556:HIS:HB3	2.02	0.41
1:L:340:ILE:HG23	1:L:556:HIS:HB3	2.02	0.41
1:M:511:ILE:HD13	1:M:519:ILE:HD11	2.02	0.41
1:G:326:GLN:HB2	1:G:570:VAL:HG23	2.02	0.41
1:I:486:SER:OG	1:I:502:THR:O	2.29	0.41
1:J:335:GLU:OE1	1:J:505:ARG:NH1	2.53	0.41
1:A:604:PRO:O	1:N:531:GLN:NE2	2.54	0.41
1:A:335:GLU:OE1	1:A:505:ARG:NH1	2.53	0.41
1:D:326:GLN:HB2	1:D:570:VAL:HG23	2.02	0.41
1:N:340:ILE:HG23	1:N:556:HIS:HB3	2.02	0.41
1:A:350:ILE:O	1:A:358:THR:OG1	2.32	0.41
1:B:378:SER:O	1:B:383:GLU:N	2.48	0.41
1:B:340:ILE:HG23	1:B:556:HIS:HB3	2.02	0.41
1:L:326:GLN:HB2	1:L:570:VAL:HG23	2.02	0.41
1:L:511:ILE:HD13	1:L:519:ILE:HD11	2.02	0.41
1:M:340:ILE:HG23	1:M:556:HIS:HB3	2.02	0.41
1:A:358:THR:HG22	1:B:391:VAL:HG13	2.03	0.41
1:B:512:LEU:HB3	1:C:326:GLN:NE2	2.24	0.41
1:C:340:ILE:HG23	1:C:556:HIS:HB3	2.03	0.41
1:F:264:LEU:HD22	1:F:313:LEU:HD22	2.03	0.41
1:K:264:LEU:HD22	1:K:313:LEU:HD22	2.03	0.41
1:M:378:SER:O	1:M:383:GLU:N	2.48	0.41
1:N:326:GLN:HB2	1:N:570:VAL:HG23	2.02	0.41
1:O:378:SER:O	1:O:383:GLU:N	2.48	0.41
1:C:241:THR:HB	1:D:215:THR:HA	2.02	0.41
1:E:264:LEU:HD22	1:E:313:LEU:HD22	2.03	0.41
1:E:537:PRO:HB3	1:F:406:SER:HB2	2.03	0.41
1:H:264:LEU:HD22	1:H:313:LEU:HD22	2.03	0.41
1:I:264:LEU:HD22	1:I:313:LEU:HD22	2.03	0.41
1:K:335:GLU:OE1	1:K:505:ARG:NH1	2.53	0.41
1:O:340:ILE:HG23	1:O:556:HIS:HB3	2.02	0.41
1:B:520:VAL:HG12	1:C:580:SER:HA	2.03	0.41
1:H:326:GLN:HB2	1:H:570:VAL:HG23	2.02	0.41
1:J:264:LEU:HD22	1:J:313:LEU:HD22	2.03	0.41
1:M:192:LEU:HD23	1:M:192:LEU:HA	1.91	0.41
1:M:326:GLN:HB2	1:M:570:VAL:HG23	2.02	0.41
1:A:340:ILE:HG23	1:A:556:HIS:HB3	2.02	0.40
1:C:264:LEU:HD22	1:C:313:LEU:HD22	2.03	0.40
1:C:326:GLN:HB2	1:C:570:VAL:HG23	2.02	0.40
1:C:459:LYS:HE2	1:C:459:LYS:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:THR:HA	1:D:390:ILE:O	2.21	0.40
1:I:192:LEU:HA	1:I:192:LEU:HD23	1.91	0.40
1:K:326:GLN:HB2	1:K:570:VAL:HG23	2.02	0.40
1:A:326:GLN:HB2	1:A:570:VAL:HG23	2.02	0.40
1:D:264:LEU:HD22	1:D:313:LEU:HD22	2.03	0.40
1:F:459:LYS:HB3	1:F:459:LYS:HE2	1.90	0.40
1:H:535:LYS:NZ	1:H:541:ASP:OD1	2.38	0.40
1:H:524:LEU:HD22	1:I:431:VAL:HG21	2.03	0.40
1:K:230:LEU:HD13	1:K:230:LEU:HA	1.95	0.40
1:L:264:LEU:HD22	1:L:313:LEU:HD22	2.03	0.40
1:O:326:GLN:HB2	1:O:570:VAL:HG23	2.02	0.40
1:B:264:LEU:HD22	1:B:313:LEU:HD22	2.03	0.40
1:B:348:TRP:NE1	1:B:548:LEU:O	2.47	0.40
1:G:264:LEU:HD22	1:G:313:LEU:HD22	2.03	0.40
1:G:587:ILE:HA	1:G:587:ILE:HD12	1.97	0.40
1:J:545:LEU:HD22	1:J:548:LEU:HD12	2.04	0.40
1:J:326:GLN:HB2	1:J:570:VAL:HG23	2.02	0.40
1:B:326:GLN:HB2	1:B:570:VAL:HG23	2.02	0.40
1:D:486:SER:OG	1:D:502:THR:O	2.29	0.40
