



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 04:21 PM JST

PDB ID : 6LY8 / pdb_00006ly8
EMDB ID : EMD-30014
Title : V/A-ATPase from *Thermus thermophilus*, the soluble domain, including V1, d, two EG stalks, and N-terminal domain of α -subunit.
Authors : Kishikawa, J.; Nakanishi, A.; Furuta, A.; Kato, T.; Namba, K.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2020-02-13
Resolution : 3.50 Å (reported)
Based on initial model : 5Y5Y

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

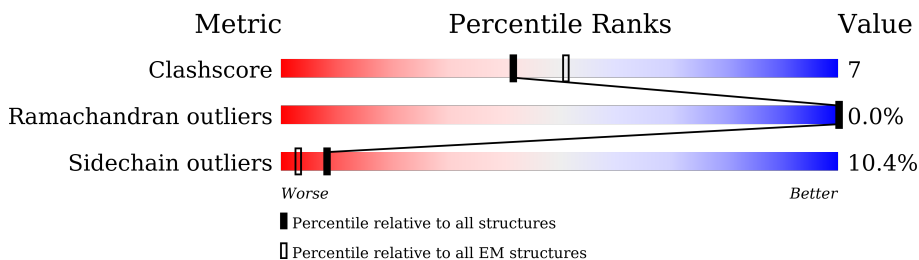
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	578	78% 19% .
1	B	578	78% 19% .
1	C	578	78% 20% .
2	D	478	77% 18% . .
2	E	478	73% 21% . .
2	F	478	76% 18% . .
3	G	223	77% 17% . 6%
4	H	104	68% 21% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26631 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	B	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	C	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	E	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	F	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		

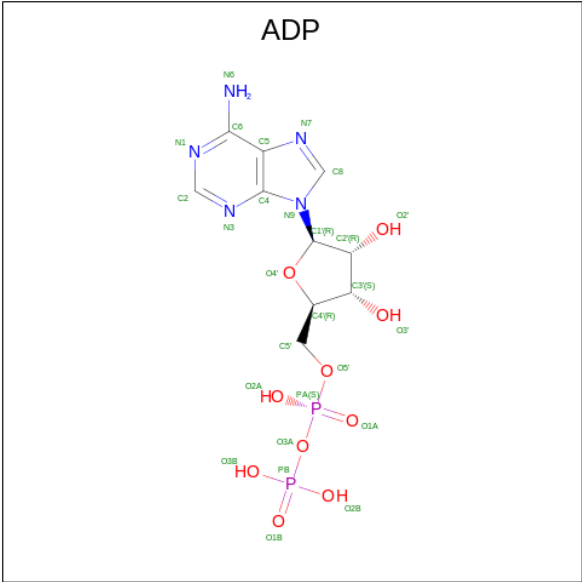
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total	C	N	O	S	0	0
			1642	1033	307	300	2		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total	C	N	O	S	0	0
			758	479	131	145	3		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

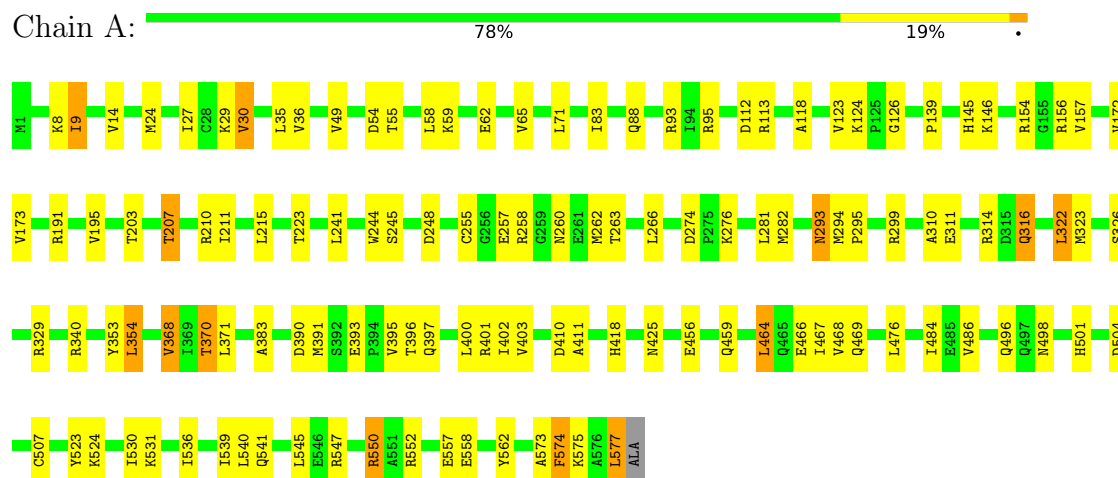


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

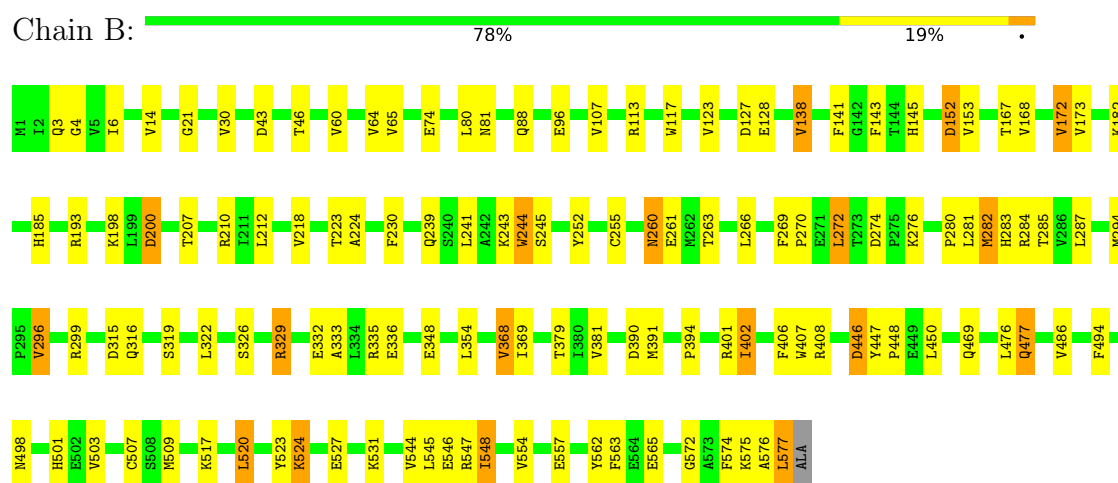
3 Residue-property plots

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

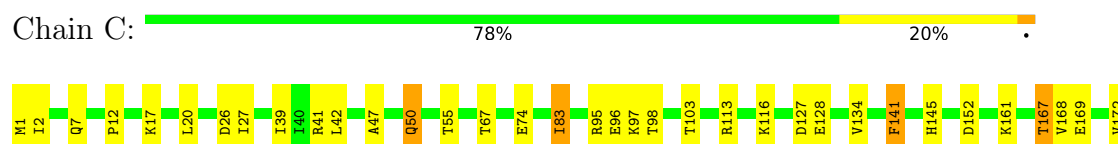
- Molecule 1: V-type ATP synthase alpha chain

