



Full wwPDB EM Model Validation Report ⓘ

Mar 12, 2020 – 09:44 AM EDT

PDB ID : 6PB4
EMDB ID : EMD-20286
Title : The E. coli class-II CAP-dependent transcription activation complex with de novo RNA transcript at the state 2
Authors : Liu, B.; Shi, W.
Deposited on : 2019-06-13
Resolution : 4.35 Å(reported)

This is a Full wwPDB EM 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

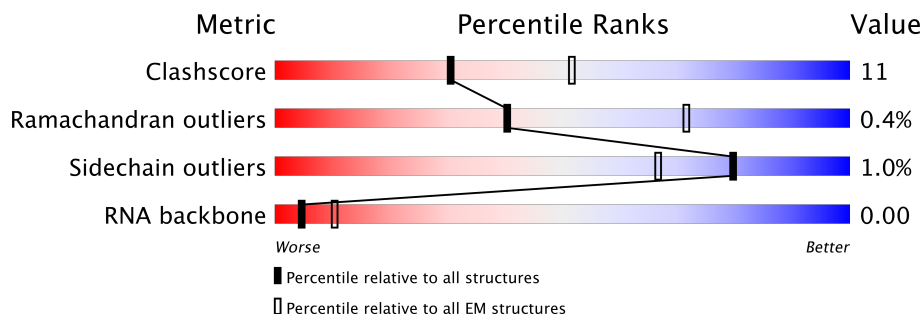
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.35 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 on 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	329	54% 15% 30%
1	B	329	54% 15% 31%
2	C	1342	69% 30% .
3	D	1407	69% 25% . 5%
4	E	91	70% 16% 13%
5	F	628	55% 20% . 23%
6	G	210	71% 22% 6%

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Mol	Chain	Length	Quality of chain
6	H	210	<div><div></div><div>71%</div><div>21%</div><div>6%</div></div>
7	1	78	<div><div></div><div>76%</div><div>23%</div><div></div></div>
8	2	78	<div><div></div><div>76%</div><div>24%</div><div></div></div>
9	3	3	<div><div></div><div>67%</div><div>33%</div><div></div></div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 69953 atoms, of which 34440 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
1	B	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1340	Total	C	H	N	O	S	0	0
			21151	6631	10581	1841	2055	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1337	Total	C	H	N	O	S	0	0
			21012	6531	10616	1853	1962	50		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	79	Total	C	H	N	O	S	0	0
			1261	382	634	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	483	Total	C	H	N	O	S	0	0
			7918	2455	3990	704	746	23		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a protein called cAMP-activated global transcriptional regulator CRP.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	197	Total	C	H	N	O	S	0	0
			3156	986	1600	273	288	9		
6	H	197	Total	C	H	N	O	S	0	0
			3156	986	1600	273	288	9		

- Molecule 7 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	1	78	Total	C	H	N	O	P	0	0
			2481	765	890	264	484	78		

- Molecule 8 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	78	Total	C	H	N	O	P	0	0
			2485	767	873	313	454	78		

- Molecule 9 is a RNA chain called Nascent RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	3	Total	C	H	N	O	P	0	0
			109	30	32	15	27	5		

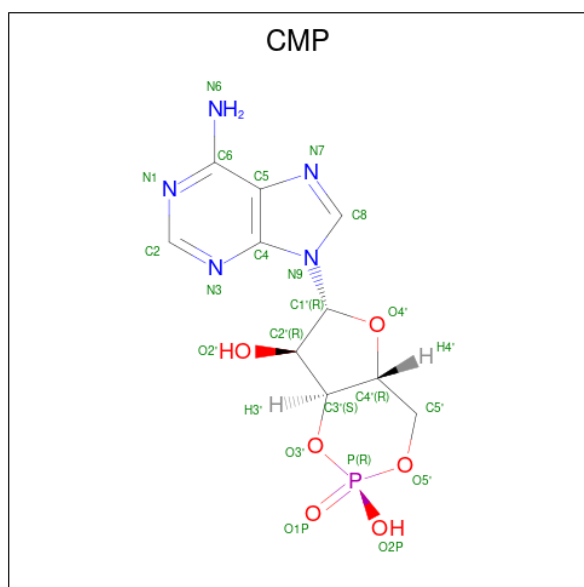
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P) (labeled as "Ligand of Interest" by author).

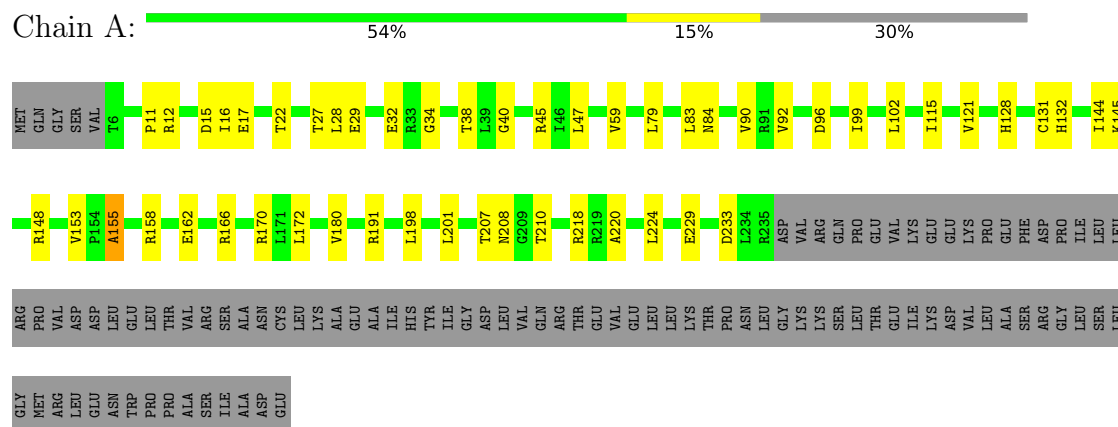


Mol	Chain	Residues	Atoms					AltConf	
12	G	1	Total 33	C 10	H 11	N 5	O 6	P 1	0
12	H	1	Total 33	C 10	H 11	N 5	O 6	P 1	0