1:G:322:VAL:HG11	1:H:251:ARG:HH22	1.86	0.40
1:J:486:SER:OG	1:J:502:THR:O	2.29	0.40
1:K:545:LEU:HD22	1:K:548:LEU:HD12	2.04	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	386/624 (62%)	344 (89%)	42 (11%)	0	100	100
1	B	386/624 (62%)	344 (89%)	42 (11%)	0	100	100
1	C	386/624 (62%)	345 (89%)	41 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	E	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	F	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	G	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	H	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	I	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	J	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	K	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	L	386/624 (62%)	344 (89%)	42 (11%)	0	100	100
1	M	386/624 (62%)	344 (89%)	42 (11%)	0	100	100
1	N	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
1	O	386/624 (62%)	345 (89%)	41 (11%)	0	100	100
All	All	5790/9360 (62%)	5171 (89%)	619 (11%)	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	326/510 (64%)	326 (100%)	0	100	100
1	B	326/510 (64%)	326 (100%)	0	100	100
1	C	326/510 (64%)	326 (100%)	0	100	100
1	D	326/510 (64%)	326 (100%)	0	100	100
1	E	326/510 (64%)	326 (100%)	0	100	100
1	F	326/510 (64%)	326 (100%)	0	100	100
1	G	326/510 (64%)	326 (100%)	0	100	100
1	H	326/510 (64%)	326 (100%)	0	100	100
1	I	326/510 (64%)	326 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	326/510 (64%)	326 (100%)	0	100	100
1	K	326/510 (64%)	326 (100%)	0	100	100
1	L	326/510 (64%)	326 (100%)	0	100	100
1	M	326/510 (64%)	326 (100%)	0	100	100
1	N	326/510 (64%)	326 (100%)	0	100	100
1	O	326/510 (64%)	326 (100%)	0	100	100
All	All	4890/7650 (64%)	4890 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	434	ASN
1	G	472	ASN
1	G	483	GLN
1	G	608	ASN
1	O	472	ASN
1	O	483	GLN
1	O	517	GLN
1	O	608	ASN
1	A	254	HIS
1	A	470	HIS
1	A	472	ASN
1	A	483	GLN
1	A	608	ASN
1	B	472	ASN
1	B	483	GLN
1	B	608	ASN
1	C	470	HIS
1	C	483	GLN
1	C	608	ASN
1	D	299	ASN
1	D	472	ASN
1	D	483	GLN
1	D	608	ASN
1	E	424	ASN
1	E	470	HIS
1	E	472	ASN
1	E	483	GLN

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Mol	Chain	Res	Type
1	E	608	ASN
1	F	472	ASN
1	F	483	GLN
1	F	608	ASN
1	H	434	ASN
1	H	470	HIS
1	H	472	ASN
1	H	483	GLN
1	H	608	ASN
1	I	472	ASN
1	I	483	GLN
1	I	608	ASN
1	J	434	ASN
1	J	472	ASN
1	J	483	GLN
1	J	608	ASN
1	K	472	ASN
1	K	483	GLN
1	K	608	ASN
1	L	472	ASN
1	L	483	GLN
1	L	608	ASN
1	M	472	ASN
1	M	483	GLN
1	M	608	ASN
1	N	424	ASN
1	N	470	HIS
1	N	472	ASN
1	N	483	GLN
1	N	608	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.