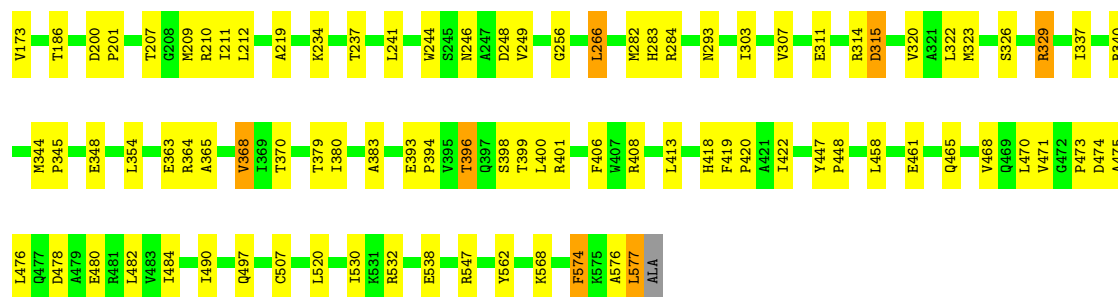


- Molecule 1: V-type ATP synthase alpha chain

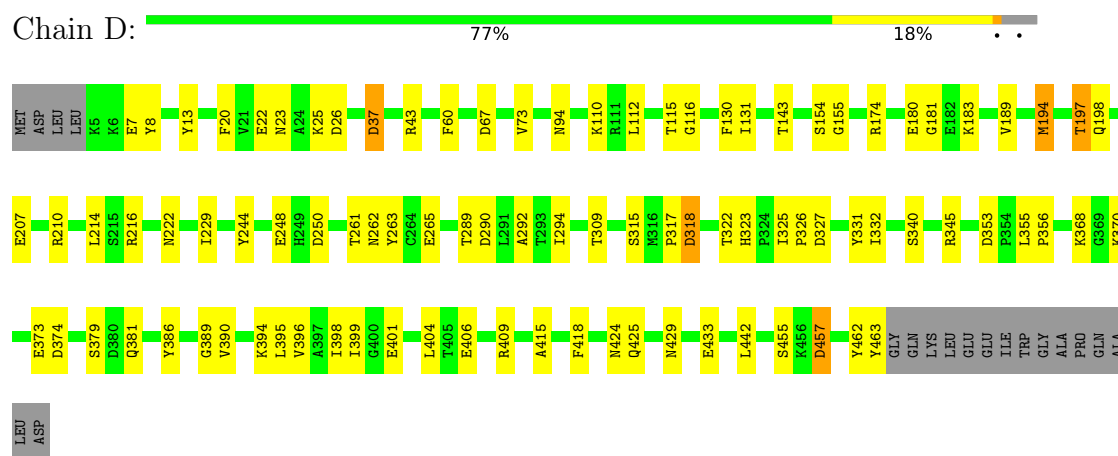


- Molecule 1: V-type ATP synthase alpha chain



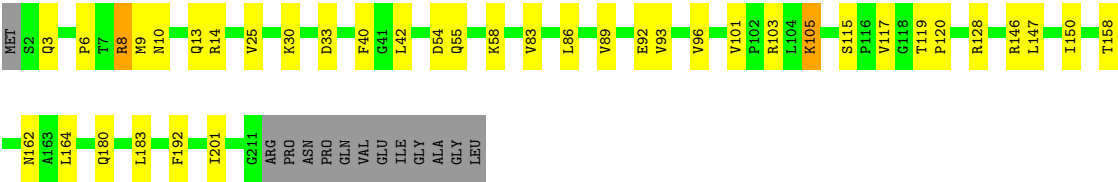


• Molecule 2: V-type ATP synthase beta chain

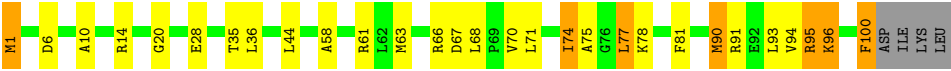




• Molecule 3: V-type ATP synthase subunit D



• Molecule 4: V-type ATP synthase subunit F



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71196	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.37	0/4568	0.48	0/6198
1	B	0.35	0/4568	0.47	0/6198
1	C	0.36	0/4568	0.48	0/6198
2	D	0.36	0/3663	0.48	0/4960
2	E	0.35	0/3663	0.48	0/4960
2	F	0.37	0/3663	0.49	0/4960
3	G	0.29	0/1662	0.44	0/2235
4	H	0.26	0/769	0.50	0/1039
All	All	0.35	0/27124	0.47	0/36748

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
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	419	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4490	61	0
1	B	4472	0	4491	62	0
1	C	4472	0	4491	60	0
2	D	3596	0	3624	42	0
2	E	3596	0	3624	56	0
2	F	3596	0	3624	46	0
3	G	1642	0	1718	24	0
4	H	758	0	764	18	0
5	A	27	0	12	0	0
All	All	26631	0	26838	354	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 7.