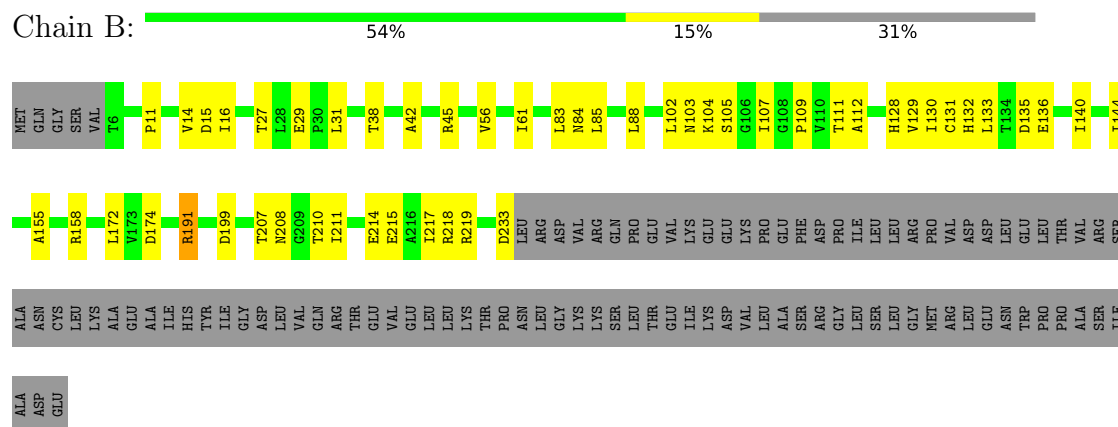
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

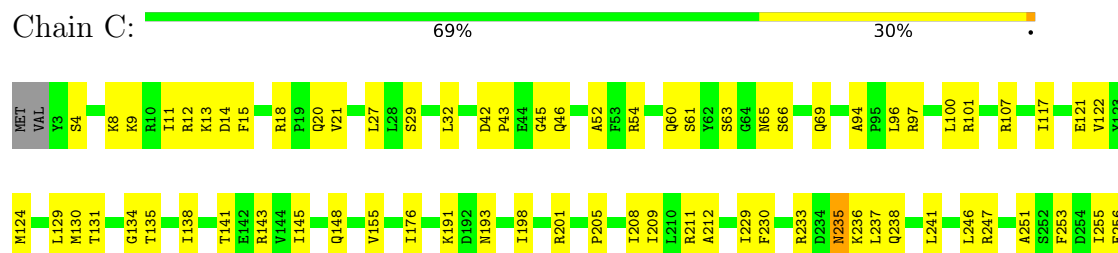
- Molecule 1: DNA-directed RNA polymerase subunit alpha

