wwPDB EM Map/Model Validation Report (i)

Oct 17, 2016 – 01:13 PM EDT

PDB ID	:	5GW5
EMDB ID:	:	EMD-9541
Title	:	Structure of TRiC-AMP-PNP
Authors	:	Zang, Y.; Jin, M.; Wang, H.; Cong, Y.
Deposited on	:	2016-09-08
Resolution	:	4.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

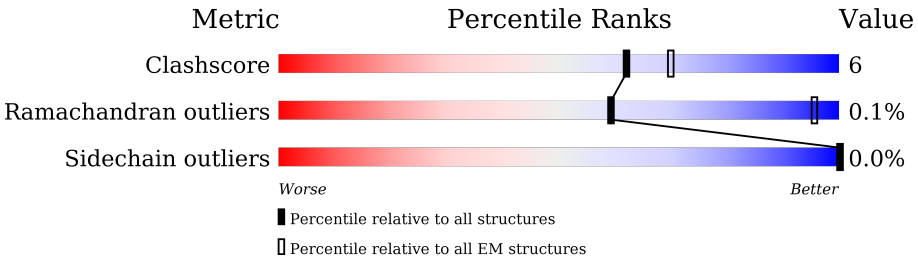
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	559	67% 31% .
1	a	559	97% .
2	B	527	76% 23% .
2	b	527	98% .
3	D	528	71% 27% .
3	d	528	98% .
4	E	562	68% 26% 6%
4	e	562	94% 6%
5	G	534	73% 24% .

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Mol	Chain	Length	Quality of chain
5	g	534	97%
6	H	550	69% 25% 6%
6	h	550	94% 6%
7	Q	568	70% 25%
7	q	568	95%
8	Z	546	72% 26%
8	z	546	98%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 64544 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		
1	A	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		
2	B	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		
3	D	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		
4	E	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		
5	G	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		
6	H	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		

- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		
7	Q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

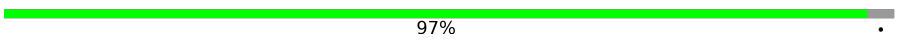
Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		
8	Z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

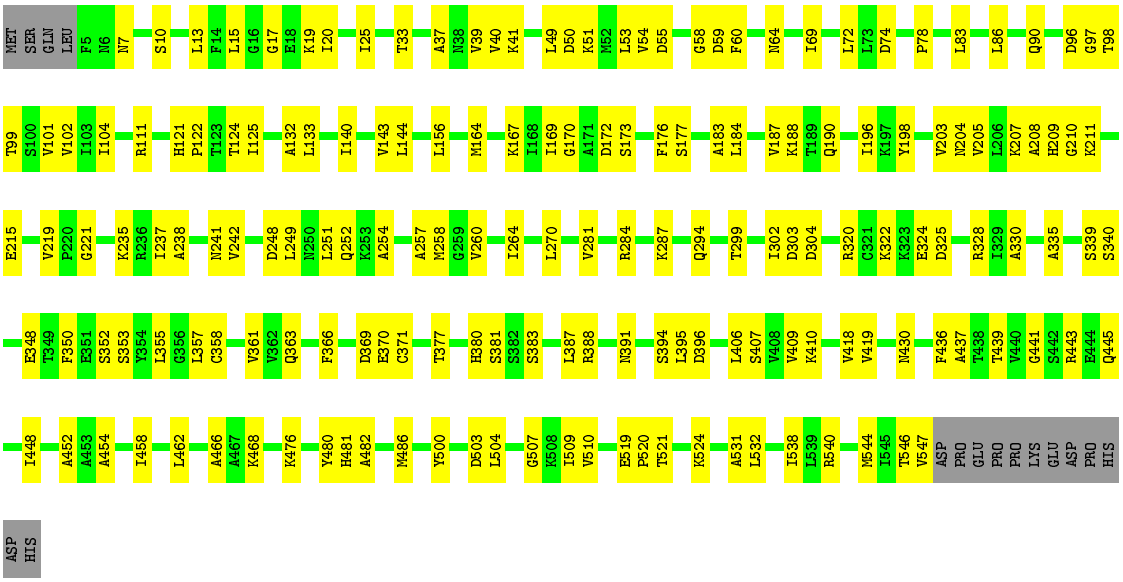
- Molecule 1: T-complex protein 1 subunit alpha

Chain a:



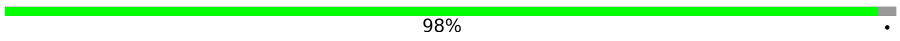
- Molecule 1: T-complex protein 1 subunit alpha

Chain A:



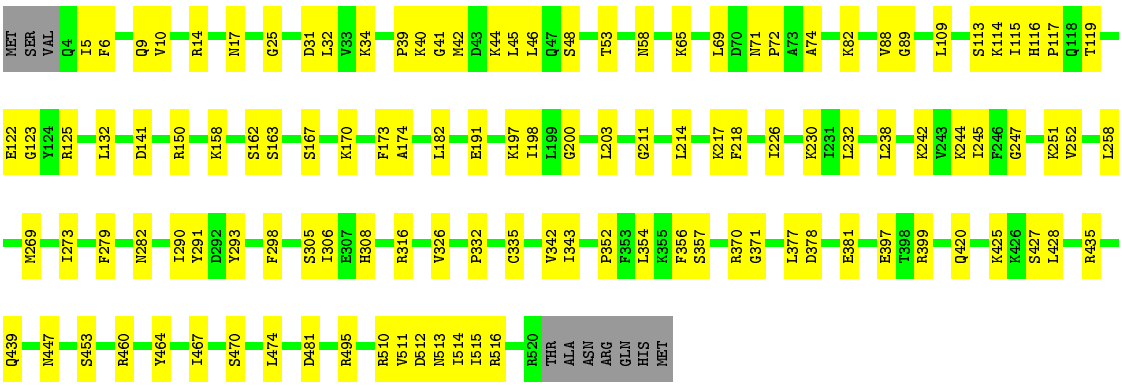
- Molecule 2: T-complex protein 1 subunit beta

Chain b:



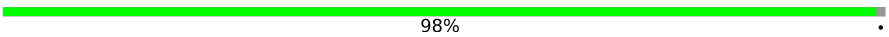
- Molecule 2: T-complex protein 1 subunit beta

Chain B:



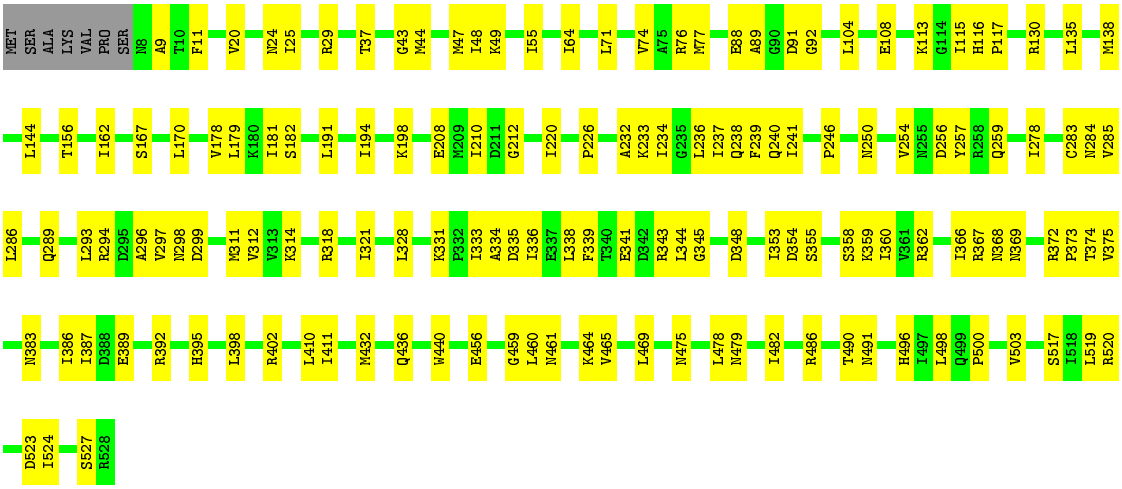
- Molecule 3: T-complex protein 1 subunit delta

Chain d:



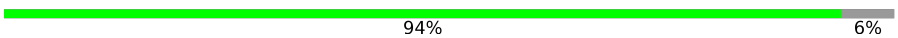
- Molecule 3: T-complex protein 1 subunit delta

Chain D:



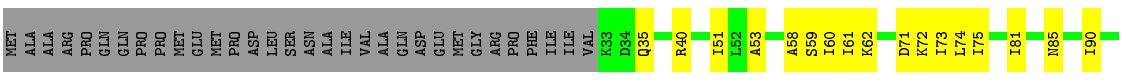
- Molecule 4: T-complex protein 1 subunit epsilon

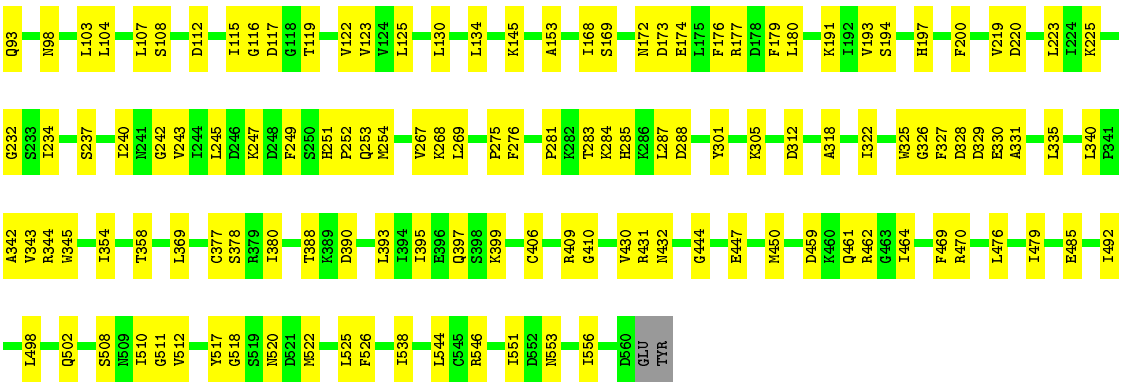
Chain e:



- Molecule 4: T-complex protein 1 subunit epsilon

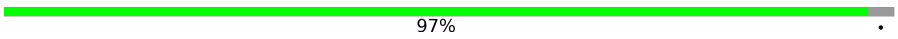
Chain E:





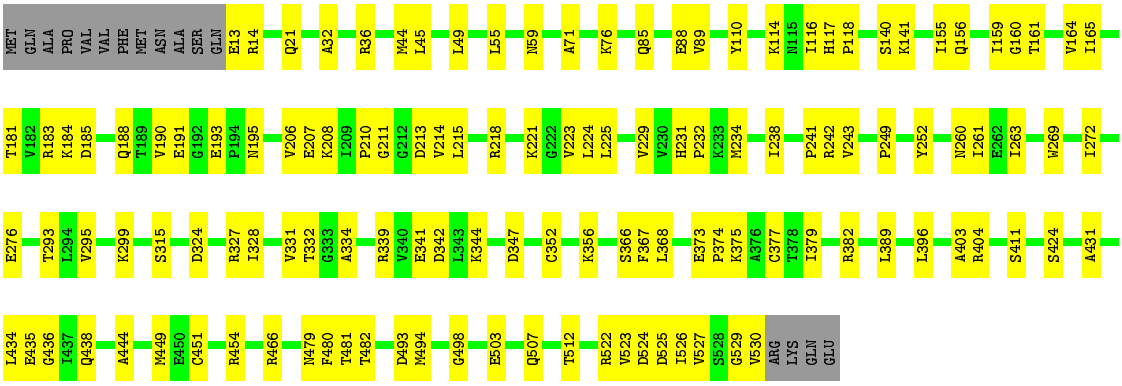
• Molecule 5: T-complex protein 1 subunit gamma

Chain g:



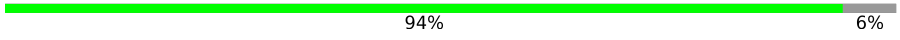
• Molecule 5: T-complex protein 1 subunit gamma

Chain G:



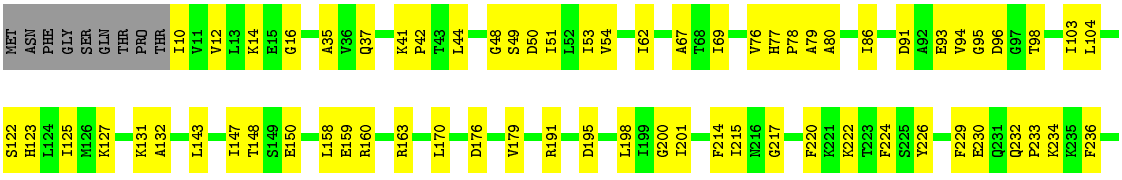
• Molecule 6: T-complex protein 1 subunit eta

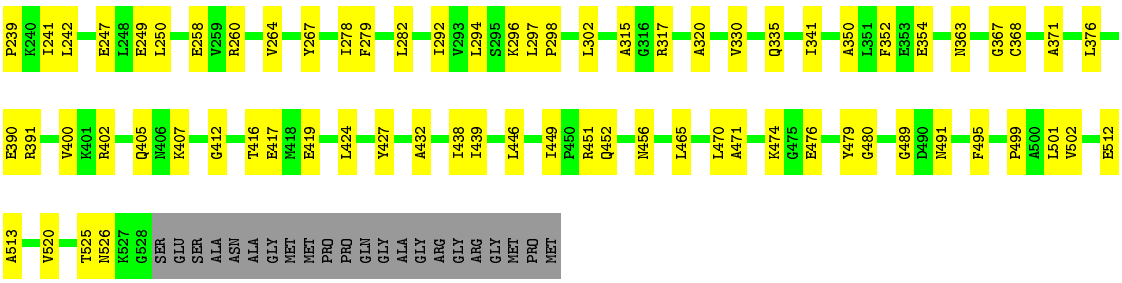
Chain h:



• Molecule 6: T-complex protein 1 subunit eta

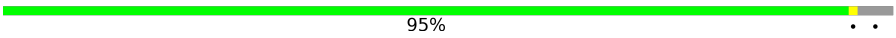
Chain H:





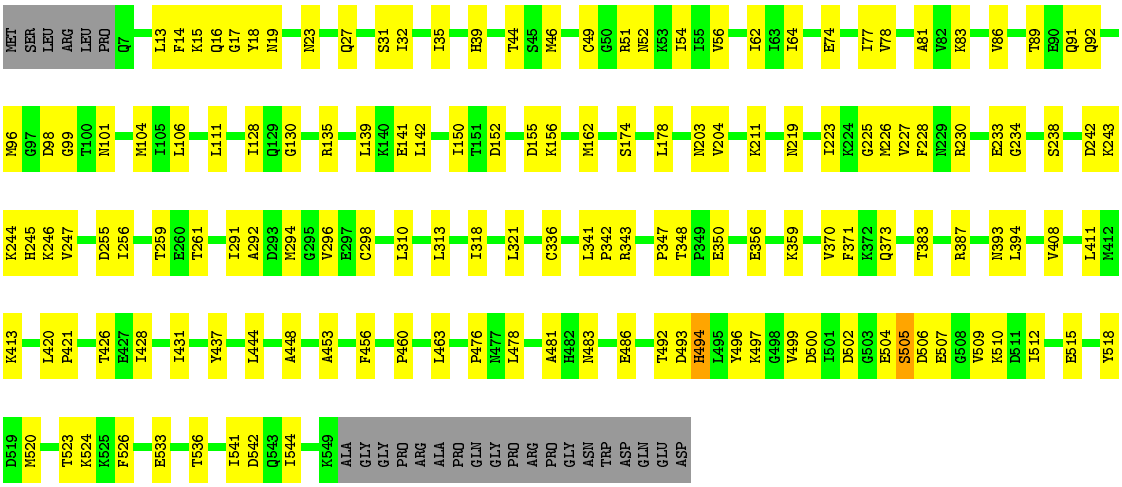
• Molecule 7: T-complex protein 1 subunit theta

Chain q:



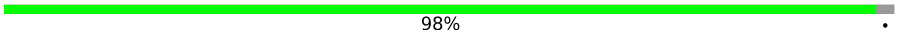
• Molecule 7: T-complex protein 1 subunit theta

Chain Q:



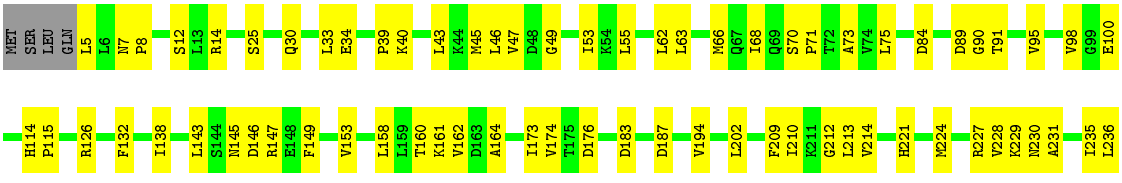
• Molecule 8: T-complex protein 1 subunit zeta

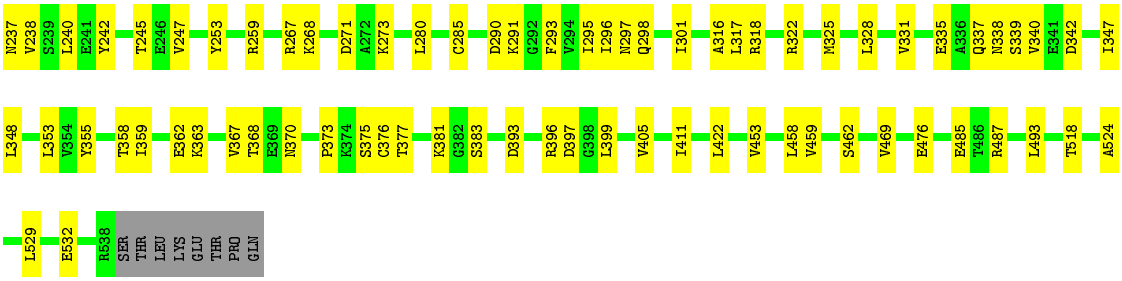
Chain z:



• Molecule 8: T-complex protein 1 subunit zeta

Chain Z:




N237 V238 S239 L240 E241 Y242 T245 E246 V247 Y253 R259 R267 K268 D271 A272 K273 L280 C285 D290 K291 G292 F293 Y294 I295 I296 N297 Q298 I301 A316 L317 R318 R322 M325 L328 V331 E335 A336 Q337 N338 S339 V340 E341 D342 I347
L348 L353 V354 Y355 T358 I359 E362 K363 V367 T368 E369 N370 P373 K374 S375 C376 T377 K381 G382 S383 D393 R396 D397 G398 L399 V405 I411 L422 V453 L458 V459 S462 V469 E476 E485 T486 R487 L493 T518 A524
L529 E532 R538 SER THR LEU LYS GLU THR PRO GLN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	67990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	Not provided	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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.23	0/4140	0.41	0/5585
1	a	0.23	0/4140	0.41	0/5585
2	B	0.23	0/3969	0.39	0/5348
2	b	0.23	0/3969	0.40	0/5348
3	D	0.23	0/4022	0.39	0/5421
3	d	0.23	0/4022	0.39	0/5421
4	E	0.23	0/4117	0.40	0/5539
4	e	0.23	0/4117	0.39	0/5539
5	G	0.22	0/4029	0.39	0/5442
5	g	0.22	0/4029	0.40	0/5442
6	H	0.23	0/4018	0.39	0/5422
6	h	0.23	0/4018	0.40	0/5422
7	Q	0.29	1/4175 (0.0%)	0.40	0/5636
7	q	0.29	1/4175 (0.0%)	0.41	0/5636
8	Z	0.23	0/4162	0.41	0/5624
8	z	0.23	0/4162	0.39	0/5624
All	All	0.24	2/65264 (0.0%)	0.40	0/88034

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	q	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	q	413	LYS	C-N	11.30	1.55	1.34
7	Q	413	LYS	C-N	11.25	1.55	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	q	491	LYS	Peptide
7	q	505	SER	Peptide

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	4103	0	4269	124	0
1	a	4103	0	4269	0	0
2	B	3930	0	4034	88	0
2	b	3930	0	4034	0	0
3	D	3985	0	4157	101	0
3	d	3985	0	4157	0	0
4	E	4068	0	4163	107	0
4	e	4068	0	4163	0	0
5	G	3982	0	4123	87	0
5	g	3982	0	4123	0	0
6	H	3969	0	4055	93	0
6	h	3969	0	4055	0	0
7	Q	4125	0	4260	104	0
7	q	4125	0	4260	0	0
8	Z	4110	0	4204	95	0
8	z	4110	0	4204	0	0
All	All	64544	0	66530	724	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 6.