All (354) 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:C:576:ALA:O	1:C:577:LEU:CD2	1.80	1.29
1:C:576:ALA:O	1:C:577:LEU:HD22	1.38	1.20
1:C:576:ALA:O	1:C:577:LEU:HD23	1.62	0.98
4:H:94:VAL:HG12	4:H:100:PHE:C	1.92	0.89
1:A:577:LEU:HD23	1:A:577:LEU:H	1.42	0.85
1:C:210:ARG:NH1	1:C:507:CYS:SG	2.51	0.82
1:C:576:ALA:C	1:C:577:LEU:HD23	2.01	0.81
2:E:91:ARG:NH2	2:E:104:PRO:O	2.15	0.80
1:C:401:ARG:NH2	2:F:265:GLU:OE2	2.15	0.79
1:C:576:ALA:C	1:C:577:LEU:CD2	2.50	0.79
2:F:225:ASP:OD1	2:F:225:ASP:N	2.18	0.75
1:B:294:MET:O	1:B:299:ARG:NH1	2.20	0.74
1:A:210:ARG:NH1	1:A:507:CYS:SG	2.60	0.74
1:C:547:ARG:O	1:C:562:TYR:OH	2.04	0.74
1:C:74:GLU:OE2	1:C:113:ARG:NH2	2.22	0.73
1:B:74:GLU:OE1	1:B:113:ARG:NH2	2.23	0.72
1:B:210:ARG:NH1	1:B:494:PHE:O	2.23	0.71
1:B:224:ALA:HB3	1:B:381:VAL:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:NH1	1:C:169:GLU:OE2	2.25	0.68
2:E:274:ARG:NH1	2:E:276:GLU:OE2	2.25	0.68
2:F:318:ASP:N	2:F:318:ASP:OD1	2.25	0.68
1:A:550:ARG:NH1	1:A:562:TYR:OH	2.26	0.68
2:D:406:GLU:OE1	2:D:409:ARG:NH1	2.26	0.68
1:C:234:LYS:HD2	1:C:383:ALA:HB1	1.77	0.67
4:H:63:MET:HG2	4:H:68:LEU:HD12	1.76	0.67
1:C:1:MET:HG2	1:C:2:ILE:HG13	1.75	0.66
1:C:470:LEU:HG	1:C:471:VAL:HG13	1.76	0.66
2:E:374:ASP:OD1	2:E:374:ASP:N	2.30	0.65
1:A:29:LYS:HG2	1:A:36:VAL:HG12	1.78	0.65
1:A:340:ARG:NH2	2:F:276:GLU:OE2	2.30	0.65
2:D:318:ASP:OD1	2:D:318:ASP:N	2.29	0.65
2:F:197:THR:OG1	2:F:198:GLN:N	2.31	0.64
2:E:323:HIS:HB3	2:E:326:PRO:HD2	1.79	0.64
2:D:197:THR:OG1	2:D:198:GLN:N	2.30	0.64
2:F:11:ILE:HG22	2:F:21:VAL:HG12	1.79	0.64
2:E:407:ASN:ND2	2:E:408:ASP:OD1	2.31	0.64
1:B:326:SER:HB3	1:B:329:ARG:HB2	1.79	0.63
3:G:103:ARG:HH21	3:G:146:ARG:HD3	1.62	0.63
1:A:391:MET:O	1:A:397:GLN:NE2	2.30	0.62
1:B:200:ASP:OD1	1:B:200:ASP:N	2.31	0.62
3:G:25:VAL:HG23	3:G:164:LEU:HD23	1.81	0.61
1:B:332:GLU:OE1	1:B:335:ARG:NH1	2.32	0.61
1:A:577:LEU:HD23	1:A:577:LEU:N	2.14	0.61
1:A:467:ILE:HD11	2:D:394:LYS:HG2	1.83	0.61
1:A:370:THR:OG1	1:A:371:LEU:N	2.32	0.60
1:B:207:THR:HG23	1:B:241:LEU:HD13	1.83	0.60
1:B:401:ARG:NH2	2:E:265:GLU:OE2	2.34	0.60
2:F:325:ILE:HB	2:F:326:PRO:HD3	1.82	0.60
1:B:185:HIS:HE1	1:B:193:ARG:HH12	1.50	0.59
1:C:167:THR:OG1	1:C:168:VAL:N	2.32	0.59
1:B:4:GLY:O	1:B:64:VAL:N	2.32	0.59
2:D:325:ILE:HB	2:D:326:PRO:HD3	1.84	0.59
2:F:78:ASP:OD1	2:F:78:ASP:N	2.34	0.59
1:A:210:ARG:NH2	1:A:496:GLN:O	2.36	0.59
1:B:517:LYS:HD3	1:B:563:PHE:HZ	1.68	0.59
1:A:293:ASN:OD1	1:A:293:ASN:N	2.36	0.59
2:D:37:ASP:N	2:D:37:ASP:OD1	2.35	0.59
1:C:393:GLU:HB3	1:C:396:THR:HG22	1.85	0.59
1:A:577:LEU:H	1:A:577:LEU:CD2	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:PRO:HA	1:B:280:PRO:HA	1.85	0.58
4:H:66:ARG:HB3	4:H:68:LEU:HG	1.83	0.58
1:A:504:ASP:OD2	1:A:552:ARG:NH1	2.36	0.58
1:C:127:ASP:OD1	1:C:128:GLU:N	2.32	0.58
2:E:325:ILE:HB	2:E:326:PRO:HD3	1.84	0.58
2:E:405:THR:OG1	2:E:406:GLU:N	2.36	0.58
2:E:150:LEU:HD21	2:E:337:ILE:HD12	1.85	0.58
1:B:260:ASN:ND2	1:B:261:GLU:OE2	2.36	0.58
1:B:252:TYR:HB3	1:B:287:LEU:HD12	1.86	0.58
2:F:154:SER:OG	2:F:155:GLY:N	2.36	0.58
2:E:340:SER:HB2	2:E:353:ASP:HB2	1.85	0.57
1:C:311:GLU:OE2	1:C:364:ARG:NE	2.35	0.57
1:B:336:GLU:OE2	2:D:289:THR:OG1	2.17	0.57
1:A:393:GLU:HG2	1:A:395:VAL:H	1.70	0.57
2:D:455:SER:OG	2:D:457:ASP:OD1	2.16	0.56
2:F:27:LEU:HD23	2:F:75:LEU:HD13	1.86	0.56
2:F:49:GLU:OE1	2:F:274:ARG:NH2	2.38	0.56
4:H:100:PHE:CD2	4:H:100:PHE:N	2.73	0.56
1:A:459:GLN:HG3	2:D:345:ARG:HD2	1.87	0.56
4:H:14:ARG:NH1	4:H:20:GLY:O	2.37	0.56
1:C:315:ASP:HA	1:C:370:THR:HG21	1.86	0.56
2:E:169:ARG:NH1	2:E:207:GLU:OE2	2.38	0.56
2:F:11:ILE:HD13	2:F:11:ILE:H	1.71	0.56
2:F:136:SER:OG	2:F:430:ARG:NH1	2.39	0.56
2:E:154:SER:OG	2:E:155:GLY:N	2.39	0.56
3:G:158:THR:HG22	3:G:162:ASN:HD21	1.70	0.56
2:D:154:SER:OG	2:D:155:GLY:N	2.40	0.55
2:E:51:SER:OG	2:E:52:GLU:N	2.40	0.55
2:F:148:GLN:NE2	2:F:361:LEU:HB2	2.22	0.55
3:G:8:ARG:HD3	3:G:9:MET:H	1.72	0.55
1:A:558:GLU:OE1	1:A:558:GLU:N	2.39	0.54
2:F:318:ASP:O	3:G:3:GLN:NE2	2.35	0.54
1:B:446:ASP:OD1	1:B:446:ASP:N	2.41	0.54
1:C:473:PRO:HA	1:C:476:LEU:HD23	1.88	0.54
2:D:317:PRO:HG3	2:D:323:HIS:CD2	2.42	0.54
1:A:126:GLY:HA2	1:A:156:ARG:HH21	1.73	0.54
2:D:418:PHE:HA	2:D:442:LEU:HD21	1.90	0.53
1:C:400:LEU:O	1:C:401:ARG:HG2	2.08	0.53
2:D:13:TYR:HB3	2:D:20:PHE:HB2	1.90	0.53
2:E:210:ARG:HD2	2:E:211:THR:HG23	1.90	0.53
1:B:270:PRO:HG3	1:B:280:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:THR:OG1	2:E:10:GLY:N	2.42	0.53
1:A:112:ASP:OD1	1:A:113:ARG:N	2.41	0.53
1:A:118:ALA:HB3	1:A:139:PRO:HD2	1.90	0.53
4:H:67:ASP:OD1	4:H:67:ASP:N	2.36	0.53
1:A:468:VAL:HG22	1:A:476:LEU:HD11	1.91	0.52
1:B:547:ARG:O	1:B:562:TYR:OH	2.26	0.52
2:D:457:ASP:OD1	2:D:457:ASP:N	2.35	0.52
2:E:76:VAL:HG12	2:E:77:GLU:HG2	1.91	0.52
1:B:172:VAL:HG13	1:B:173:VAL:HG23	1.91	0.52
2:E:321:ARG:NH1	2:E:338:GLN:OE1	2.43	0.52
2:F:323:HIS:HD2	2:F:325:ILE:H	1.58	0.52
1:B:266:LEU:O	1:B:270:PRO:HG2	2.10	0.52
1:C:201:PRO:HB2	1:C:219:ALA:HB1	1.91	0.52
2:D:180:GLU:HG3	2:D:181:GLY:H	1.73	0.52
1:B:524:LYS:O	1:B:527:GLU:HG3	2.10	0.52
1:B:127:ASP:OD1	1:B:128:GLU:N	2.41	0.51
1:C:83:ILE:HD12	1:C:266:LEU:HD11	1.92	0.51
2:E:86:LYS:HG3	2:E:249:HIS:HD2	1.74	0.51
2:F:156:SER:OG	2:F:341:ARG:NH2	2.43	0.51
2:F:340:SER:HB2	2:F:353:ASP:HB2	1.91	0.51
2:D:115:THR:OG1	2:D:116:GLY:N	2.42	0.51
1:A:400:LEU:O	1:A:401:ARG:HG2	2.10	0.51