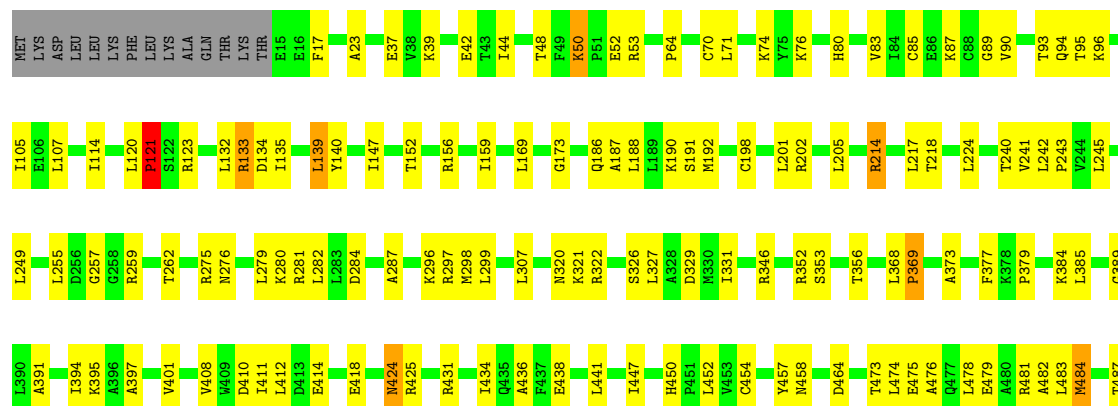


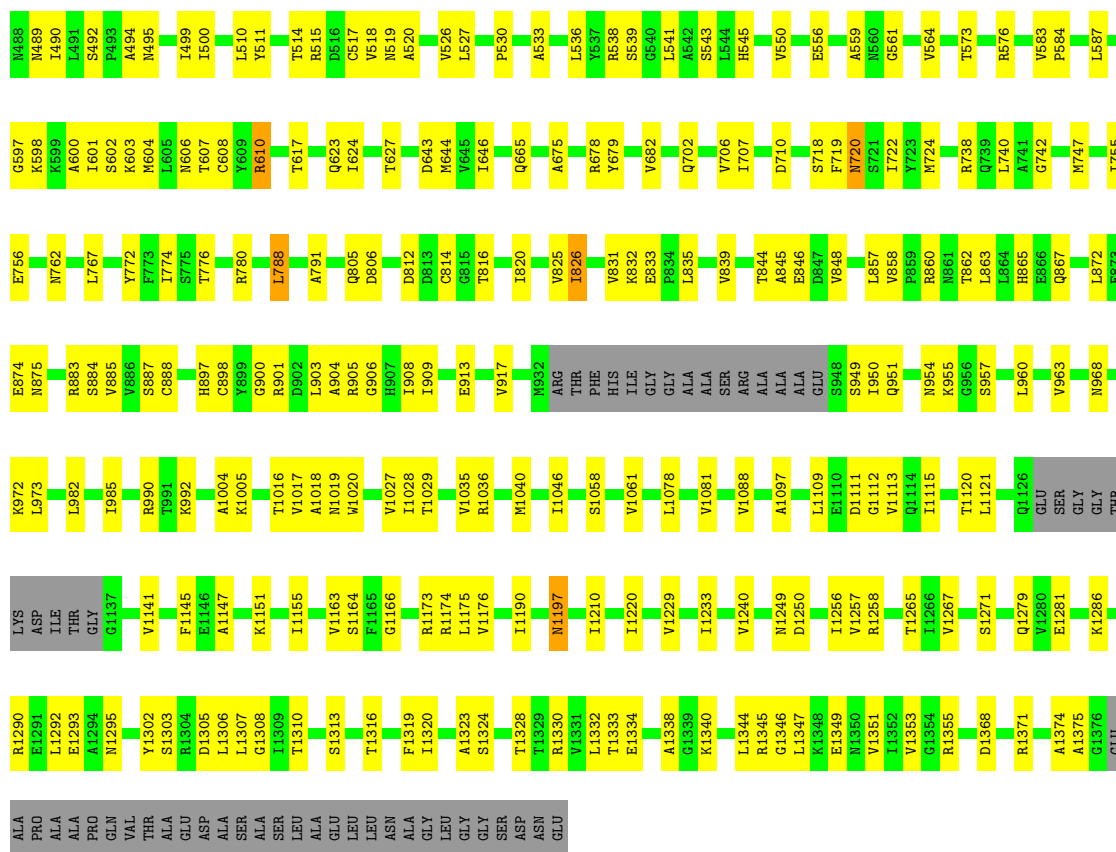
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta







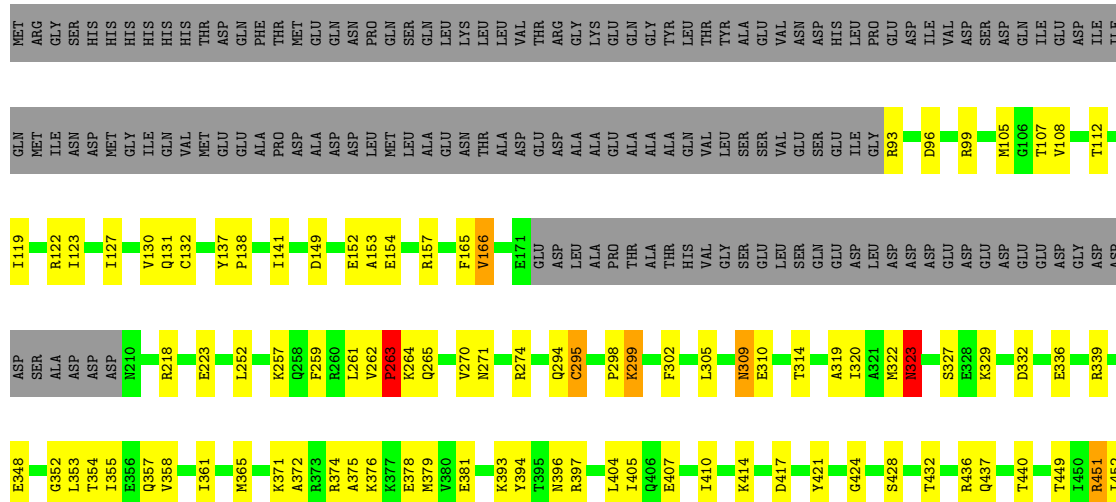
- Molecule 4: DNA-directed RNA polymerase subunit omega

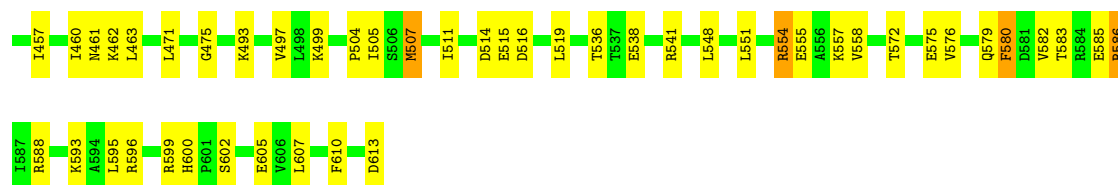
Chain E: 70% 16% 13%



- Molecule 5: RNA polymerase sigma factor RpoD

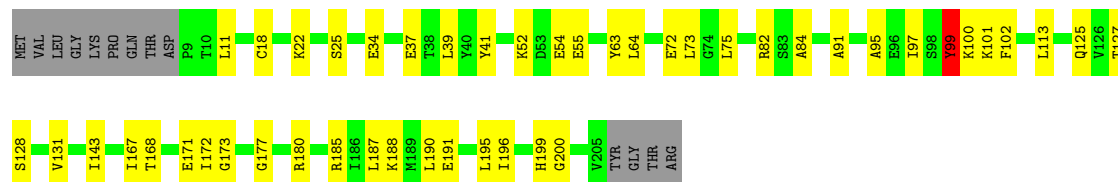
Chain F: 55% 20% 23%





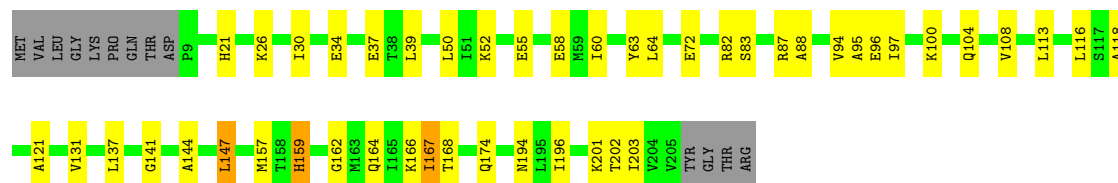
- Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain G: 71% 22% 6%