All (724) 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)
7:Q:493:ASP:O	7:Q:494:HIS:CG	2.14	1.00
1:A:252:GLN:HA	1:A:303:ASP:HB2	1.76	0.82
2:B:39:PRO:HB3	2:B:162:SER:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:193:VAL:HG13	4:E:200:PHE:HD2	1.77	0.78
7:Q:493:ASP:O	7:Q:494:HIS:CD2	2.36	0.77
8:Z:212:GLY:H	8:Z:368:THR:HG22	1.47	0.77
5:G:334:ALA:HA	5:G:347:ASP:HB2	1.66	0.77
2:B:197:LYS:HD2	2:B:377:LEU:HB3	1.67	0.75
2:B:114:LYS:HB2	3:D:11:PHE:HB2	28.81	0.73
1:A:441:GLY:HA3	6:H:470:LEU:HD11	133.93	0.71
1:A:238:ALA:HB2	1:A:242:VAL:HB	1.71	0.70
3:D:181:ILE:HG22	3:D:373:PRO:HB2	1.72	0.70
3:D:246:PRO:HG2	3:D:250:ASN:HD22	1.58	0.69
1:A:207:LYS:HB2	1:A:395:LEU:HD13	1.80	0.68
3:D:254:VAL:HG23	3:D:259:GLN:HB3	1.75	0.68
2:B:214:LEU:HD23	2:B:354:LEU:HD12	1.75	0.68
1:A:15:LEU:HD12	1:A:17:GLY:H	1.60	0.67
1:A:74:ASP:O	5:G:14:ARG:NH2	3.53	0.67
4:E:461:GLN:HG3	4:E:469:PHE:HE2	1.70	0.67
6:H:62:ILE:O	6:H:391:ARG:NH1	2.27	0.67
7:Q:23:ASN:HB3	7:Q:542:ASP:HB2	5.07	0.67
8:Z:161:LYS:NZ	8:Z:397:ASP:OD2	2.28	0.67
1:A:430:ASN:HA	1:A:452:ALA:HB1	2.01	0.66
7:Q:481:ALA:HB1	7:Q:497:LYS:HG3	1.77	0.66
8:Z:202:LEU:HD23	8:Z:381:LYS:HD3	1.77	0.66
8:Z:143:LEU:HG	8:Z:145:ASN:H	1.60	0.65
3:D:232:ALA:HA	3:D:284:ASN:HD22	1.81	0.65
4:E:380:ILE:HG12	4:E:395:ILE:HG12	1.77	0.65
3:D:372:ARG:HB2	3:D:373:PRO:HD2	1.84	0.65
7:Q:91:GLN:NE2	8:Z:383:SER:OG	2.29	0.65
3:D:383:ASN:H	3:D:386:ILE:HD12	1.62	0.64
8:Z:147:ARG:NH1	8:Z:176:ASP:OD1	2.32	0.64
3:D:198:LYS:HB2	3:D:387:ILE:HB	1.85	0.64
8:Z:68:ILE:HG21	8:Z:73:ALA:HB3	2.10	0.64
1:A:39:VAL:O	1:A:51:LYS:NZ	2.59	0.64
2:B:58:ASN:ND2	2:B:163:SER:O	2.26	0.64
2:B:244:LYS:NZ	4:E:330:GLU:OE1	9.94	0.64
6:H:224:PHE:HZ	6:H:315:ALA:HA	5.88	0.64
6:H:234:LYS:HD2	6:H:354:GLU:HB3	1.80	0.64
8:Z:240:LEU:HB2	8:Z:301:ILE:HG12	1.79	0.64
1:A:235:LYS:HB3	1:A:363:GLN:HB3	2.73	0.64
4:E:194:SER:O	4:E:197:HIS:ND1	2.31	0.64
7:Q:504:GLU:O	7:Q:505:SER:O	2.16	0.64
7:Q:502:ASP:OD2	7:Q:506:ASP:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:89:ALA:HB1	3:D:503:VAL:HG22	2.10	0.64
7:Q:336:CYS:HB2	7:Q:371:PHE:HZ	3.40	0.64
4:E:511:GLY:HA3	4:E:522:MET:HG2	2.38	0.63
6:H:42:PRO:HB2	6:H:49:SER:HB2	1.91	0.63
8:Z:229:LYS:HA	8:Z:353:LEU:HA	1.80	0.63
1:A:352:SER:HA	1:A:355:LEU:HB2	1.79	0.63
2:B:48:SER:HG	2:B:53:THR:HG1	1.53	0.63
4:E:103:LEU:HB3	4:E:544:LEU:HD11	1.90	0.63
5:G:14:ARG:HG2	5:G:527:VAL:HG12	1.81	0.63
1:A:51:LYS:HA	5:G:523:VAL:HG13	2.42	0.63
1:A:407:SER:HA	1:A:410:LYS:HE2	1.81	0.63
1:A:132:ALA:HB2	1:A:448:ILE:HG12	2.23	0.63
2:B:65:LYS:HE2	2:B:82:LYS:HG2	1.93	0.63
3:D:354:ASP:HA	3:D:359:LYS:H	1.64	0.63
1:A:546:THR:HG23	3:D:49:LYS:HD3	2.38	0.63
6:H:127:LYS:HE3	6:H:131:LYS:HE3	1.80	0.62
8:Z:459:VAL:HG11	8:Z:469:VAL:HG21	2.71	0.62
1:A:207:LYS:NZ	1:A:396:ASP:OD1	2.32	0.62
4:E:220:ASP:HB3	4:E:223:LEU:HD13	1.81	0.62
1:A:170:GLY:HA2	1:A:173:SER:HB3	1.82	0.62
7:Q:541:ILE:HG12	8:Z:45:MET:HB2	4.32	0.62
3:D:233:LYS:NZ	3:D:341:GLU:OE2	2.68	0.62
8:Z:221:HIS:HB3	8:Z:224:MET:HG3	1.81	0.62
8:Z:296:ILE:HA	8:Z:317:LEU:HB2	1.93	0.62
1:A:237:ILE:HG22	1:A:238:ALA:H	1.64	0.62
7:Q:259:THR:HG22	7:Q:261:THR:H	1.79	0.62
3:D:334:ALA:HB3	3:D:338:LEU:HD21	5.56	0.62
8:Z:221:HIS:HB3	8:Z:224:MET:HG2	3.29	0.62
2:B:48:SER:OG	2:B:53:THR:OG1	2.18	0.61
3:D:238:GLN:HB2	3:D:334:ALA:HA	1.80	0.61
4:E:240:ILE:HG22	4:E:242:GLY:H	4.17	0.61
6:H:525:THR:HA	7:Q:56:VAL:HB	1.82	0.61
1:A:249:LEU:HD13	1:A:284:ARG:NH1	5.38	0.61
3:D:278:ILE:HG21	3:D:286:LEU:HD11	2.00	0.61
6:H:512:GLU:OE2	7:Q:393:ASN:ND2	2.33	0.61
5:G:183:ARG:NH1	5:G:185:ASP:OD2	2.34	0.61
3:D:469:LEU:HD11	3:D:482:ILE:HG13	1.95	0.61
4:E:546:ARG:HH12	6:H:170:LEU:HD21	1.90	0.61
3:D:191:LEU:HG	3:D:402:ARG:HD2	1.83	0.60
3:D:236:LEU:HD13	3:D:321:ILE:HG23	1.84	0.60
4:E:247:LYS:HB3	4:E:393:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASP:HB3	2:B:399:ARG:HA	1.82	0.60
2:B:45:LEU:HD23	3:D:524:ILE:HG12	1.84	0.60
6:H:247:GLU:HB3	6:H:297:LEU:HB3	4.49	0.60
7:Q:162:MET:HG3	7:Q:411:LEU:HD11	2.40	0.60
8:Z:393:ASP:OD1	8:Z:396:ARG:NH2	2.33	0.60
1:A:437:ALA:HB1	1:A:445:GLN:HG3	1.84	0.60
2:B:6:PHE:HB3	2:B:10:VAL:HG21	5.14	0.59
5:G:411:SER:OG	5:G:503:GLU:OE1	2.20	0.59
7:Q:294:MET:HG3	7:Q:347:PRO:HG2	4.48	0.59
2:B:238:LEU:HD12	2:B:290:ILE:HG12	1.84	0.59
3:D:436:GLN:HA	3:D:440:TRP:CZ3	8.28	0.59
4:E:245:LEU:HD11	4:E:354:ILE:HD11	1.83	0.59
7:Q:247:VAL:HG22	7:Q:298:CYS:HB3	4.14	0.59
1:A:419:VAL:HB	1:A:521:THR:HG22	7.05	0.59
6:H:53:ILE:HD11	6:H:69:ILE:HG23	1.92	0.59
4:E:219:VAL:HB	4:E:431:ARG:HG3	2.00	0.59
4:E:74:LEU:HB3	4:E:93:GLN:HG2	1.88	0.59
7:Q:77:ILE:HG13	7:Q:86:VAL:HG21	1.84	0.59
5:G:324:ASP:OD1	5:G:327:ARG:NH2	8.19	0.59
6:H:402:ARG:HB3	6:H:499:PRO:HG3	2.64	0.59
8:Z:236:LEU:HG	8:Z:238:VAL:H	2.11	0.59
5:G:184:LYS:HG3	5:G:375:LYS:HE2	1.83	0.59
5:G:479:ASN:ND2	5:G:481:THR:OG1	3.11	0.59
2:B:510:ARG:HG2	4:E:71:ASP:H	1.68	0.59
4:E:388:THR:HG22	4:E:390:ASP:H	1.69	0.59
6:H:241:ILE:HD12	6:H:330:VAL:HG11	1.91	0.59
4:E:232:GLY:HA3	4:E:409:ARG:HH21	3.02	0.58
3:D:297:VAL:HB	3:D:314:LYS:HD3	1.96	0.58
4:E:556:ILE:HA	6:H:54:VAL:HB	2.06	0.58
5:G:88:GLU:O	5:G:404:ARG:NH2	6.94	0.58
2:B:14:ARG:H	2:B:17:ASN:HB2	2.50	0.58
6:H:242:LEU:HD11	6:H:341:ILE:HD13	1.84	0.58
7:Q:243:LYS:HG2	7:Q:244:LYS:HG3	1.85	0.58
3:D:210:ILE:HG22	3:D:212:GLY:H	1.68	0.58
3:D:48:ILE:HD11	3:D:64:ILE:HG23	1.88	0.58
6:H:78:PRO:HB2	7:Q:54:ILE:HG21	2.04	0.58
3:D:156:THR:HG21	3:D:496:HIS:HB3	1.96	0.57
4:E:72:LYS:HD2	4:E:90:ILE:HD13	1.86	0.57
1:A:366:PHE:HB2	1:A:369:ASP:HB3	1.93	0.57
8:Z:39:PRO:HA	8:Z:160:THR:HA	1.87	0.57
7:Q:244:LYS:H	7:Q:356:GLU:HA	2.90	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:289:GLN:HE21	3:D:318:ARG:HG2	2.33	0.57
3:D:25:ILE:HG23	3:D:104:LEU:HB3	1.99	0.57
3:D:194:ILE:HG12	3:D:375:VAL:HB	1.86	0.57
7:Q:89:THR:OG1	7:Q:104:MET:SD	2.70	0.57
8:Z:47:VAL:HG12	8:Z:49:GLY:H	1.85	0.57
1:A:124:THR:HG21	1:A:443:ARG:HD2	1.85	0.57
2:B:41:GLY:HA2	2:B:447:ASN:HB3	1.86	0.57
3:D:179:LEU:HA	3:D:182:SER:HB2	1.87	0.57
7:Q:343:ARG:NH2	8:Z:253:TYR:OH	10.20	0.57
2:B:226:ILE:HB	2:B:343:ILE:HB	4.41	0.57
8:Z:337:GLN:NE2	8:Z:339:SER:O	2.37	0.57
3:D:208:GLU:OE1	3:D:362:ARG:NH1	4.27	0.57
4:E:108:SER:HB2	4:E:119:THR:HG23	1.85	0.57
4:E:85:ASN:OD1	4:E:191:LYS:NZ	2.38	0.57
7:Q:493:ASP:C	7:Q:494:HIS:CG	2.76	0.57
1:A:10:SER:HB3	1:A:19:LYS:H	1.68	0.56
2:B:427:SER:OG	2:B:460:ARG:NH2	13.10	0.56
8:Z:458:LEU:HG	8:Z:493:LEU:HD21	1.86	0.56
1:A:391:ASN:OD1	1:A:394:SER:N	2.36	0.56
3:D:334:ALA:H	3:D:338:LEU:HD11	4.55	0.56
4:E:326:GLY:HA2	4:E:344:ARG:HB2	1.86	0.56