2:E:67:ASP:OD1	2:E:68:LEU:N	2.43	0.51
1:C:396:THR:HA	1:C:399:THR:HG22	1.92	0.51
2:F:196:ILE:HD12	2:F:201:LEU:HB2	1.93	0.51
1:A:326:SER:H	1:A:383:ALA:HB3	1.76	0.51
1:C:27:ILE:O	1:C:67:THR:OG1	2.29	0.51
1:A:390:ASP:OD1	1:A:390:ASP:N	2.44	0.51
1:A:9:ILE:HD12	1:A:58:LEU:HB2	1.93	0.51
2:F:148:GLN:HE21	2:F:361:LEU:HB2	1.76	0.51
4:H:14:ARG:HG2	4:H:20:GLY:H	1.75	0.51
1:A:310:ALA:HB2	1:A:322:LEU:HD23	1.93	0.50
1:B:527:GLU:O	1:B:531:LYS:HG2	2.11	0.50
2:E:194:MET:HA	2:E:222:ASN:HB3	1.93	0.50
1:A:172:VAL:HG23	1:A:173:VAL:HG23	1.94	0.50
1:C:474:ASP:OD1	1:C:475:ALA:N	2.43	0.50
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.50
2:E:377:GLN:H	2:E:377:GLN:NE2	2.09	0.50
2:F:194:MET:HA	2:F:222:ASN:HB3	1.93	0.50
1:C:7:GLN:HG3	1:C:17:LYS:HE2	1.94	0.50
1:B:145:HIS:CE1	1:B:316:GLN:HE22	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:321:ARG:NH2	2:E:336:GLN:OE1	2.45	0.50
1:C:246:ASN:O	1:C:246:ASN:ND2	2.45	0.49
1:B:576:ALA:HB3	1:B:577:LEU:HD23	1.94	0.49
1:C:482:LEU:HD22	1:C:530:ILE:HD12	1.93	0.49
2:F:96:ILE:HD13	2:F:98:LYS:HG2	1.95	0.49
1:C:212:LEU:HD21	1:C:422:ILE:HD13	1.94	0.49
1:B:210:ARG:NE	1:B:507:CYS:SG	2.83	0.49
1:B:296:VAL:HG12	1:B:333:ALA:HB1	1.95	0.48
1:B:43:ASP:OD1	1:B:46:THR:OG1	2.28	0.48
1:C:303:ILE:O	1:C:307:VAL:HG23	2.14	0.48
2:D:395:LEU:HD22	3:G:30:LYS:HG2	1.95	0.48
3:G:8:ARG:HG2	3:G:183:LEU:HD21	1.94	0.48
1:A:557:GLU:N	1:A:557:GLU:OE1	2.46	0.48
1:C:12:PRO:HA	1:C:55:THR:HG21	1.96	0.48
2:D:110:LYS:HD3	2:D:112:LEU:HD21	1.94	0.48
1:B:544:VAL:O	1:B:548:ILE:HG23	2.14	0.48
1:C:447:TYR:HB3	1:C:448:PRO:HD3	1.95	0.48
3:G:119:THR:N	3:G:120:PRO:HD3	2.29	0.48
4:H:100:PHE:N	4:H:100:PHE:HD2	2.12	0.48
1:A:257:GLU:HG2	1:A:258:ARG:H	1.79	0.48
1:A:322:LEU:HD13	1:A:323:MET:H	1.79	0.48
1:C:41:ARG:HG2	1:C:42:LEU:H	1.79	0.47
4:H:10:ALA:O	4:H:14:ARG:HG3	2.14	0.47
1:C:532:ARG:HH12	1:C:577:LEU:HA	1.79	0.47
1:B:486:VAL:HG21	1:B:523:TYR:HD1	1.79	0.47
1:A:260:ASN:HA	1:A:263:THR:HG22	1.95	0.47
2:E:120:ASN:ND2	2:E:122:VAL:HG22	2.29	0.47
1:B:239:GLN:HB3	1:B:269:PHE:HZ	1.80	0.47
1:C:97:LYS:HG3	1:C:98:THR:OG1	2.14	0.47
2:D:207:GLU:OE1	2:D:210:ARG:NH2	2.47	0.47
2:F:165:ALA:HB1	2:F:207:GLU:HG2	1.96	0.47
2:E:85:SER:OG	2:E:86:LYS:N	2.47	0.47
2:E:195:GLY:HA3	2:E:262:ASN:HD22	1.78	0.47
4:H:74:ILE:HG23	4:H:75:ALA:H	1.78	0.47
1:B:498:ASN:HD22	1:B:501:HIS:HB2	1.80	0.47
1:C:39:ILE:HG23	1:C:47:ALA:HB1	1.97	0.47
2:F:34:ASP:OD1	2:F:34:ASP:N	2.48	0.47
1:C:326:SER:HB3	1:C:329:ARG:HD2	1.95	0.47
2:E:175:PRO:HG2	2:E:182:GLU:HG3	1.97	0.47
2:D:37:ASP:OD2	2:D:43:ARG:NH1	2.48	0.47
1:C:241:LEU:HB2	1:C:323:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:SER:HB2	2:D:353:ASP:HB2	1.98	0.46
2:E:11:ILE:HG22	2:E:21:VAL:HG22	1.97	0.46
2:F:155:GLY:HA3	2:F:158:LEU:HD12	1.96	0.46
2:D:373:GLU:OE1	2:D:373:GLU:N	2.47	0.46
1:B:117:TRP:HB3	1:B:138:VAL:HG21	1.97	0.46
1:B:391:MET:SD	1:B:391:MET:N	2.88	0.46
4:H:90:MET:O	4:H:94:VAL:HG22	2.16	0.46
3:G:42:LEU:HD22	3:G:150:ILE:HD12	1.96	0.46
1:B:269:PHE:CD2	1:B:281:LEU:HD23	2.50	0.46
1:C:41:ARG:HG2	1:C:42:LEU:N	2.31	0.46
2:D:229:ILE:H	2:D:229:ILE:HD12	1.80	0.46
2:D:60:PHE:HD1	2:D:229:ILE:HD13	1.80	0.46
4:H:1:MET:SD	4:H:1:MET:N	2.70	0.46
2:D:263:TYR:OH	2:D:290:ASP:OD1	2.30	0.46
1:B:390:ASP:OD1	1:B:390:ASP:N	2.49	0.45
2:E:353:ASP:O	2:E:356:PRO:HD2	2.16	0.45
2:F:392:ILE:HG22	2:F:412:LEU:HD23	1.98	0.45
1:A:464:LEU:HB3	1:A:484:ILE:HD11	1.98	0.45
1:C:172:VAL:HG23	1:C:173:VAL:HG23	1.98	0.45
1:C:322:LEU:HD23	1:C:323:MET:N	2.31	0.45
2:D:8:TYR:OH	2:D:26:ASP:HB3	2.16	0.45
2:D:250:ASP:N	2:D:250:ASP:OD1	2.50	0.45
1:A:418:HIS:CD2	1:A:496:GLN:HE21	2.34	0.45
1:B:185:HIS:CE1	1:B:193:ARG:HH12	2.32	0.45
2:E:450:GLU:O	2:E:452:LYS:HD3	2.16	0.45
2:F:222:ASN:O	2:F:222:ASN:ND2	2.43	0.45
2:F:318:ASP:HB2	3:G:3:GLN:NE2	2.32	0.45
1:A:154:ARG:HE	1:A:154:ARG:HB3	1.59	0.45
1:B:274:ASP:O	1:B:276:LYS:N	2.50	0.45
2:E:399:ILE:HG13	2:E:400:GLY:H	1.80	0.45
4:H:77:LEU:HD13	4:H:78:LYS:H	1.81	0.45
2:F:334:GLU:HA	2:F:360:ARG:HH11	1.82	0.45
2:F:396:VAL:HG22	2:F:404:LEU:HD11	1.99	0.45
3:G:93:VAL:HG13	3:G:103:ARG:H	1.82	0.45
3:G:105:LYS:HE2	3:G:105:LYS:HB3	1.73	0.45
2:E:60:PHE:CE1	2:E:229:ILE:HG12	2.53	0.44
2:E:372:ARG:NH1	2:E:374:ASP:OD2	2.50	0.44
3:G:8:ARG:C	3:G:10:ASN:H	2.20	0.44
4:H:58:ALA:HA	4:H:61:ARG:HD2	1.99	0.44
1:A:8:LYS:NZ	2:F:49:GLU:OE2	2.40	0.44
1:A:30:VAL:HG22	1:A:35:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:GLU:O	1:C:484:ILE:HG12	2.17	0.44
2:E:61:GLU:HG3	2:E:227:PRO:HG3	1.99	0.44
1:B:402:ILE:HD13	1:B:402:ILE:HA	1.80	0.44
1:B:520:LEU:HD12	1:B:520:LEU:HA	1.69	0.44
3:G:158:THR:O	3:G:162:ASN:ND2	2.51	0.44
1:A:486:VAL:HG21	1:A:523:TYR:HD1	1.82	0.44
2:D:244:TYR:O	2:D:248:GLU:HB2	2.17	0.44
1:A:316:GLN:HE21	1:A:316:GLN:HB2	1.54	0.44
1:B:576:ALA:C	1:B:577:LEU:HD23	2.39	0.44
1:C:413:LEU:HD22	1:C:418:HIS:CD2	2.53	0.43
1:C:413:LEU:HD22	1:C:418:HIS:HD2	1.83	0.43
2:E:84:VAL:HA	2:E:88:MET:HE1	2.00	0.43
2:E:138:ILE:HG12	2:E:337:ILE:HD13	1.99	0.43
1:A:248:ASP:OD1	1:A:276:LYS:NZ	2.51	0.43
1:B:81:ASN:HD22	1:B:282:MET:HB3	1.83	0.43
1:B:152:ASP:OD1	1:B:152:ASP:N	2.51	0.43
2:E:91:ARG:HG3	2:E:92:ARG:H	1.83	0.43
1:A:294:MET:HB3	1:A:295:PRO:HD2	2.00	0.43
1:B:198:LYS:HA	1:B:368:VAL:HG23	2.00	0.43
1:B:241:LEU:O	1:B:245:SER:HB3	2.18	0.43
1:C:161:LYS:HG2	1:C:172:VAL:HA	2.00	0.43
2:D:174:ARG:NH2	2:D:433:GLU:OE1	2.46	0.43