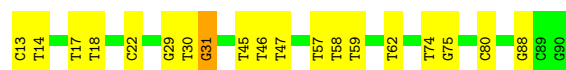
- Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain H: 71% 21% 6%



- Molecule 7: SYNTHETIC NONTEMPLATE STRAND DNA (78-MER)

Chain 1: 76% 23% 1%



- Molecule 8: SYNTHETIC TEMPLATE STRAND DNA (78-MER)

Chain 2: 76% 24% 0%



- Molecule 9: Nascent RNA

Chain 3: 67% 33% 0%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	33455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, MG, CMP

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	0.45	0/1808	0.69	0/2450
1	B	0.42	0/1789	0.71	0/2425
2	C	0.52	0/10739	0.70	2/14489 (0.0%)
3	D	0.49	0/10553	0.71	2/14248 (0.0%)
4	E	0.33	0/629	0.61	0/847
5	F	0.44	0/3982	0.70	1/5354 (0.0%)
6	G	0.40	0/1580	0.67	1/2127 (0.0%)
6	H	0.38	0/1580	0.66	0/2127
7	1	1.04	1/1777 (0.1%)	1.24	4/2741 (0.1%)
8	2	1.02	2/1815 (0.1%)	1.09	7/2800 (0.2%)
9	3	0.83	0/50	1.42	0/76
All	All	0.56	3/36302 (0.0%)	0.77	17/49684 (0.0%)

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	A	0	3
1	B	0	2
2	C	0	9
3	D	0	17
5	F	0	10
6	G	0	2
6	H	0	2
All	All	0	45

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	47	DT	C3'-O3'	6.44	1.52	1.44
8	2	42	DG	C3'-O3'	5.68	1.51	1.44
8	2	34	DA	C3'-O3'	5.41	1.50	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	332	ASP	CB-CG-OD1	7.01	124.61	118.30
3	D	710	ASP	CB-CG-OD1	6.71	124.34	118.30
7	1	31	DG	O4'-C1'-N9	6.65	112.66	108.00
8	2	41	DC	P-O3'-C3'	6.47	127.47	119.70
8	2	42	DG	P-O3'-C3'	5.88	126.76	119.70
8	2	47	DA	C4'-C3'-C2'	-5.69	97.98	103.10
3	D	352	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	C	944	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	C	107	ARG	NE-CZ-NH1	5.35	122.98	120.30
8	2	39	DT	O4'-C1'-N1	5.32	111.72	108.00
7	1	47	DT	P-O3'-C3'	5.30	126.06	119.70
7	1	57	DT	N3-C4-O4	5.30	123.08	119.90
8	2	41	DC	OP2-P-O3'	5.21	116.67	105.20
6	G	180	ARG	NE-CZ-NH1	5.21	122.90	120.30
8	2	50	DT	N3-C4-O4	5.20	123.02	119.90
8	2	66	DT	N3-C4-O4	5.03	122.92	119.90
7	1	62	DT	N3-C4-O4	5.02	122.91	119.90

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	VAL	Peptide
1	A	155	ALA	Peptide
1	A	191	ARG	Peptide
1	B	109	PRO	Peptide
1	B	191	ARG	Peptide
2	C	1004	ASP	Peptide
2	C	1059	ARG	Peptide
2	C	1232	MET	Peptide
2	C	1234	LYS	Peptide
2	C	235	ASN	Peptide
2	C	29	SER	Peptide
2	C	516	ASP	Peptide
2	C	581	THR	Peptide

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Mol	Chain	Res	Type	Group
2	C	662	SER	Peptide
3	D	120	LEU	Peptide
3	D	121	PRO	Peptide
3	D	1293	GLU	Peptide
3	D	1324	SER	Peptide
3	D	139	LEU	Peptide
3	D	331	ILE	Peptide
3	D	369	PRO	Peptide
3	D	484	MET	Peptide
3	D	518	VAL	Peptide
3	D	541	LEU	Peptide
3	D	584	PRO	Peptide
3	D	776	THR	Peptide
3	D	788	LEU	Peptide
3	D	826	ILE	Peptide
3	D	845	ALA	Peptide
3	D	904	ALA	Peptide
3	D	963	VAL	Peptide
5	F	112	THR	Peptide
5	F	165	PHE	Peptide
5	F	263	PRO	Peptide
5	F	294	GLN	Peptide
5	F	295	CYS	Peptide
5	F	299	LYS	Peptide
5	F	323	ASN	Peptide
5	F	396	ASN	Peptide
5	F	572	THR	Peptide
5	F	582	VAL	Peptide
6	G	200	GLY	Peptide
6	G	99	TYR	Peptide
6	H	159	HIS	Peptide
6	H	167	ILE	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	1786	1813	1813	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1767	1789	1789	32	0
2	C	10570	10581	10582	283	0
3	D	10396	10616	10615	254	0
4	E	627	634	634	20	0
5	F	3928	3990	3990	89	0
6	G	1556	1600	1600	31	0
6	H	1556	1600	1600	29	0
7	1	1591	890	891	15	0
8	2	1612	873	876	17	0
9	3	77	32	33	6	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
12	G	22	11	11	3	0
12	H	22	11	11	2	0
All	All	35513	34440	34445	739	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 11.