7:Q:356:GLU:HB2	7:Q:373:GLN:HA	1.87	0.56
1:A:443:ARG:NH1	3:D:459:GLY:O	2.31	0.56
6:H:191:ARG:O	6:H:405:GLN:NE2	2.38	0.56
2:B:342:VAL:HB	2:B:357:SER:HB3	1.91	0.56
7:Q:54:ILE:HG12	7:Q:64:ILE:HG12	1.86	0.56
1:A:358:CYS:HA	1:A:377:THR:HA	1.87	0.56
1:A:53:LEU:HD11	1:A:69:ILE:HA	1.88	0.56
4:E:247:LYS:HG3	4:E:249:PHE:H	1.70	0.56
5:G:431:ALA:HA	5:G:434:LEU:HD12	6.37	0.56
1:A:249:LEU:HD23	1:A:340:SER:HA	3.04	0.55
1:A:264:ILE:HG21	1:A:270:LEU:HB2	1.88	0.55
1:A:544:MET:HA	3:D:47:MET:HB2	1.88	0.55
4:E:174:GLU:OE1	4:E:177:ARG:NH2	5.97	0.55
4:E:283:THR:HG23	4:E:284:LYS:H	4.30	0.55
2:B:113:SER:O	2:B:453:SER:OG	25.83	0.55
1:A:51:LYS:HD3	5:G:525:ASP:HB3	1.87	0.55
6:H:147:ILE:HG13	6:H:150:GLU:HB2	2.06	0.55
8:Z:33:LEU:HD12	8:Z:95:VAL:HG11	1.88	0.55
1:A:462:LEU:HG	1:A:504:LEU:HD11	1.87	0.55
2:B:40:LYS:NZ	2:B:474:LEU:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:232:GLN:OE1	6:H:233:PRO:HD2	6.79	0.55
7:Q:56:VAL:HG22	7:Q:62:ILE:HG12	4.72	0.55
4:E:284:LYS:HE3	6:H:260:ARG:HD2	1.88	0.55
7:Q:223:ILE:HG22	7:Q:225:GLY:H	1.72	0.55
4:E:251:HIS:HB3	4:E:254:MET:HG3	2.51	0.55
6:H:163:ARG:NH1	6:H:176:ASP:OD1	2.35	0.55
2:B:252:VAL:HG21	2:B:258:LEU:HB2	4.21	0.55
2:B:214:LEU:HB3	2:B:354:LEU:HB2	1.88	0.55
7:Q:486:GLU:CD	7:Q:492:THR:HG22	2.26	0.55
8:Z:367:VAL:O	8:Z:370:ASN:ND2	2.40	0.55
1:A:242:VAL:HG23	1:A:294:GLN:HB2	1.89	0.55
1:A:50:ASP:HB3	1:A:64:ASN:HB3	1.89	0.55
2:B:513:ASN:OD1	2:B:514:ILE:N	2.48	0.55
7:Q:492:THR:OG1	7:Q:493:ASP:N	2.39	0.55
2:B:117:PRO:HD3	3:D:9:ALA:HB3	34.95	0.54
5:G:466:ARG:HA	7:Q:444:LEU:HD21	60.60	0.54
2:B:251:LYS:HD2	4:E:288:ASP:HB3	6.08	0.54
5:G:160:GLY:O	5:G:161:THR:OG1	2.25	0.54
5:G:193:GLU:HG2	5:G:195:ASN:H	1.79	0.54
7:Q:219:ASN:O	7:Q:387:ARG:NH1	2.40	0.54
6:H:298:PRO:HB3	6:H:317:ARG:HE	4.98	0.54
1:A:173:SER:HA	1:A:176:PHE:HB2	1.91	0.54
1:A:325:ASP:OD1	1:A:328:ARG:NH2	2.39	0.54
2:B:116:HIS:NE2	4:E:485:GLU:O	2.47	0.54
4:E:285:HIS:CE1	4:E:287:LEU:HD13	2.43	0.54
2:B:515:ILE:HD11	4:E:60:ILE:HD13	3.51	0.54
5:G:339:ARG:NH2	5:G:342:ASP:OD1	2.37	0.54
1:A:58:GLY:O	5:G:76:LYS:NZ	2.68	0.54
4:E:145:LYS:HB3	4:E:464:ILE:HG21	1.88	0.54
7:Q:246:LYS:HB2	7:Q:296:VAL:HA	1.96	0.54
3:D:144:LEU:HD13	3:D:182:SER:HB3	1.88	0.54
1:A:219:VAL:O	1:A:383:SER:OG	2.25	0.54
2:B:511:VAL:HG11	4:E:73:ILE:HG13	1.89	0.54
6:H:412:GLY:O	6:H:491:ASN:ND2	2.33	0.54
1:A:15:LEU:HD12	1:A:17:GLY:N	2.23	0.54
3:D:298:ASN:OD1	3:D:299:ASP:N	2.42	0.54
4:E:269:LEU:HD21	4:E:322:ILE:HD12	4.02	0.54
1:A:209:HIS:CD2	5:G:190:VAL:HG13	7.92	0.54
8:Z:100:GLU:HG2	8:Z:453:VAL:HB	1.93	0.54
1:A:519:GLU:HG2	1:A:524:LYS:HE2	1.89	0.54
3:D:29:ARG:NH1	3:D:108:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:35:ILE:HD11	7:Q:81:ALA:HB1	1.89	0.54
2:B:232:LEU:HD11	2:B:326:VAL:HG11	2.91	0.53
4:E:107:LEU:HB2	4:E:544:LEU:HD22	1.93	0.53
7:Q:150:ILE:HG12	7:Q:152:ASP:H	1.74	0.53
7:Q:27:GLN:HE22	7:Q:544:ILE:HG12	5.68	0.53
1:A:111:ARG:HG3	1:A:454:ALA:HB2	1.90	0.53
1:A:17:GLY:HA3	1:A:547:VAL:HA	2.01	0.53
2:B:65:LYS:HG2	2:B:82:LYS:HE2	1.90	0.53
5:G:208:LYS:HD2	5:G:389:LEU:HB3	1.90	0.53
7:Q:500:ASP:HB2	7:Q:509:VAL:HA	3.17	0.53
3:D:234:ILE:O	3:D:345:GLY:N	2.38	0.53
6:H:42:PRO:O	6:H:49:SER:N	2.41	0.53
6:H:499:PRO:HG2	6:H:502:VAL:HG23	1.91	0.53
7:Q:243:LYS:HE2	7:Q:244:LYS:HE3	1.91	0.53
4:E:53:ALA:HB1	4:E:98:ASN:HD21	1.73	0.53
5:G:45:LEU:HD23	5:G:59:ASN:HB3	1.90	0.53
6:H:471:ALA:HA	6:H:474:LYS:HD2	1.99	0.53
5:G:238:ILE:HG21	5:G:293:THR:HG21	1.90	0.53
7:Q:238:SER:HB2	7:Q:359:LYS:HG2	2.11	0.53
4:E:461:GLN:HG3	4:E:469:PHE:CE2	2.44	0.53
5:G:188:GLN:HE21	5:G:191:GLU:H	1.56	0.53
7:Q:493:ASP:HB3	7:Q:494:HIS:CD2	3.69	0.53
7:Q:493:ASP:O	7:Q:494:HIS:ND1	2.42	0.53
4:E:275:PRO:HB3	4:E:325:TRP:HB2	1.90	0.53
2:B:197:LYS:HD3	2:B:381:GLU:HB2	1.90	0.52
3:D:355:SER:H	3:D:358:SER:HB2	1.73	0.52
5:G:231:HIS:ND1	5:G:232:PRO:HD2	2.25	0.52
8:Z:295:ILE:HB	8:Z:316:ALA:HA	1.91	0.52
1:A:143:VAL:HG23	1:A:144:LEU:HG	6.09	0.52
1:A:363:GLN:HE21	1:A:370:GLU:HG2	1.74	0.52
8:Z:237:ASN:HB3	8:Z:338:ASN:HA	1.91	0.52
8:Z:301:ILE:O	8:Z:318:ARG:NH1	2.44	0.52
1:A:503:ASP:HB2	1:A:510:VAL:HG22	1.91	0.52
1:A:78:PRO:HB3	3:D:55:ILE:HD13	2.96	0.52
4:E:115:ILE:HG22	4:E:117:ASP:H	1.74	0.52
1:A:167:LYS:HB2	1:A:169:ILE:HG22	1.92	0.52
2:B:510:ARG:O	4:E:71:ASP:N	3.28	0.52
4:E:112:ASP:HA	4:E:116:GLY:HA2	1.96	0.52
4:E:172:ASN:OD1	4:E:173:ASP:N	2.43	0.52
5:G:85:GLN:HE21	5:G:89:VAL:HG22	6.42	0.52
7:Q:14:PHE:HB2	8:Z:70:SER:HB2	3.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD23	1:A:102:VAL:HG13	1.91	0.52
4:E:75:ILE:HG12	4:E:81:ILE:HG12	2.65	0.52
7:Q:341:LEU:HD12	7:Q:342:PRO:HD2	1.91	0.52
2:B:230:LYS:H	2:B:282:ASN:HB2	1.75	0.52
6:H:14:LYS:HG3	6:H:16:GLY:H	1.72	0.52
8:Z:7:ASN:HB2	8:Z:8:PRO:HD2	2.06	0.52
3:D:436:GLN:HA	3:D:440:TRP:CE3	7.55	0.52
3:D:368:ASN:OD1	3:D:369:ASN:N	2.44	0.52
5:G:160:GLY:HA2	5:G:165:ILE:HD13	1.97	0.52
8:Z:245:THR:HG22	8:Z:247:VAL:H	1.75	0.52
3:D:241:ILE:N	3:D:296:ALA:O	2.92	0.51
2:B:247:GLY:HA2	4:E:285:HIS:CE1	4.79	0.51
1:A:40:VAL:HB	1:A:99:THR:HG23	2.19	0.51
2:B:516:ARG:HA	4:E:75:ILE:HB	1.92	0.51
1:A:248:ASP:HB3	1:A:339:SER:HA	1.93	0.51
5:G:249:PRO:HB3	5:G:299:LYS:HB2	1.91	0.51
6:H:247:GLU:HB3	6:H:249:GLU:OE1	2.10	0.51
4:E:444:GLY:HA3	4:E:512:VAL:HG23	1.92	0.51
1:A:144:LEU:HD21	1:A:419:VAL:HG23	9.34	0.51
7:Q:227:VAL:HG13	7:Q:370:VAL:HG12	1.97	0.51
8:Z:153:VAL:HG11	8:Z:405:VAL:HG21	1.93	0.51
1:A:187:VAL:HA	1:A:381:SER:O	3.10	0.51
3:D:234:ILE:HG12	3:D:285:VAL:HB	2.00	0.51
7:Q:13:LEU:HD21	7:Q:18:TYR:HB2	1.93	0.51
8:Z:210:ILE:HB	8:Z:377:THR:HB	1.93	0.51
8:Z:46:LEU:HD11	8:Z:62:LEU:HD23	1.92	0.51
2:B:242:LYS:HB3	2:B:245:ILE:HD12	3.75	0.51
6:H:224:PHE:CZ	6:H:226:TYR:HB2	2.45	0.51
7:Q:150:ILE:HG22	7:Q:152:ASP:H	4.19	0.51
7:Q:141:GLU:OE1	7:Q:437:TYR:OH	4.21	0.51
7:Q:83:LYS:HG2	8:Z:53:ILE:HD12	1.91	0.51
5:G:356:LYS:HB2	5:G:367:PHE:HB2	2.96	0.51
7:Q:506:ASP:O	7:Q:507:GLU:C	2.49	0.51
6:H:296:LYS:HE2	6:H:320:ALA:HA	1.99	0.50
6:H:44:LEU:HD23	6:H:452:GLN:HB3	2.72	0.50
2:B:191:GLU:O	2:B:316:ARG:NH1	2.54	0.50
2:B:197:LYS:HB3	2:B:377:LEU:HD13	1.94	0.50
6:H:48:GLY:HA2	6:H:456:ASN:HB3	1.92	0.50
3:D:254:VAL:HG22	3:D:259:GLN:HG3	4.27	0.50
6:H:258:GLU:OE1	6:H:260:ARG:NH1	11.56	0.50
3:D:331:LYS:HD2	3:D:343:ARG:HG2	3.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:510:LYS:NZ	7:Q:515:GLU:OE1	7.71	0.50
3:D:237:ILE:HD11	3:D:286:LEU:HD22	2.06	0.50
3:D:353:ILE:N	3:D:360:ILE:O	2.39	0.50
4:E:243:VAL:HG21	4:E:354:ILE:HG12	1.99	0.50
6:H:37:GLN:HE21	6:H:103:ILE:HG23	1.90	0.50
3:D:411:ILE:HB	3:D:478:LEU:HD21	7.08	0.50