3:G:58:LYS:HG2	4:H:78:LYS:HG3	2.00	0.43
1:B:212:LEU:HD22	1:B:407:TRP:CE2	2.53	0.43
2:E:151:PRO:HG2	2:E:336:GLN:HB2	2.00	0.43
2:F:301:VAL:HG23	2:F:304:LYS:HB2	2.01	0.43
1:A:59:LYS:N	1:A:62:GLU:OE2	2.51	0.43
1:A:464:LEU:HD13	1:A:464:LEU:HA	1.71	0.43
1:C:348:GLU:OE2	2:E:280:ARG:NH2	2.34	0.43
1:C:465:GLN:HA	1:C:468:VAL:HB	2.00	0.43
2:E:152:ILE:HB	2:E:313:ILE:HG13	2.01	0.43
2:E:232:ILE:HD12	2:E:270:ILE:HD12	2.00	0.43
2:D:292:ALA:HB2	2:D:332:ILE:HD13	2.01	0.43
2:E:26:ASP:N	2:E:26:ASP:OD1	2.52	0.43
2:F:341:ARG:O	2:F:345:ARG:HG2	2.19	0.43
4:H:96:LYS:HD3	4:H:96:LYS:HA	1.83	0.43
1:C:209:MET:HA	1:C:497:GLN:HE22	1.83	0.43
2:F:305:LYS:HE2	2:F:305:LYS:HB3	1.69	0.43
3:G:96:VAL:HG12	3:G:101:VAL:O	2.19	0.43
1:A:14:VAL:HG22	1:A:49:VAL:HB	2.01	0.43
2:E:218:VAL:HG12	2:E:219:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:ILE:HG12	2:F:19:LEU:HD13	2.01	0.43
1:A:393:GLU:OE1	1:A:396:THR:OG1	2.37	0.42
2:D:355:LEU:HD21	2:D:386:TYR:HD2	1.83	0.42
2:E:6:LYS:O	2:E:6:LYS:HG2	2.18	0.42
3:G:40:PHE:HD1	3:G:40:PHE:HA	1.72	0.42
1:A:498:ASN:ND2	1:A:501:HIS:HB2	2.34	0.42
1:B:406:PHE:CE2	1:B:408:ARG:HG2	2.54	0.42
4:H:95:ARG:HD3	4:H:95:ARG:HA	1.62	0.42
1:C:314:ARG:HD2	1:C:368:VAL:HG12	2.02	0.42
2:D:8:TYR:HB2	2:D:73:VAL:O	2.19	0.42
2:F:260:MET:HE1	2:F:294:ILE:HD11	2.01	0.42
1:B:3:GLN:HG2	1:B:65:VAL:HG22	2.01	0.42
2:D:396:VAL:CG2	2:D:404:LEU:HD11	2.50	0.42
2:E:120:ASN:HD22	2:E:122:VAL:H	1.66	0.42
2:D:194:MET:HA	2:D:222:ASN:HB3	2.00	0.42
1:A:311:GLU:HG2	1:A:314:ARG:NH1	2.35	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.78	0.42
1:A:573:ALA:O	1:A:577:LEU:CD2	2.67	0.42
2:E:175:PRO:HB2	2:E:182:GLU:HA	2.00	0.42
1:A:27:ILE:HD11	1:A:71:LEU:HB2	2.00	0.42
1:A:401:ARG:HD3	2:D:262:ASN:ND2	2.34	0.42
1:B:167:THR:OG1	1:B:168:VAL:N	2.52	0.42
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.86	0.42
1:C:141:PHE:CG	1:C:283:HIS:HD2	2.38	0.42
2:E:399:ILE:HG13	2:E:400:GLY:N	2.35	0.42
1:B:477:GLN:HE21	1:B:477:GLN:HB2	1.59	0.42
2:D:22:GLU:HG2	2:D:23:ASN:H	1.84	0.42
3:G:6:PRO:O	3:G:10:ASN:ND2	2.53	0.42
1:A:207:THR:O	1:A:207:THR:OG1	2.35	0.41
1:A:574:PHE:HA	1:A:577:LEU:HD21	2.01	0.41
1:C:406:PHE:CE2	1:C:408:ARG:HB2	2.56	0.41
3:G:42:LEU:HB3	3:G:147:LEU:HD13	2.01	0.41
1:A:241:LEU:O	1:A:245:SER:HB3	2.19	0.41
1:C:394:PRO:O	1:C:398:SER:OG	2.32	0.41
2:D:389:GLY:HA3	2:D:415:ALA:HB2	2.02	0.41
3:G:103:ARG:NH2	3:G:146:ARG:HB2	2.35	0.41
1:A:410:ASP:OD1	1:A:411:ALA:N	2.53	0.41
2:D:261:THR:O	2:D:265:GLU:HG2	2.20	0.41
2:F:86:LYS:HD2	2:F:249:HIS:CD2	2.55	0.41
1:C:256:GLY:HA3	1:C:329:ARG:HG2	2.03	0.41
2:E:377:GLN:H	2:E:377:GLN:HE21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ILE:H	2:F:96:ILE:HG13	1.43	0.41
2:F:267:LEU:HD12	2:F:267:LEU:HA	1.82	0.41
3:G:14:ARG:HD3	3:G:14:ARG:HA	1.80	0.41
2:D:374:ASP:OD1	2:D:374:ASP:N	2.33	0.41
3:G:180:GLN:HE21	3:G:180:GLN:HB2	1.69	0.41
1:B:447:TYR:HB3	1:B:448:PRO:HD3	2.03	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.41
1:C:576:ALA:C	1:C:577:LEU:HD22	2.21	0.41
2:F:146:ARG:HD2	2:F:252:HIS:HD2	1.86	0.41
1:A:145:HIS:ND1	1:A:146:LYS:O	2.53	0.41
1:A:539:ILE:HG23	1:A:574:PHE:HZ	1.84	0.41
1:B:182:LYS:HE3	1:B:182:LYS:HB2	1.93	0.41
1:C:50:GLN:O	1:C:50:GLN:HG3	2.21	0.41
2:F:8:TYR:HB2	2:F:73:VAL:O	2.21	0.41
1:C:574:PHE:HD1	1:C:574:PHE:HA	1.72	0.41
2:E:23:ASN:ND2	2:E:23:ASN:O	2.54	0.41
2:E:453:ARG:HH11	2:E:453:ARG:HB2	1.86	0.41
1:A:402:ILE:HG23	1:A:403:VAL:HG13	2.03	0.41
1:B:6:ILE:HG23	1:B:14:VAL:HG13	2.03	0.41
2:E:201:LEU:HD11	2:E:221:LEU:HD13	2.02	0.41
2:E:207:GLU:CD	2:E:210:ARG:HH12	2.24	0.41
2:E:277:ILE:HG12	3:G:192:PHE:CZ	2.55	0.41
2:F:48:ILE:HD11	2:F:58:GLN:NE2	2.36	0.41
2:F:57:ILE:HG22	2:F:58:GLN:H	1.86	0.41
1:A:54:ASP:O	1:A:55:THR:OG1	2.30	0.41
1:A:195:VAL:HG11	1:A:368:VAL:HG21	2.03	0.41
1:B:21:GLY:HA2	2:E:67:ASP:OD2	2.21	0.40
2:D:355:LEU:HB2	2:D:356:PRO:HD3	2.03	0.40
2:D:462:TYR:O	2:D:463:TYR:HB3	2.21	0.40
1:B:348:GLU:HG3	1:B:394:PRO:HD3	2.04	0.40
2:F:376:LYS:H	2:F:376:LYS:HG2	1.70	0.40
4:H:91:ARG:HA	4:H:91:ARG:HD3	1.74	0.40
1:A:262:MET:HE2	1:A:262:MET:HB2	1.96	0.40
2:D:67:ASP:OD1	2:D:67:ASP:N	2.54	0.40
2:E:395:LEU:O	2:E:399:ILE:HG12	2.21	0.40
2:F:443:LEU:HD23	2:F:443:LEU:HA	1.91	0.40
3:G:158:THR:HG22	3:G:162:ASN:ND2	2.36	0.40
1:A:255:CYS:SG	1:A:299:ARG:HB3	2.62	0.40
1:B:243:LYS:HD2	1:B:244:TRP:CZ3	2.57	0.40
1:B:572:GLY:O	1:B:575:LYS:HG2	2.21	0.40
1:C:344:MET:HG2	1:C:345:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:ILE:HD13	2:E:398:ILE:HA	1.90	0.40
1:A:9:ILE:CD1	1:A:58:LEU:HB2	2.51	0.40
1:B:141:PHE:HE2	1:B:283:HIS:CD2	2.39	0.40
1:C:237:THR:O	1:C:241:LEU:HG	2.21	0.40
1:C:365:ALA:HB2	1:C:380:ILE:HD12	2.03	0.40
1:C:458:LEU:HD21	1:C:490:ILE:HG21	2.02	0.40
2:E:153:PHE:CE2	2:E:336:GLN:HG3	2.56	0.40
2:F:321:ARG:HE	2:F:321:ARG:HB3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/578 (100%)	515 (90%)	60 (10%)	0	100	100
1	B	575/578 (100%)	517 (90%)	58 (10%)	0	100	100
1	C	575/578 (100%)	516 (90%)	58 (10%)	1 (0%)	44	75
2	D	457/478 (96%)	407 (89%)	50 (11%)	0	100	100
2	E	457/478 (96%)	401 (88%)	56 (12%)	0	100	100
2	F	457/478 (96%)	400 (88%)	57 (12%)	0	100	100
3	G	208/223 (93%)	190 (91%)	18 (9%)	0	100	100
4	H	98/104 (94%)	78 (80%)	20 (20%)	0	100	100
All	All	3402/3495 (97%)	3024 (89%)	377 (11%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	420	PRO