All (739) 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)
12:G:301:CMP:C2	12:G:301:CMP:H2	0.97	1.50
12:H:301:CMP:H2	12:H:301:CMP:C2	0.97	1.49
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.36	1.03
3:D:464:ASP:OD1	9:3:3:G:O2'	1.84	0.94
7:1:45:DT:O4	8:2:46:DA:N6	2.00	0.93
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.51	0.92
3:D:905:ARG:NH1	3:D:908:ILE:O	2.05	0.89
7:1:31:DG:O6	8:2:60:DC:N4	2.10	0.85
1:A:155:ALA:HB1	1:A:172:LEU:HD11	1.58	0.84
5:F:437:GLN:OE1	8:2:26:DA:N6	2.11	0.84
1:A:45:ARG:NE	1:B:38:THR:OG1	2.11	0.82
2:C:684:ASN:OD1	2:C:687:ARG:NH2	2.13	0.82
2:C:909:LYS:NZ	6:G:25:SER:O	2.13	0.81
3:D:50:LYS:NZ	3:D:52:GLU:OE1	2.14	0.81
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.52	0.80
3:D:147:ILE:O	3:D:156:ARG:NH1	2.15	0.79
2:C:27:LEU:O	2:C:528:ARG:NH1	2.14	0.79
2:C:592:ARG:NH2	2:C:601:ASP:OD1	2.16	0.79
5:F:436:ARG:NH2	8:2:26:DA:O4'	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:THR:O	3:D:1313:SER:OG	2.01	0.78
1:B:104:LYS:NZ	1:B:105:SER:O	2.16	0.78
3:D:951:GLN:OE1	3:D:1016:THR:OG1	2.02	0.78
3:D:556:GLU:O	3:D:564:VAL:N	2.18	0.77
3:D:1271:SER:OG	3:D:1290:ARG:NH1	2.18	0.77
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.66	0.76
2:C:1272:GLU:OE1	2:C:1272:GLU:N	2.19	0.76
5:F:576:VAL:O	5:F:580:PHE:N	2.18	0.76
3:D:702:GLN:O	3:D:718:SER:OG	2.03	0.76
3:D:872:LEU:O	3:D:875:ASN:N	2.19	0.76
6:H:26:LYS:N	6:H:88:ALA:O	2.18	0.76
2:C:452:ARG:NH1	2:C:453:ILE:O	2.19	0.76
2:C:576:SER:OG	2:C:659:GLN:O	2.02	0.75
7:1:46:DT:O4	8:2:45:DA:N6	2.19	0.75
6:G:168:THR:OG1	8:2:48:DT:OP1	2.04	0.75
2:C:148:GLN:NE2	2:C:533:LEU:O	2.20	0.75
2:C:18:ARG:NH2	2:C:620:ASN:O	2.18	0.75
3:D:257:GLY:O	3:D:259:ARG:NH1	2.20	0.74
2:C:13:LYS:O	2:C:1183:ALA:N	2.21	0.74
2:C:46:GLN:OE1	2:C:46:GLN:N	2.21	0.74
3:D:42:GLU:OE2	5:F:451:ARG:NH1	2.21	0.74
2:C:696:ASP:OD2	2:C:827:ARG:NH2	2.21	0.74
3:D:875:ASN:O	3:D:990:ARG:NH2	2.21	0.73
2:C:478:ARG:NH2	8:2:25:DT:OP1	2.21	0.73
3:D:805:GLN:NE2	3:D:806:ASP:OD1	2.21	0.73
2:C:43:PRO:O	2:C:54:ARG:NH2	2.21	0.73
5:F:348:GLU:O	5:F:352:GLY:N	2.21	0.73
5:F:96:ASP:OD2	5:F:99:ARG:NH1	2.22	0.72
3:D:1334:GLU:O	3:D:1340:LYS:NZ	2.22	0.72
2:C:318:SER:OG	2:C:320:ASP:OD1	2.03	0.72
3:D:475:GLU:OE1	4:E:28:ARG:NH2	2.23	0.72
3:D:901:ARG:NH2	3:D:906:GLY:O	2.23	0.72
2:C:989:LEU:O	2:C:997:TRP:NE1	2.23	0.71
2:C:205:PRO:O	2:C:208:ILE:HG22	1.90	0.71
3:D:1155:ILE:O	3:D:1210:ILE:N	2.22	0.71
5:F:585:GLU:OE1	5:F:586:ARG:NH1	2.23	0.71
6:G:125:GLN:O	6:G:128:SER:OG	2.06	0.71
1:A:90:VAL:O	1:A:210:THR:OG1	2.06	0.71
2:C:700:VAL:HG12	2:C:1117:LEU:HD23	1.72	0.71
3:D:844:THR:HG21	3:D:858:VAL:HG11	1.73	0.71
6:G:143:ILE:HG23	6:G:172:ILE:HD11	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:548:LEU:HA	5:F:551:LEU:HD13	1.72	0.71
2:C:958:LYS:O	2:C:961:SER:OG	2.03	0.70
2:C:1252:SER:OG	2:C:1256:GLN:N	2.24	0.70
2:C:727:VAL:HG23	2:C:773:LEU:HD12	1.74	0.70
3:D:1345:ARG:N	3:D:1349:GLU:OE1	2.24	0.70
7:1:74:DT:OP1	7:1:75:DG:N2	2.24	0.70
2:C:1281:TYR:OH	3:D:431:ARG:O	2.09	0.70
2:C:339:ASN:O	2:C:343:HIS:N	2.24	0.70
2:C:398:SER:O	2:C:401:GLY:N	2.23	0.69