6:H:241:ILE:HA	6:H:292:ILE:HB	1.93	0.50
1:A:468:LYS:HE3	1:A:507:GLY:HA3	2.53	0.50
4:E:267:VAL:N	4:E:377:CYS:O	2.39	0.50
5:G:482:THR:HA	5:G:493:ASP:HA	1.94	0.50
1:A:476:LYS:HG2	6:H:432:ALA:HB1	132.05	0.50
7:Q:96:MET:HG3	7:Q:98:ASP:H	1.76	0.49
8:Z:5:LEU:O	8:Z:14:ARG:NH2	5.65	0.49
2:B:167:SER:HA	2:B:170:LYS:HB2	3.39	0.49
4:E:104:LEU:HD22	4:E:123:VAL:HG13	2.28	0.49
5:G:494:MET:O	5:G:498:GLY:HA2	2.51	0.49
2:B:170:LYS:O	2:B:174:ALA:N	2.41	0.49
6:H:452:GLN:NE2	6:H:456:ASN:OD1	6.27	0.49
5:G:155:ILE:HD11	5:G:403:ALA:HB2	1.94	0.49
8:Z:174:VAL:HG13	8:Z:399:LEU:HD23	1.95	0.49
1:A:215:GLU:HB2	1:A:388:ARG:HD2	5.53	0.49
3:D:77:MET:SD	3:D:517:SER:OG	2.65	0.49
7:Q:292:ALA:HB2	7:Q:318:ILE:HD11	1.94	0.49
3:D:500:PRO:HG2	3:D:503:VAL:HG23	1.97	0.49
6:H:368:CYS:HB2	6:H:371:ALA:HB2	1.95	0.49
1:A:210:GLY:HA3	1:A:388:ARG:HH21	1.78	0.49
1:A:322:LYS:HE2	1:A:324:GLU:HB2	1.95	0.49
4:E:237:SER:OG	4:E:409:ARG:N	2.43	0.49
6:H:250:LEU:HD13	6:H:302:LEU:HD22	1.94	0.49
2:B:252:VAL:HG21	2:B:258:LEU:HG	1.94	0.49
2:B:218:PHE:HB3	2:B:306:ILE:HG12	2.25	0.49
3:D:285:VAL:HG22	3:D:311:MET:HB3	2.20	0.49
4:E:180:LEU:HD11	4:E:430:VAL:HG22	1.93	0.49
5:G:213:ASP:OD1	5:G:214:VAL:N	2.46	0.49
7:Q:32:ILE:HG12	7:Q:111:LEU:HB3	2.22	0.49
2:B:198:ILE:HB	2:B:370:ARG:HD2	1.94	0.49
5:G:85:GLN:NE2	5:G:512:THR:OG1	2.46	0.49
7:Q:420:LEU:HD11	7:Q:524:LYS:HG3	6.06	0.49
3:D:486:ARG:HG3	3:D:490:THR:HG21	1.94	0.48
5:G:242:ARG:NH1	5:G:243:VAL:O	2.45	0.48
5:G:503:GLU:HG2	5:G:507:GLN:HG3	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:35:ILE:O	7:Q:39:HIS:N	2.41	0.48
1:A:219:VAL:HG12	1:A:221:GLY:H	2.96	0.48
2:B:218:PHE:HB2	2:B:305:SER:O	2.12	0.48
3:D:523:ASP:OD1	3:D:524:ILE:N	2.45	0.48
5:G:21:GLN:NE2	5:G:524:ASP:OD1	2.46	0.48
6:H:279:PHE:HA	6:H:282:LEU:HB3	1.95	0.48
2:B:46:LEU:HB3	3:D:527:SER:HB3	2.50	0.48
4:E:344:ARG:HE	4:E:345:TRP:HD1	7.07	0.48
6:H:200:GLY:O	6:H:376:LEU:N	2.58	0.48
6:H:214:PHE:HD1	6:H:376:LEU:HD13	1.77	0.48
6:H:417:GLU:HG2	6:H:449:ILE:HB	2.57	0.48
5:G:434:LEU:HD11	5:G:438:GLN:HE21	1.76	0.48
6:H:91:ASP:HA	6:H:95:GLY:HA2	1.95	0.48
7:Q:242:ASP:O	7:Q:245:HIS:NE2	2.58	0.48
7:Q:49:CYS:O	7:Q:51:ARG:NH1	8.11	0.48
8:Z:280:LEU:HD21	8:Z:348:LEU:HD11	1.95	0.48
7:Q:44:THR:O	7:Q:51:ARG:N	2.33	0.48
8:Z:158:LEU:O	8:Z:162:VAL:HG22	2.19	0.48
1:A:133:LEU:HD22	1:A:532:LEU:HD13	1.94	0.48
6:H:335:GLN:HG2	6:H:341:ILE:HG12	2.09	0.48
6:H:424:LEU:HD23	6:H:427:TYR:HD2	1.88	0.48
6:H:480:GLY:N	6:H:489:GLY:O	2.44	0.48
1:A:156:LEU:HD13	1:A:409:VAL:HG13	3.78	0.48
3:D:432:MET:HG3	3:D:440:TRP:CD1	2.49	0.48
4:E:312:ASP:HB3	4:E:369:LEU:HD12	1.94	0.48
8:Z:485:GLU:OE2	8:Z:487:ARG:NH2	2.45	0.48
2:B:173:PHE:HZ	2:B:203:LEU:HB3	1.79	0.48
3:D:220:ILE:HD11	3:D:312:VAL:HB	1.96	0.48
3:D:335:ASP:OD1	3:D:336:ILE:N	2.43	0.48
4:E:553:ASN:HB3	6:H:51:ILE:HG13	1.96	0.48
6:H:236:PHE:HB2	6:H:352:PHE:HB3	2.51	0.48
8:Z:238:VAL:O	8:Z:297:ASN:ND2	2.58	0.48
8:Z:194:VAL:HG22	8:Z:376:CYS:HB2	2.14	0.48
1:A:287:LYS:HG3	1:A:348:GLU:HA	2.46	0.48
7:Q:135:ARG:NH1	7:Q:533:GLU:OE2	2.42	0.48
7:Q:15:LYS:HA	8:Z:68:ILE:HA	1.95	0.48
1:A:183:ALA:O	1:A:187:VAL:HG23	3.99	0.47
3:D:328:LEU:HA	3:D:366:ILE:HD12	5.65	0.47
4:E:268:LYS:HB2	4:E:318:ALA:HA	2.51	0.47
6:H:125:ILE:HA	6:H:438:ILE:HD13	1.96	0.47
7:Q:230:ARG:NH2	7:Q:233:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:298:GLN:NE2	8:Z:322:ARG:HG2	2.29	0.47
2:B:109:LEU:HA	2:B:113:SER:HB2	2.63	0.47
3:D:113:LYS:HB3	4:E:492:ILE:HD11	58.47	0.47
3:D:392:ARG:HA	3:D:395:HIS:HD2	1.79	0.47
5:G:55:LEU:HD11	8:Z:75:LEU:HD21	6.24	0.47
1:A:190:GLN:HA	1:A:196:ILE:H	2.84	0.47
4:E:247:LYS:HG2	4:E:343:VAL:HG13	1.97	0.47
5:G:141:LYS:HE2	5:G:480:PHE:HZ	1.78	0.47
5:G:32:ALA:O	5:G:36:ARG:HG3	2.22	0.47
1:A:258:MET:HB3	5:G:344:LYS:HA	3.55	0.47
8:Z:213:LEU:HD12	8:Z:328:LEU:HD23	1.96	0.47
5:G:229:VAL:HG11	5:G:234:MET:HG3	6.78	0.47
1:A:164:MET:HB3	1:A:169:ILE:HG23	1.97	0.47
2:B:115:ILE:HG23	2:B:425:LYS:HB3	1.96	0.47
3:D:256:ASP:OD1	3:D:257:TYR:N	2.48	0.47
4:E:40:ARG:HH12	6:H:35:ALA:HB1	1.79	0.47
8:Z:242:TYR:HB2	8:Z:267:ARG:HH21	1.99	0.47
1:A:208:ALA:N	1:A:387:LEU:O	2.96	0.47
1:A:303:ASP:OD1	1:A:304:ASP:N	2.45	0.47
1:A:96:ASP:OD1	1:A:97:GLY:N	2.47	0.47
3:D:167:SER:HA	3:D:170:LEU:HB2	2.10	0.47
3:D:461:ASN:HB3	3:D:464:LYS:HB3	1.95	0.47
2:B:513:ASN:HB3	4:E:72:LYS:HD2	3.88	0.47
5:G:263:ILE:HD13	5:G:269:TRP:HA	4.90	0.47
6:H:222:LYS:HD3	6:H:363:ASN:ND2	2.29	0.47
3:D:37:THR:O	3:D:44:MET:N	2.45	0.47
2:B:326:VAL:HG22	2:B:335:CYS:HB3	1.97	0.47
5:G:295:VAL:N	5:G:315:SER:O	2.45	0.47
5:G:436:GLY:HA2	7:Q:476:PRO:HB2	110.71	0.47
3:D:372:ARG:O	3:D:374:THR:N	2.48	0.47
3:D:20:VAL:HG11	3:D:523:ASP:HA	2.05	0.47
4:E:125:LEU:HD11	4:E:476:LEU:HD23	1.96	0.47
5:G:181:THR:HG23	5:G:373:GLU:HB3	3.03	0.47
6:H:480:GLY:HA3	6:H:491:ASN:ND2	2.31	0.47
7:Q:98:ASP:OD1	7:Q:99:GLY:N	2.50	0.47
1:A:111:ARG:HD2	1:A:454:ALA:HB2	4.02	0.47
6:H:10:ILE:HB	7:Q:19:ASN:HB3	5.29	0.46
1:A:140:ILE:HG22	1:A:144:LEU:HD23	1.97	0.46
5:G:110:TYR:HD1	5:G:114:LYS:HG3	1.81	0.46
5:G:260:ASN:OD1	5:G:261:ILE:N	3.00	0.46
7:Q:14:PHE:CE2	8:Z:25:SER:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:235:ILE:HG23	8:Z:325:MET:HE3	1.97	0.46
8:Z:43:LEU:HD21	8:Z:55:LEU:HB3	2.04	0.46
1:A:211:LYS:HB2	1:A:388:ARG:HD3	5.40	0.46
2:B:116:HIS:CG	2:B:117:PRO:HD2	2.56	0.46
4:E:58:ALA:O	4:E:62:LYS:HG3	2.15	0.46
8:Z:238:VAL:HG21	8:Z:340:VAL:HG23	3.46	0.46
5:G:44:MET:HB3	8:Z:529:LEU:O	2.14	0.46
1:A:86:LEU:HD21	1:A:101:VAL:HG12	1.98	0.46
1:A:251:LEU:HD12	1:A:302:ILE:HG12	2.10	0.46
6:H:143:LEU:HD21	6:H:419:GLU:HG2	2.09	0.46
1:A:122:PRO:HA	1:A:125:ILE:HD12	1.97	0.46
1:A:406:LEU:HD12	1:A:409:VAL:HB	2.79	0.46
2:B:88:VAL:HG23	2:B:89:GLY:H	1.81	0.46
3:D:284:ASN:O	3:D:311:MET:N	2.75	0.46
4:E:107:LEU:HD21	4:E:122:VAL:HG22	1.97	0.46
2:B:514:ILE:HG13	4:E:73:ILE:HB	1.97	0.46
7:Q:291:ILE:HG12	7:Q:347:PRO:HG3	1.97	0.46
4:E:397:GLN:HG3	4:E:399:LYS:HG2	2.01	0.46
8:Z:12:SER:OG	8:Z:532:GLU:OE2	2.49	0.46
4:E:115:ILE:HG23	4:E:432:ASN:HD21	2.81	0.46
4:E:358:THR:HG22	4:E:377:CYS:HB3	1.98	0.46
5:G:263:ILE:HD11	5:G:272:ILE:HG13	1.98	0.46
2:B:122:GLU:OE2	2:B:125:ARG:NH1	5.97	0.46
7:Q:162:MET:SD	7:Q:518:TYR:OH	2.61	0.46
8:Z:45:MET:HG3	8:Z:53:ILE:HG23	1.97	0.46
3:D:283:CYS:SG	3:D:344:LEU:HD11	4.01	0.46
4:E:328:ASP:OD1	4:E:329:ASP:N	2.55	0.46
5:G:331:VAL:HG23	5:G:332:THR:HG23	2.22	0.46
8:Z:273:LYS:HB3	8:Z:340:VAL:HG21	1.97	0.46
8:Z:214:VAL:HG12	8:Z:377:THR:HG21	1.99	0.46
1:A:20:ILE:HG22	1:A:25:ILE:HB	1.98	0.46
1:A:480:TYR:HB3	1:A:500:TYR:HD2	2.38	0.46
4:E:234:ILE:HG22	4:E:410:GLY:HA2	3.28	0.46