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	468/468 (100%)	421 (90%)	47 (10%)	6	26
1	B	468/468 (100%)	418 (89%)	50 (11%)	5	24
1	C	468/468 (100%)	427 (91%)	41 (9%)	8	31
2	D	386/401 (96%)	354 (92%)	32 (8%)	9	32
2	E	386/401 (96%)	341 (88%)	45 (12%)	4	21
2	F	386/401 (96%)	339 (88%)	47 (12%)	4	20
3	G	166/176 (94%)	152 (92%)	14 (8%)	9	32
4	H	76/80 (95%)	60 (79%)	16 (21%)	1	5
All	All	2804/2863 (98%)	2512 (90%)	292 (10%)	8	25

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	24	MET
1	A	30	VAL
1	A	65	VAL
1	A	83	ILE
1	A	88	GLN
1	A	93	ARG
1	A	95	ARG
1	A	123	VAL
1	A	124	LYS
1	A	157	VAL
1	A	191	ARG
1	A	203	THR
1	A	207	THR
1	A	211	ILE
1	A	215	LEU
1	A	223	THR
1	A	244	TRP
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	274	ASP
1	A	281	LEU
1	A	282	MET
1	A	293	ASN
1	A	316	GLN
1	A	322	LEU
1	A	329	ARG
1	A	353	TYR
1	A	354	LEU
1	A	368	VAL
1	A	370	THR
1	A	425	ASN
1	A	456	GLU
1	A	464	LEU
1	A	466	GLU
1	A	469	GLN
1	A	524	LYS
1	A	530	ILE
1	A	531	LYS
1	A	536	ILE
1	A	540	LEU
1	A	541	GLN
1	A	545	LEU
1	A	547	ARG
1	A	550	ARG
1	A	574	PHE
1	A	575	LYS
1	A	577	LEU
1	B	30	VAL
1	B	60	VAL
1	B	80	LEU
1	B	88	GLN
1	B	96	GLU
1	B	107	VAL
1	B	123	VAL
1	B	138	VAL
1	B	143	PHE
1	B	152	ASP
1	B	153	VAL
1	B	172	VAL
1	B	200	ASP
1	B	218	VAL