2:C:719:LYS:O	2:C:779:ARG:NE	2.25	0.69
3:D:53:ARG:NH2	3:D:87:LYS:O	2.25	0.69
9:3:1:GTP:H2'	9:3:2:A:H5'	1.74	0.69
2:C:866:ASP:OD1	2:C:870:ILE:N	2.25	0.69
6:G:173:GLY:O	6:G:177:GLY:N	2.25	0.69
1:A:84:ASN:O	1:A:128:HIS:NE2	2.26	0.69
2:C:563:THR:OG1	2:C:572:ILE:O	2.04	0.69
2:C:494:ASN:ND2	8:2:24:DA:OP1	2.25	0.68
3:D:1319:PHE:O	3:D:1323:ALA:N	2.27	0.68
1:B:215:GLU:OE2	1:B:219:ARG:NH2	2.27	0.68
2:C:560:PRO:O	3:D:780:ARG:NH2	2.26	0.68
2:C:339:ASN:N	2:C:343:HIS:O	2.26	0.68
2:C:18:ARG:NH1	2:C:621:SER:O	2.26	0.68
2:C:1332:SER:HB3	3:D:245:LEU:HD21	1.76	0.68
5:F:511:ILE:HD12	5:F:519:LEU:HD13	1.74	0.68
3:D:188:LEU:O	3:D:191:SER:OG	2.09	0.67
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.67	0.67
2:C:850:ILE:O	2:C:851:THR:OG1	2.13	0.67
2:C:804:PHE:CD1	2:C:1098:LEU:HD11	2.29	0.67
9:3:1:GTP:C2'	9:3:2:A:H5'	2.24	0.67
1:A:158:ARG:O	1:A:162:GLU:N	2.28	0.67
2:C:1307:ASN:O	2:C:1312:ASN:N	2.28	0.67
2:C:504:GLU:O	2:C:508:SER:N	2.28	0.67
2:C:557:ARG:NH2	2:C:606:LEU:O	2.28	0.67
3:D:665:GLN:OE1	3:D:678:ARG:NH2	2.28	0.66
6:G:99:TYR:O	6:G:101:LYS:N	2.27	0.66
2:C:1303:LYS:NZ	2:C:1314:GLN:O	2.27	0.66
5:F:376:LYS:O	5:F:379:MET:N	2.28	0.66
2:C:1259:LEU:O	2:C:1267:GLY:N	2.28	0.66
2:C:211:ARG:NH1	2:C:357:ASN:O	2.29	0.66
3:D:536:LEU:O	3:D:539:SER:OG	2.14	0.66
3:D:885:VAL:O	3:D:1258:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:326:SER:OG	3:D:329:ASP:N	2.28	0.66
6:G:185:ARG:NH2	8:2:51:DG:N7	2.43	0.65
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.78	0.65
3:D:198:CYS:SG	3:D:202:ARG:NH1	2.69	0.65
2:C:646:SER:OG	2:C:649:GLN:OE1	2.12	0.65
2:C:408:SER:O	2:C:431:LYS:NZ	2.26	0.65
3:D:425:ARG:NH1	3:D:457:TYR:O	2.29	0.65
2:C:4:SER:O	2:C:8:LYS:N	2.30	0.65
2:C:65:ASN:OD1	2:C:66:SER:N	2.30	0.65
3:D:816:THR:O	3:D:860:ARG:NH2	2.30	0.65
5:F:600:HIS:O	5:F:602:SER:N	2.29	0.65
3:D:883:ARG:NH1	3:D:898:CYS:SG	2.70	0.64
2:C:233:ARG:NH1	2:C:238:GLN:OE1	2.30	0.64
2:C:663:VAL:O	2:C:666:SER:OG	2.05	0.64
2:C:135:THR:OG1	2:C:143:ARG:O	2.14	0.64
2:C:582:ASN:N	2:C:586:PHE:O	2.31	0.64
2:C:592:ARG:O	2:C:653:MET:N	2.30	0.64
5:F:407:GLU:HA	5:F:410:ILE:HD12	1.79	0.64
1:B:207:THR:OG1	1:B:208:ASN:N	2.29	0.64
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.31	0.64
2:C:397:LEU:O	2:C:398:SER:OG	2.16	0.64
2:C:801:ARG:O	2:C:1096:ILE:HD13	1.97	0.64
2:C:758:ARG:NH2	2:C:833:ILE:O	2.31	0.64
3:D:320:ASN:ND2	3:D:322:ARG:O	2.31	0.63
3:D:275:ARG:NH1	3:D:298:MET:O	2.30	0.63
3:D:957:SER:N	3:D:985:ILE:O	2.31	0.63
6:H:37:GLU:OE2	6:H:100:LYS:NZ	2.29	0.63
1:A:207:THR:HG23	1:A:208:ASN:O	1.99	0.63
5:F:132:CYS:SG	5:F:257:LYS:NZ	2.59	0.63
2:C:701:GLY:N	2:C:1182:ILE:O	2.32	0.63
2:C:1295:SER:O	2:C:1301:ARG:NH2	2.32	0.63
2:C:257:ALA:N	2:C:260:LYS:O	2.32	0.63
3:D:454:CYS:O	3:D:458:ASN:N	2.32	0.63
2:C:1252:SER:N	2:C:1257:GLN:O	2.32	0.62
2:C:935:THR:N	2:C:1040:ASP:OD2	2.30	0.62
2:C:1088:ASP:OD2	2:C:1092:THR:OG1	2.17	0.62
3:D:418:GLU:OE2	4:E:3:ARG:NE	2.33	0.62
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.33	0.62
2:C:1325:VAL:HG13	3:D:249:LEU:HD11	1.81	0.62
2:C:94:ALA:CB	2:C:129:LEU:HD11	2.21	0.61