7:Q:228:PHE:HD2	7:Q:321:LEU:HD21	1.95	0.46
3:D:181:ILE:HB	3:D:373:PRO:CB	4.20	0.45
5:G:140:SER:HB3	5:G:411:SER:HB2	1.98	0.45
8:Z:285:CYS:HB3	8:Z:291:LYS:HG3	4.76	0.45
1:A:257:ALA:HB3	1:A:260:VAL:HG22	2.00	0.45
2:B:273:ILE:HD12	2:B:298:PHE:CE1	2.51	0.45
3:D:138:MET:HB2	3:D:478:LEU:HD11	1.98	0.45
4:E:251:HIS:ND1	4:E:252:PRO:HD2	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:476:GLU:HB2	6:H:479:TYR:CE2	2.51	0.45
8:Z:5:LEU:HB2	8:Z:14:ARG:HH12	2.57	0.45
5:G:424:SER:HB3	5:G:449:MET:HB2	2.12	0.45
5:G:525:ASP:OD1	5:G:526:ILE:N	2.50	0.45
6:H:250:LEU:HD22	6:H:302:LEU:HD22	3.64	0.45
6:H:239:PRO:HB2	6:H:292:ILE:HG12	1.98	0.45
6:H:86:ILE:HG21	6:H:513:ALA:HB2	2.46	0.45
7:Q:428:ILE:HD11	7:Q:460:PRO:HG3	1.98	0.45
7:Q:14:PHE:HB3	8:Z:70:SER:HB2	1.98	0.45
1:A:418:VAL:HA	1:A:520:PRO:HA	1.98	0.45
4:E:51:ILE:HD12	4:E:130:LEU:HB3	1.98	0.45
4:E:522:MET:O	4:E:526:PHE:N	3.28	0.45
5:G:435:GLU:OE2	7:Q:483:ASN:ND2	115.84	0.45
7:Q:128:ILE:HG23	7:Q:536:THR:HB	4.64	0.45
8:Z:335:GLU:HB2	8:Z:347:ILE:HG23	1.99	0.45
1:A:53:LEU:HD13	1:A:72:LEU:HB2	1.99	0.45
3:D:130:ARG:HD3	3:D:440:TRP:HH2	1.82	0.45
4:E:225:LYS:O	4:E:406:CYS:N	2.79	0.45
4:E:517:TYR:HD2	4:E:525:LEU:HD13	4.66	0.45
8:Z:173:ILE:HG12	8:Z:209:PHE:HB2	2.02	0.45
3:D:254:VAL:HG13	3:D:259:GLN:HB3	5.30	0.45
7:Q:463:LEU:HB2	7:Q:499:VAL:HG11	1.97	0.45
5:G:181:THR:HG23	5:G:373:GLU:HG2	1.98	0.45
5:G:211:GLY:O	5:G:382:ARG:NE	2.48	0.45
3:D:135:LEU:HD11	3:D:411:ILE:HD13	3.23	0.45
7:Q:139:LEU:HD23	7:Q:142:LEU:HD12	1.99	0.45
8:Z:268:LYS:HA	8:Z:271:ASP:HB2	2.00	0.45
6:H:350:ALA:HB3	6:H:367:GLY:HA3	1.99	0.45
5:G:225:LEU:HD11	5:G:328:ILE:HD11	2.41	0.44
6:H:215:ILE:HG22	6:H:217:GLY:H	1.96	0.44
6:H:526:ASN:HD21	7:Q:74:GLU:HB3	1.82	0.44
8:Z:89:ASP:OD1	8:Z:90:GLY:N	2.49	0.44
1:A:90:GLN:HB3	1:A:98:THR:HG22	1.99	0.44
3:D:91:ASP:OD1	3:D:92:GLY:N	2.51	0.44
5:G:215:LEU:O	5:G:218:ARG:NH1	2.32	0.44
6:H:37:GLN:O	6:H:41:LYS:HG3	2.17	0.44
7:Q:486:GLU:CD	7:Q:492:THR:CG2	2.86	0.44
3:D:162:ILE:HB	3:D:389:GLU:HG2	4.89	0.44
5:G:234:MET:SD	5:G:315:SER:HA	2.57	0.44
6:H:122:SER:HA	6:H:125:ILE:HD12	2.00	0.44
8:Z:337:GLN:HE22	8:Z:342:ASP:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:40:LYS:HG2	8:Z:493:LEU:HD13	2.00	0.44
1:A:101:VAL:HG13	1:A:531:ALA:HB2	1.98	0.44
5:G:339:ARG:HG2	5:G:341:GLU:H	1.82	0.44
7:Q:155:ASP:OD1	7:Q:156:LYS:N	2.50	0.44
7:Q:408:VAL:HG13	7:Q:411:LEU:HD12	1.99	0.44
7:Q:428:ILE:HG13	7:Q:478:LEU:HB3	4.29	0.44
5:G:45:LEU:N	8:Z:529:LEU:O	2.82	0.44
1:A:121:HIS:CG	1:A:122:PRO:HD2	2.55	0.44
1:A:254:ALA:HB2	1:A:281:VAL:HG13	2.00	0.44
1:A:363:GLN:NE2	1:A:370:GLU:OE2	2.50	0.44
2:B:9:GLN:O	2:B:516:ARG:NH2	8.83	0.44
6:H:77:HIS:CE1	6:H:79:ALA:HB3	2.60	0.44
7:Q:16:GLN:HG2	7:Q:17:GLY:H	1.83	0.44
7:Q:211:LYS:HB2	7:Q:394:LEU:HD21	2.00	0.44
1:A:173:SER:O	1:A:177:SER:N	2.37	0.44
1:A:37:ALA:O	1:A:41:LYS:HG3	2.18	0.44
2:B:170:LYS:HA	2:B:173:PHE:HB2	2.00	0.44
1:A:49:LEU:HD22	5:G:522:ARG:HG3	3.74	0.44
1:A:242:VAL:HG13	1:A:358:CYS:HB3	2.30	0.44
3:D:130:ARG:HD3	3:D:440:TRP:CH2	2.53	0.44
4:E:251:HIS:CD2	4:E:253:GLN:HB2	5.26	0.44
6:H:104:LEU:HD11	6:H:446:LEU:HD23	2.00	0.44
7:Q:46:MET:HB2	7:Q:101:ASN:HB3	2.06	0.44
1:A:121:HIS:NE2	3:D:456:GLU:O	2.51	0.44
1:A:59:ASP:OD1	1:A:60:PHE:N	2.46	0.44
2:B:269:MET:O	2:B:273:ILE:HG12	2.18	0.44
3:D:220:ILE:HD12	3:D:226:PRO:HD2	2.61	0.44
5:G:206:VAL:HG12	5:G:379:ILE:HB	2.00	0.44
8:Z:84:ASP:OD1	8:Z:91:THR:OG1	2.31	0.44
2:B:167:SER:HA	2:B:170:LYS:HB3	1.99	0.44
6:H:67:ALA:N	6:H:98:THR:OG1	2.69	0.44
6:H:77:HIS:HB3	6:H:80:ALA:HB3	2.00	0.44
8:Z:126:ARG:HD2	8:Z:518:THR:HA	2.00	0.44
2:B:197:LYS:NZ	2:B:378:ASP:OD1	2.49	0.43
3:D:24:ASN:HB3	3:D:74:VAL:HG21	2.71	0.43
5:G:13:GLU:OE2	5:G:14:ARG:NH1	2.51	0.43
6:H:201:ILE:HG21	6:H:390:GLU:HG3	1.99	0.43
6:H:158:LEU:HD22	6:H:400:VAL:HG13	2.00	0.43
8:Z:162:VAL:HG23	8:Z:164:ALA:H	1.99	0.43
8:Z:358:THR:HG23	8:Z:363:LYS:HG2	1.99	0.43
3:D:296:ALA:HB3	3:D:314:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:333:ILE:HG13	3:D:339:PHE:HD1	4.66	0.43
5:G:156:GLN:HA	5:G:159:ILE:HD12	4.80	0.43
2:B:119:THR:O	2:B:123:GLY:N	2.51	0.43
3:D:116:HIS:CG	3:D:117:PRO:HD2	2.53	0.43
4:E:153:ALA:HB2	4:E:469:PHE:CD1	2.69	0.43
4:E:168:ILE:HG23	4:E:179:PHE:HD2	1.92	0.43
6:H:224:PHE:CZ	6:H:315:ALA:HA	5.16	0.43
8:Z:331:VAL:HG22	8:Z:375:SER:HB3	2.39	0.43
2:B:115:ILE:HD11	2:B:428:LEU:HB2	2.33	0.43
2:B:420:GLN:NE2	2:B:464:TYR:OH	10.30	0.43
1:A:54:VAL:O	5:G:529:GLY:N	2.58	0.43
1:A:466:ALA:HB2	1:A:504:LEU:HD13	1.99	0.43
1:A:481:HIS:NE2	1:A:500:TYR:O	2.52	0.43
2:B:158:LYS:HA	2:B:170:LYS:HD2	3.34	0.43
4:E:193:VAL:HG13	4:E:200:PHE:CD2	2.53	0.43
4:E:51:ILE:HG21	4:E:134:LEU:HB2	2.02	0.43
4:E:59:SER:HA	4:E:62:LYS:HD2	2.06	0.43
5:G:159:ILE:HG23	5:G:164:VAL:HG23	2.00	0.43
5:G:379:ILE:HD13	5:G:396:LEU:HD21	2.04	0.43
6:H:160:ARG:HD3	6:H:495:PHE:HE2	1.85	0.43
1:A:33:THR:HG21	1:A:538:ILE:HD13	3.44	0.43
2:B:42:MET:HB3	3:D:520:ARG:O	2.19	0.43
6:H:264:VAL:HA	6:H:267:TYR:CD2	2.53	0.43
4:E:301:TYR:O	4:E:305:LYS:HG2	4.62	0.43
6:H:159:GLU:HG3	6:H:179:VAL:HG11	4.27	0.43
7:Q:255:ASP:OD1	7:Q:256:ILE:N	2.54	0.43
7:Q:421:PRO:O	7:Q:426:THR:OG1	2.23	0.43
1:A:104:ILE:HG13	1:A:458:ILE:HD11	2.01	0.43
4:E:177:ARG:HA	4:E:180:LEU:HB3	2.01	0.43
4:E:281:PRO:HD3	6:H:267:TYR:CZ	3.16	0.43
6:H:520:VAL:HA	7:Q:52:ASN:O	2.19	0.43
8:Z:30:GLN:HE22	8:Z:100:GLU:HB2	2.06	0.43
2:B:512:ASP:OD1	4:E:72:LYS:NZ	3.27	0.43
5:G:207:GLU:HG2	5:G:224:LEU:HD22	3.63	0.43
2:B:31:ASP:HA	2:B:34:LYS:HD3	2.02	0.43
2:B:132:LEU:HD22	2:B:495:ARG:HG3	2.01	0.43
8:Z:459:VAL:HG11	8:Z:469:VAL:HG11	2.00	0.43
1:A:350:PHE:HB2	1:A:353:SER:HB2	2.01	0.42
1:A:184:LEU:HD13	1:A:406:LEU:HD11	2.01	0.42
3:D:71:LEU:HA	3:D:76:ARG:HH21	1.84	0.42
5:G:181:THR:HG21	5:G:221:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:VAL:HG12	3:D:182:SER:OG	2.19	0.42
4:E:459:ASP:OD1	4:E:470:ARG:NH2	9.75	0.42
5:G:49:LEU:HD21	8:Z:71:PRO:HG3	1.99	0.42
1:A:55:ASP:HB2	5:G:530:VAL:HG22	2.01	0.42
6:H:229:PHE:CG	6:H:230:GLU:N	4.28	0.42
7:Q:130:GLY:HA3	7:Q:448:ALA:HB3	2.01	0.42
3:D:191:LEU:HD22	3:D:398:LEU:HB3	2.01	0.42
4:E:378:SER:HB3	4:E:397:GLN:O	2.19	0.42
1:A:49:LEU:HB3	5:G:522:ARG:O	2.24	0.42
7:Q:203:ASN:OD1	7:Q:204:VAL:N	4.73	0.42
8:Z:63:LEU:HA	8:Z:66:MET:HG2	2.40	0.42
2:B:150:ARG:HG3	2:B:182:LEU:HD11	2.01	0.42
4:E:283:THR:HG23	4:E:284:LYS:N	4.62	0.42
4:E:335:LEU:HB3	4:E:340:LEU:O	2.31	0.42
4:E:517:TYR:CD2	4:E:525:LEU:HD13	4.36	0.42
6:H:94:VAL:HG12	6:H:96:ASP:H	1.84	0.42
7:Q:313:LEU:HB3	7:Q:318:ILE:HB	2.56	0.42
1:A:237:ILE:HG22	1:A:238:ALA:N	2.31	0.42