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Mol	Chain	Res	Type
1	B	223	THR
1	B	230	PHE
1	B	244	TRP
1	B	255	CYS
1	B	260	ASN
1	B	263	THR
1	B	272	LEU
1	B	282	MET
1	B	284	ARG
1	B	285	THR
1	B	296	VAL
1	B	315	ASP
1	B	319	SER
1	B	322	LEU
1	B	329	ARG
1	B	354	LEU
1	B	368	VAL
1	B	369	ILE
1	B	379	THR
1	B	402	ILE
1	B	446	ASP
1	B	450	LEU
1	B	469	GLN
1	B	476	LEU
1	B	477	GLN
1	B	503	VAL
1	B	509	MET
1	B	520	LEU
1	B	524	LYS
1	B	546	GLU
1	B	548	ILE
1	B	554	VAL
1	B	557	GLU
1	B	565	GLU
1	B	574	PHE
1	B	577	LEU
1	C	20	LEU
1	C	26	ASP
1	C	50	GLN
1	C	83	ILE
1	C	95	ARG
1	C	96	GLU

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Mol	Chain	Res	Type
1	C	103	THR
1	C	116	LYS
1	C	134	VAL
1	C	141	PHE
1	C	145	HIS
1	C	152	ASP
1	C	167	THR
1	C	186	THR
1	C	200	ASP
1	C	207	THR
1	C	211	ILE
1	C	244	TRP
1	C	248	ASP
1	C	249	VAL
1	C	266	LEU
1	C	282	MET
1	C	284	ARG
1	C	293	ASN
1	C	315	ASP
1	C	320	VAL
1	C	329	ARG
1	C	337	ILE
1	C	340	ARG
1	C	354	LEU
1	C	363	GLU
1	C	368	VAL
1	C	379	THR
1	C	396	THR
1	C	461	GLU
1	C	478	ASP
1	C	520	LEU
1	C	538	GLU
1	C	568	LYS
1	C	574	PHE
1	C	577	LEU
2	D	7	GLU
2	D	25	LYS
2	D	37	ASP
2	D	94	ASN
2	D	130	PHE
2	D	131	ILE
2	D	143	THR

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Mol	Chain	Res	Type
2	D	183	LYS
2	D	189	VAL
2	D	194	MET
2	D	197	THR
2	D	214	LEU
2	D	216	ARG
2	D	294	ILE
2	D	309	THR
2	D	315	SER
2	D	318	ASP
2	D	322	THR
2	D	327	ASP
2	D	331	TYR
2	D	368	LYS
2	D	370	LYS
2	D	379	SER
2	D	381	GLN
2	D	390	VAL
2	D	398	ILE
2	D	399	ILE
2	D	401	GLU
2	D	424	ASN
2	D	425	GLN
2	D	429	ASN
2	D	457	ASP
2	E	7	GLU
2	E	26	ASP
2	E	43	ARG
2	E	73	VAL
2	E	81	ARG
2	E	82	LEU
2	E	89	LEU
2	E	94	ASN
2	E	98	LYS
2	E	100	ILE
2	E	111	ARG
2	E	120	ASN
2	E	130	PHE
2	E	131	ILE
2	E	133	THR
2	E	137	THR
2	E	143	THR

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Mol	Chain	Res	Type
2	E	148	GLN
2	E	150	LEU
2	E	180	GLU
2	E	183	LYS
2	E	194	MET
2	E	206	GLN
2	E	257	LEU
2	E	258	THR
2	E	270	ILE
2	E	274	ARG
2	E	290	ASP
2	E	294	ILE
2	E	304	LYS
2	E	327	ASP
2	E	336	GLN
2	E	355	LEU
2	E	372	ARG
2	E	374	ASP
2	E	377	GLN
2	E	379	SER
2	E	384	SER
2	E	405	THR
2	E	413	GLN
2	E	427	GLN
2	E	437	GLN
2	E	452	LYS
2	E	453	ARG
2	E	459	ILE
2	F	9	THR
2	F	11	ILE
2	F	26	ASP
2	F	37	ASP
2	F	53	GLU
2	F	54	TYR
2	F	63	THR
2	F	73	VAL
2	F	78	ASP
2	F	79	VAL
2	F	96	ILE
2	F	111	ARG
2	F	112	LEU
2	F	126	LYS