5:F:372:ALA:O	5:F:376:LYS:NZ	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.81	0.61
2:C:718:ALA:N	2:C:781:ASP:O	2.33	0.61
3:D:424:ASN:HA	3:D:434:ILE:HG22	1.81	0.61
3:D:604:MET:O	3:D:607:THR:OG1	2.17	0.61
1:A:131:CYS:SG	1:A:132:HIS:N	2.74	0.61
5:F:299:LYS:O	5:F:302:PHE:N	2.34	0.61
1:A:59:VAL:HG22	1:A:144:ILE:HG23	1.81	0.61
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.82	0.61
1:A:11:PRO:HB2	1:A:28:LEU:HD11	1.83	0.60
3:D:519:ASN:OD1	3:D:520:ALA:N	2.34	0.60
5:F:309:ASN:OD1	5:F:314:THR:OG1	2.14	0.60
5:F:596:ARG:O	5:F:600:HIS:ND1	2.33	0.60
1:A:155:ALA:CB	1:A:172:LEU:HD11	2.30	0.60
2:C:261:VAL:HG11	2:C:264:GLU:OE2	2.01	0.60
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.83	0.60
3:D:675:ALA:O	3:D:679:TYR:N	2.34	0.60
5:F:575:GLU:O	5:F:579:GLN:N	2.33	0.60
2:C:903:ARG:NH2	2:C:908:GLU:O	2.34	0.60
3:D:85:CYS:O	3:D:89:GLY:N	2.34	0.60
3:D:133:ARG:NH2	7:1:88:DG:OP1	2.35	0.60
3:D:385:LEU:HB3	3:D:391:ALA:HB3	1.84	0.60
1:B:131:CYS:SG	1:B:132:HIS:N	2.75	0.60
3:D:490:ILE:O	3:D:499:ILE:HG22	2.02	0.59
7:1:46:DT:O4	8:2:45:DA:C6	2.55	0.59
1:A:96:ASP:O	1:A:148:ARG:N	2.35	0.59
3:D:255:LEU:N	3:D:259:ARG:O	2.34	0.59
3:D:275:ARG:O	3:D:279:LEU:N	2.36	0.59
3:D:169:LEU:O	3:D:173:GLY:N	2.35	0.59
2:C:697:LYS:O	2:C:799:ASN:ND2	2.36	0.58
5:F:131:GLN:HB2	5:F:261:LEU:HD21	1.84	0.58
5:F:554:ARG:NE	5:F:555:GLU:OE2	2.33	0.58
2:C:759:SER:OG	2:C:762:ASN:N	2.36	0.58
3:D:356:THR:N	3:D:447:ILE:O	2.36	0.58
3:D:863:LEU:HD21	3:D:901:ARG:NH1	2.19	0.58
2:C:1088:ASP:OD1	2:C:1091:GLY:N	2.36	0.58
3:D:70:CYS:SG	3:D:74:LYS:N	2.77	0.58
3:D:408:VAL:O	3:D:412:LEU:N	2.33	0.58
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.36	0.58
2:C:593:LYS:O	2:C:600:THR:N	2.36	0.58
3:D:114:ILE:HG22	3:D:307:LEU:HD12	1.86	0.58
1:B:112:ALA:N	1:B:128:HIS:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:21:HIS:ND1	6:H:96:GLU:OE2	2.37	0.58
3:D:1035:VAL:N	3:D:1113:VAL:O	2.34	0.58
7:1:46:DT:C4	8:2:45:DA:N6	2.71	0.58
3:D:473:THR:OG1	4:E:28:ARG:NH2	2.37	0.58
3:D:436:ALA:HB3	3:D:484:MET:O	2.04	0.57
5:F:404:LEU:HD12	5:F:405:ILE:HG13	1.86	0.57
6:G:11:LEU:HD22	6:G:41:TYR:OH	2.03	0.57
1:B:61:ILE:CG2	1:B:140:ILE:HD11	2.35	0.57
3:D:121:PRO:O	3:D:123:ARG:NH1	2.38	0.57
3:D:1279:GLN:NE2	3:D:1281:GLU:OE1	2.38	0.57
2:C:559:CYS:SG	2:C:662:SER:N	2.78	0.57
3:D:1267:VAL:HG23	3:D:1302:TYR:CA	2.35	0.57
2:C:1127:LYS:NZ	2:C:1203:ASP:OD2	2.37	0.57
2:C:594:VAL:HG11	2:C:650:VAL:HB	1.87	0.57
3:D:1265:THR:N	3:D:1305:ASP:OD2	2.38	0.56
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.70	0.56
6:H:72:GLU:HG3	6:H:116:LEU:HD11	1.86	0.56
3:D:201:LEU:HD22	3:D:217:LEU:HD22	1.85	0.56
5:F:138:PRO:HD2	5:F:353:LEU:HD12	1.87	0.56
3:D:1286:LYS:O	3:D:1290:ARG:N	2.37	0.56
6:H:196:ILE:HD11	6:H:202:THR:HB	1.87	0.56
2:C:1292:THR:O	2:C:1297:ASP:N	2.36	0.56
3:D:385:LEU:O	3:D:389:GLY:N	2.38	0.56
1:B:199:ASP:N	1:B:199:ASP:OD1	2.38	0.56
2:C:542:ARG:NH1	7:1:80:DC:O5'	2.38	0.56
3:D:643:ASP:O	3:D:720:ASN:ND2	2.38	0.56
5:F:353:LEU:HD21	5:F:357:GLN:HB2	1.86	0.56
3:D:1249:ASN:OD1	3:D:1250:ASP:N	2.39	0.56