6:H:148:THR:HG22	6:H:407:LYS:HD2	2.02	0.42
7:Q:106:LEU:HD11	7:Q:456:PHE:CE1	2.72	0.42
7:Q:431:ILE:HA	7:Q:453:ALA:HB1	2.00	0.42
8:Z:146:ASP:O	8:Z:149:PHE:N	2.51	0.42
1:A:188:LYS:HB2	1:A:198:TYR:CE1	3.39	0.42
1:A:210:GLY:CA	1:A:388:ARG:HH21	2.33	0.42
1:A:540:ARG:HA	3:D:44:MET:SD	2.59	0.42
7:Q:106:LEU:HD11	7:Q:456:PHE:HE1	2.06	0.42
1:A:7:ASN:HB3	1:A:20:ILE:HD12	2.01	0.42
1:A:299:THR:O	1:A:320:ARG:HA	2.20	0.42
2:B:25:GLY:HA3	2:B:71:ASN:HD22	2.23	0.42
2:B:308:HIS:O	2:B:308:HIS:ND1	2.53	0.42
4:E:517:TYR:CG	4:E:518:GLY:N	2.88	0.42
5:G:110:TYR:HE2	5:G:444:ALA:HB2	1.84	0.42
6:H:451:ARG:HA	6:H:465:LEU:HD11	5.41	0.42
8:Z:40:LYS:HG3	8:Z:462:SER:HB2	2.02	0.42
1:A:441:GLY:HA2	1:A:445:GLN:OE1	2.28	0.42
2:B:211:GLY:O	2:B:356:PHE:HB2	2.19	0.42
4:E:344:ARG:HH21	4:E:345:TRP:HE1	10.18	0.42
4:E:450:MET:HE1	4:E:538:ILE:HG21	2.33	0.42
5:G:451:CYS:SG	5:G:454:ARG:NH2	3.97	0.42
6:H:37:GLN:HG3	6:H:103:ILE:HA	2.01	0.42
8:Z:114:HIS:CG	8:Z:115:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:SER:HA	2:B:481:ASP:HA	2.05	0.42
3:D:117:PRO:HB2	3:D:519:LEU:HB3	2.07	0.42
3:D:410:LEU:HD13	3:D:498:LEU:HD22	2.15	0.42
4:E:61:ILE:HD11	4:E:123:VAL:HB	2.02	0.42
4:E:327:PHE:CE2	4:E:342:ALA:HB1	2.54	0.42
5:G:252:TYR:CD1	5:G:276:GLU:HA	3.24	0.42
6:H:220:PHE:HD1	6:H:222:LYS:H	1.66	0.42
6:H:294:LEU:HD23	6:H:315:ALA:HB3	2.70	0.42
8:Z:132:PHE:HD2	8:Z:422:LEU:HD12	1.85	0.42
7:Q:343:ARG:HG3	8:Z:259:ARG:NH1	6.41	0.42
6:H:77:HIS:HE1	6:H:79:ALA:HB3	1.96	0.42
1:A:377:THR:HG22	1:A:380:HIS:CD2	5.62	0.41
1:A:436:PHE:O	1:A:439:THR:OG1	2.27	0.41
5:G:117:HIS:CG	5:G:118:PRO:HD2	2.55	0.41
6:H:93:GLU:HG3	6:H:501:LEU:HD21	11.38	0.41
7:Q:226:MET:HA	7:Q:383:THR:OG1	2.20	0.41
7:Q:348:THR:HG22	7:Q:350:GLU:H	1.85	0.41
8:Z:293:PHE:HE1	8:Z:348:LEU:HD21	2.54	0.41
8:Z:359:ILE:HG13	8:Z:362:GLU:H	1.85	0.41
6:H:12:VAL:O	7:Q:78:VAL:HB	2.40	0.41
6:H:195:ASP:HB3	6:H:198:LEU:HG	2.04	0.41
7:Q:242:ASP:HB3	7:Q:245:HIS:CE1	2.54	0.41
7:Q:92:GLN:HA	7:Q:526:PHE:HE2	1.85	0.41
8:Z:296:ILE:O	8:Z:296:ILE:HG22	2.20	0.41
2:B:291:TYR:HE2	2:B:293:TYR:CD2	4.93	0.41
2:B:72:PRO:HG3	2:B:514:ILE:HG21	2.31	0.41
4:E:447:GLU:HG2	4:E:479:ILE:HB	2.02	0.41
3:D:475:ASN:ND2	4:E:462:ARG:HH12	125.11	0.41
5:G:110:TYR:HB3	5:G:116:ILE:HD12	2.00	0.41
8:Z:236:LEU:HD11	8:Z:238:VAL:HG12	2.03	0.41
1:A:13:LEU:HG	1:A:15:LEU:HD23	2.03	0.41
1:A:330:ALA:O	1:A:335:ALA:N	2.50	0.41
1:A:377:THR:OG1	1:A:380:HIS:HB3	2.20	0.41
7:Q:520:MET:HG3	7:Q:523:THR:H	5.04	0.41
7:Q:541:ILE:HG13	8:Z:43:LEU:O	4.36	0.41
8:Z:227:ARG:HG2	8:Z:355:TYR:HB2	2.02	0.41
8:Z:98:VAL:HG13	8:Z:524:ALA:HB2	2.36	0.41
1:A:238:ALA:HB1	1:A:241:ASN:O	3.06	0.41
2:B:397:GLU:OE2	2:B:399:ARG:NE	2.38	0.41
3:D:138:MET:HG3	3:D:411:ILE:HD13	2.03	0.41
5:G:181:THR:HG21	5:G:377:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:227:VAL:HB	7:Q:383:THR:HG21	2.52	0.41
7:Q:496:TYR:O	7:Q:512:ILE:HG12	2.20	0.41
7:Q:15:LYS:HG2	8:Z:68:ILE:HG12	2.02	0.41
1:A:172:ASP:HB2	1:A:176:PHE:CE2	2.60	0.41
1:A:238:ALA:CB	1:A:242:VAL:HB	2.46	0.41
3:D:194:ILE:HA	3:D:375:VAL:O	2.29	0.41
3:D:348:ASP:HB2	3:D:367:ARG:HE	1.85	0.41
3:D:460:LEU:HB3	3:D:465:VAL:HG21	2.04	0.41
3:D:479:ASN:O	3:D:491:ASN:HA	2.20	0.41
5:G:208:LYS:HB3	5:G:389:LEU:HD13	2.03	0.41
5:G:241:PRO:HG3	5:G:352:CYS:HB3	2.01	0.41
6:H:143:LEU:HD13	6:H:416:THR:HG23	2.54	0.41
8:Z:228:VAL:HG11	8:Z:231:ALA:HB2	2.58	0.41
2:B:88:VAL:HG23	2:B:89:GLY:N	2.36	0.41
3:D:293:LEU:HG	3:D:294:ARG:HG2	2.05	0.41
1:A:540:ARG:NH2	3:D:43:GLY:O	4.28	0.41
1:A:242:VAL:HG11	1:A:361:VAL:HG23	2.22	0.41
4:E:200:PHE:HZ	4:E:234:ILE:HB	2.23	0.41
4:E:510:ILE:HG23	4:E:520:ASN:HB3	2.88	0.41
6:H:132:ALA:HB2	6:H:439:ILE:HG12	2.53	0.41
8:Z:30:GLN:O	8:Z:34:GLU:N	2.53	0.41
2:B:232:LEU:HD21	2:B:326:VAL:HG11	2.02	0.41
4:E:276:PHE:CE2	4:E:331:ALA:HB1	2.56	0.41
4:E:327:PHE:HE2	4:E:342:ALA:HB1	1.85	0.41
4:E:498:LEU:HD22	4:E:510:ILE:HG22	2.02	0.41
5:G:223:VAL:HB	5:G:368:LEU:HD12	2.03	0.41
5:G:331:VAL:HG12	5:G:374:PRO:HG3	3.55	0.41
8:Z:476:GLU:OE2	8:Z:487:ARG:NH1	4.10	0.41
2:B:511:VAL:HG13	4:E:72:LYS:HA	2.03	0.41
4:E:107:LEU:HD23	4:E:123:VAL:HG22	2.74	0.41
5:G:210:PRO:HA	5:G:389:LEU:HD11	2.11	0.41
8:Z:370:ASN:HB2	8:Z:373:PRO:HB3	2.10	0.41
5:G:225:LEU:HB2	5:G:366:SER:HB3	3.39	0.41
4:E:551:ILE:HA	6:H:50:ASP:O	2.20	0.41
7:Q:27:GLN:O	7:Q:31:SER:N	2.87	0.41
8:Z:183:ASP:HB2	8:Z:187:ASP:HB2	5.30	0.41
1:A:363:GLN:HG3	1:A:371:CYS:O	2.21	0.40
1:A:482:ALA:O	1:A:486:MET:HG3	2.27	0.40
2:B:200:GLY:N	2:B:371:GLY:O	2.54	0.40
2:B:435:ARG:O	2:B:439:GLN:HG2	2.23	0.40
2:B:32:LEU:HD22	2:B:44:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:SER:OG	2:B:481:ASP:OD1	2.39	0.40
7:Q:234:GLY:HA2	7:Q:310:LEU:HD11	5.25	0.40
6:H:123:HIS:CE1	7:Q:49:CYS:HG	7.50	0.40
8:Z:138:ILE:HB	8:Z:411:ILE:HG13	5.20	0.40
2:B:217:LYS:HB2	2:B:352:PRO:HB2	2.04	0.40
2:B:69:LEU:HD13	2:B:74:ALA:HB1	2.13	0.40
4:E:35:GLN:HB2	6:H:76:VAL:HG21	4.51	0.40
7:Q:174:SER:HB3	7:Q:178:LEU:HG	2.03	0.40
5:G:71:ALA:HB3	8:Z:7:ASN:HB2	2.02	0.40
2:B:279:PHE:HE1	2:B:332:PRO:HA	1.87	0.40
3:D:115:ILE:HD11	4:E:492:ILE:HD13	60.11	0.40
3:D:71:LEU:O	3:D:76:ARG:NE	2.99	0.40
1:A:204:ASN:OD1	1:A:205:VAL:N	2.55	0.40
2:B:162:SER:O	2:B:163:SER:OG	2.33	0.40
4:E:169:SER:HA	4:E:176:PHE:HB2	2.52	0.40
4:E:502:GLN:NE2	4:E:508:SER:O	2.55	0.40
5:G:206:VAL:HG12	5:G:379:ILE:HD12	2.04	0.40
8:Z:230:ASN:HB2	8:Z:290:ASP:O	2.52	0.40
1:A:357:LEU:O	1:A:377:THR:OG1	4.62	0.40
1:A:369:ASP:OD1	1:A:370:GLU:N	2.55	0.40
1:A:480:TYR:CD2	1:A:509:ILE:HG21	2.57	0.40
3:D:239:PHE:CG	3:D:240:GLN:N	2.91	0.40
3:D:88:GLU:O	3:D:402:ARG:NH2	6.70	0.40
6:H:278:ILE:O	6:H:282:LEU:HG	5.16	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	541/559 (97%)	507 (94%)	33 (6%)	1 (0%)	52 86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	a	541/559 (97%)	501 (93%)	39 (7%)	1 (0%)	52 86
2	B	515/527 (98%)	490 (95%)	23 (4%)	2 (0%)	39 80
2	b	515/527 (98%)	486 (94%)	29 (6%)	0	100 100
3	D	519/528 (98%)	494 (95%)	25 (5%)	0	100 100
3	d	519/528 (98%)	494 (95%)	24 (5%)	1 (0%)	52 86
4	E	526/562 (94%)	502 (95%)	24 (5%)	0	100 100
4	e	526/562 (94%)	503 (96%)	23 (4%)	0	100 100
5	G	516/534 (97%)	496 (96%)	20 (4%)	0	100 100
5	g	516/534 (97%)	491 (95%)	25 (5%)	0	100 100
6	H	517/550 (94%)	497 (96%)	20 (4%)	0	100 100
6	h	517/550 (94%)	497 (96%)	20 (4%)	0	100 100
7	Q	541/568 (95%)	520 (96%)	19 (4%)	2 (0%)	39 80
7	q	541/568 (95%)	516 (95%)	25 (5%)	0	100 100
8	Z	532/546 (97%)	513 (96%)	19 (4%)	0	100 100
8	z	532/546 (97%)	518 (97%)	14 (3%)	0	100 100
All	All	8414/8748 (96%)	8025 (95%)	382 (4%)	7 (0%)	59 90