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Mol	Chain	Res	Type
2	F	128	GLU
2	F	131	ILE
2	F	133	THR
2	F	137	THR
2	F	141	MET
2	F	148	GLN
2	F	150	LEU
2	F	172	THR
2	F	180	GLU
2	F	182	GLU
2	F	183	LYS
2	F	187	PHE
2	F	197	THR
2	F	206	GLN
2	F	222	ASN
2	F	225	ASP
2	F	232	ILE
2	F	254	LEU
2	F	257	LEU
2	F	259	ASP
2	F	270	ILE
2	F	290	ASP
2	F	294	ILE
2	F	309	THR
2	F	315	SER
2	F	318	ASP
2	F	343	LEU
2	F	376	LYS
2	F	393	ARG
2	F	405	THR
2	F	412	LEU
2	F	429	ASN
2	F	459	ILE
3	G	8	ARG
3	G	13	GLN
3	G	33	ASP
3	G	54	ASP
3	G	55	GLN
3	G	83	VAL
3	G	86	LEU
3	G	89	VAL
3	G	92	GLU

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Mol	Chain	Res	Type
3	G	105	LYS
3	G	115	SER
3	G	117	VAL
3	G	128	ARG
3	G	201	ILE
4	H	1	MET
4	H	6	ASP
4	H	28	GLU
4	H	35	THR
4	H	36	LEU
4	H	44	LEU
4	H	70	VAL
4	H	71	LEU
4	H	74	ILE
4	H	77	LEU
4	H	81	PHE
4	H	90	MET
4	H	93	LEU
4	H	95	ARG
4	H	96	LYS
4	H	100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	81	ASN
1	A	88	GLN
1	A	196	GLN
1	A	425	ASN
1	A	469	GLN
1	A	496	GLN
1	A	571	GLN
1	B	3	GLN
1	B	7	GLN
1	B	50	GLN
1	B	81	ASN
1	B	88	GLN
1	B	185	HIS
1	B	202	ASN
1	B	316	GLN
1	B	418	HIS

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Mol	Chain	Res	Type
1	B	477	GLN
1	B	496	GLN
1	B	498	ASN
1	C	50	GLN
1	C	238	GLN
1	C	283	HIS
1	C	316	GLN
1	C	469	GLN
1	C	496	GLN
1	C	497	GLN
2	D	94	ASN
2	D	142	ASN
2	D	148	GLN
2	D	170	GLN
2	D	206	GLN
2	D	249	HIS
2	D	252	HIS
2	D	262	ASN
2	D	310	GLN
2	D	407	ASN
2	D	413	GLN
2	D	424	ASN
2	D	425	GLN
2	E	23	ASN
2	E	120	ASN
2	E	142	ASN
2	E	148	GLN
2	E	252	HIS
2	E	323	HIS
2	E	363	ASN
2	E	377	GLN
2	E	407	ASN
2	E	427	GLN
2	E	437	GLN
2	E	448	GLN
2	F	46	GLN
2	F	58	GLN
2	F	129	GLN
2	F	142	ASN
2	F	148	GLN
2	F	166	GLN
2	F	252	HIS

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Mol	Chain	Res	Type
2	F	310	GLN
2	F	323	HIS
2	F	363	ASN
2	F	388	ASN
2	F	413	GLN
2	F	429	ASN
2	F	448	GLN
3	G	10	ASN
3	G	13	GLN
3	G	17	GLN
3	G	55	GLN
3	G	95	ASN
3	G	162	ASN
3	G	180	GLN
4	H	11	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	A	600	1	24,29,29	0.95	1 (4%)	29,45,45	1.45	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	1	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ADP	C5-C4	2.40	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ADP	C3'-C2'-C1'	3.37	106.05	100.98
5	A	600	ADP	N3-C2-N1	-3.19	123.69	128.68
5	A	600	ADP	PA-O3A-PB	-3.05	122.35	132.83
5	A	600	ADP	C4-C5-N7	-2.24	107.07	109.40
5	A	600	ADP	C2'-C3'-C4'	2.05	106.62	102.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

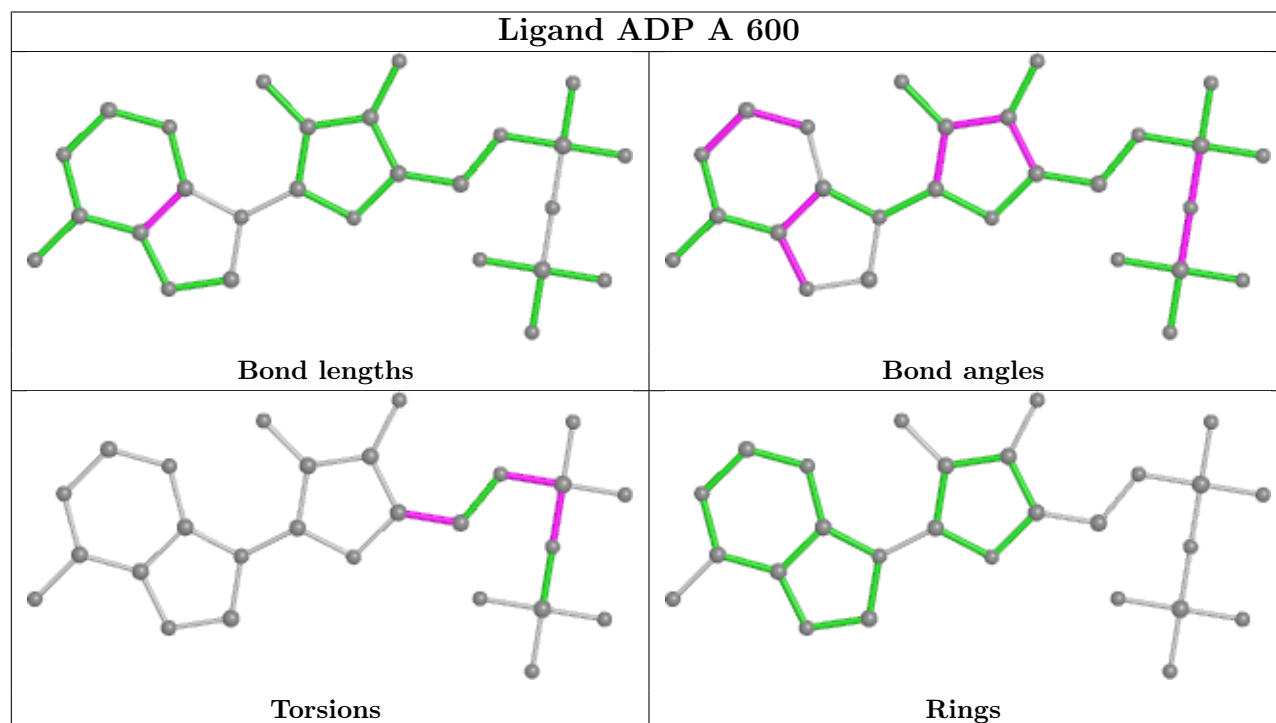
Mol	Chain	Res	Type	Atoms
5	A	600	ADP	O4'-C4'-C5'-O5'
5	A	600	ADP	C3'-C4'-C5'-O5'
5	A	600	ADP	PB-O3A-PA-O1A
5	A	600	ADP	PB-O3A-PA-O2A
5	A	600	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30014. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.