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Q	505	SER
7	Q	494	HIS
2	B	5	ILE
3	d	213	VAL
2	B	467	ILE
1	a	203	VAL
1	A	203	VAL

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	455/471 (97%)	455 (100%)	0	100	100
1	a	455/471 (97%)	455 (100%)	0	100	100
2	B	432/441 (98%)	432 (100%)	0	100	100
2	b	432/441 (98%)	432 (100%)	0	100	100
3	D	447/453 (99%)	447 (100%)	0	100	100
3	d	447/453 (99%)	447 (100%)	0	100	100
4	E	454/483 (94%)	454 (100%)	0	100	100
4	e	454/483 (94%)	454 (100%)	0	100	100
5	G	441/455 (97%)	441 (100%)	0	100	100
5	g	441/455 (97%)	441 (100%)	0	100	100
6	H	432/454 (95%)	432 (100%)	0	100	100
6	h	432/454 (95%)	432 (100%)	0	100	100
7	Q	454/473 (96%)	454 (100%)	0	100	100
7	q	454/473 (96%)	453 (100%)	1 (0%)	95	97
8	Z	451/463 (97%)	451 (100%)	0	100	100
8	z	451/463 (97%)	451 (100%)	0	100	100
All	All	7132/7386 (97%)	7131 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	q	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	417	ASN
1	A	190	GLN
2	b	192	HIS
2	b	304	ASN
2	b	420	GLN
2	B	420	GLN
3	d	250	ASN
3	d	284	ASN
3	D	250	ASN
3	D	284	ASN

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Mol	Chain	Res	Type
3	D	395	HIS
4	e	111	GLN
4	e	397	GLN
4	e	432	ASN
4	e	502	GLN
4	E	42	HIS
4	E	241	ASN
4	E	466	GLN
4	E	502	GLN
5	g	85	GLN
5	g	188	GLN
5	g	479	ASN
5	G	85	GLN
5	G	188	GLN
5	G	438	GLN
6	H	232	GLN
6	H	435	GLN
6	H	526	ASN
7	q	373	GLN
7	q	494	HIS
7	Q	91	GLN
7	Q	129	GLN
7	Q	314	ASN
7	Q	373	GLN
7	Q	494	HIS
8	z	230	ASN
8	z	237	ASN
8	z	356	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.