3:D:1267:VAL:HG23	3:D:1302:TYR:HA	1.86	0.56
3:D:64:PRO:O	3:D:95:THR:OG1	2.15	0.56
2:C:528:ARG:NE	2:C:575:LEU:HD11	2.21	0.56
2:C:843:THR:OG1	2:C:846:GLY:O	2.11	0.56
3:D:438:GLU:OE2	4:E:3:ARG:NH2	2.38	0.56
6:G:190:LEU:HD22	6:G:195:LEU:HD12	1.88	0.56
1:B:83:LEU:HD21	3:D:526:VAL:HG21	1.88	0.56
6:G:167:ILE:HD11	6:G:171:GLU:H	1.71	0.56
1:B:15:ASP:OD1	1:B:16:ILE:N	2.40	0.55
2:C:899:GLU:OE1	2:C:902:LEU:HD23	2.06	0.55
2:C:990:ASP:OD1	2:C:991:LYS:N	2.39	0.55
3:D:1229:VAL:O	3:D:1233:ILE:HD12	2.07	0.55
2:C:565:GLU:OE1	2:C:565:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:THR:HG22	2:C:758:ARG:H	1.72	0.55
3:D:282:LEU:HD11	3:D:287:ALA:HB3	1.89	0.55
2:C:1065:LYS:NZ	9:3:3:G:OP1	2.40	0.55
2:C:786:GLY:N	2:C:789:THR:OG1	2.37	0.55
4:E:22:VAL:HG22	4:E:25:ARG:NH2	2.21	0.55
1:B:61:ILE:HG23	1:B:140:ILE:HD11	1.88	0.55
2:C:1042:LEU:HD13	2:C:1046:VAL:HG12	1.88	0.55
2:C:839:VAL:HG23	2:C:1046:VAL:HG13	1.89	0.55
3:D:1035:VAL:O	3:D:1112:GLY:N	2.40	0.55
3:D:514:THR:OG1	3:D:576:ARG:NE	2.40	0.55
3:D:353:SER:HB3	3:D:447:ILE:HD11	1.89	0.55
6:H:60:ILE:HD12	6:H:174:GLN:HG2	1.89	0.55
2:C:1269:ARG:N	8:2:15:DC:OP1	2.40	0.55
1:A:17:GLU:OE2	1:A:27:THR:HG23	2.06	0.55
3:D:820:ILE:HG23	3:D:884:SER:HB2	1.88	0.55
2:C:788:SER:O	2:C:795:ALA:N	2.37	0.55
3:D:1141:VAL:CG2	3:D:1240:VAL:HG11	2.37	0.55
3:D:825:VAL:HG23	3:D:832:LYS:HB2	1.89	0.55
2:C:1240:ASP:O	2:C:1262:LYS:NZ	2.40	0.54
5:F:305:LEU:CD1	5:F:319:ALA:HB2	2.37	0.54
3:D:1004:ALA:N	3:D:1017:VAL:O	2.40	0.54
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.40	0.54
3:D:559:ALA:O	3:D:561:GLY:N	2.40	0.54
1:B:107:ILE:HG23	1:B:133:LEU:O	2.08	0.54
2:C:241:LEU:HD21	2:C:246:LEU:HD12	1.88	0.54
2:C:444:ASP:OD2	2:C:551:HIS:NE2	2.36	0.54
2:C:766:ASN:OD1	2:C:767:GLN:N	2.40	0.54
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.89	0.54
2:C:63:SER:OG	2:C:480:SER:OG	2.15	0.54
2:C:936:ARG:HG3	2:C:1042:LEU:HD12	1.90	0.54
3:D:1306:LEU:HD23	3:D:1307:LEU:N	2.22	0.54
2:C:198:ILE:O	2:C:201:ARG:N	2.41	0.54
2:C:349:GLU:O	2:C:353:VAL:HG23	2.08	0.54
2:C:97:ARG:NH1	2:C:121:GLU:OE2	2.40	0.54
3:D:858:VAL:HG12	3:D:862:THR:OG1	2.07	0.54
2:C:318:SER:O	2:C:322:LEU:N	2.39	0.54
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.90	0.54
2:C:595:THR:HG1	2:C:600:THR:HG1	1.54	0.54
3:D:368:LEU:HD22	3:D:441:LEU:HD23	1.89	0.54
3:D:960:LEU:HD11	3:D:982:LEU:HD12	1.89	0.54
5:F:119:ILE:HD13	5:F:379:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:282:LEU:HD21	3:D:287:ALA:HB2	1.90	0.53
3:D:520:ALA:HB3	3:D:543:SER:HB2	1.91	0.53
6:G:37:GLU:OE1	6:G:37:GLU:N	2.41	0.53
2:C:402:ARG:NH2	2:C:419:ILE:O	2.42	0.53
3:D:1111:ASP:OD1	3:D:1112:GLY:N	2.41	0.53
5:F:137:TYR:CE2	5:F:361:ILE:HG21	2.43	0.53
2:C:448:LEU:HD12	2:C:553:THR:HG22	1.91	0.53
2:C:96:LEU:HD23	2:C:124:MET:O	2.07	0.53
3:D:583:VAL:HG11	3:D:587:LEU:HD11	1.91	0.53
3:D:844:THR:CG2	3:D:858:VAL:HG11	2.37	0.53
2:C:545:PHE:O	2:C:549:ASP:N	2.41	0.53
3:D:1220:ILE:CG2	3:D:1229:VAL:HG22	2.39	0.53
3:D:93:THR:HG22	3:D:94:GLN:H	1.73	0.53
7:1:22:DC:H42	8:2:69:DG:H1	1.56	0.53
6:G:131:VAL:HG22	6:H:131:VAL:HG22	1.91	0.53
1:B:155:ALA:N	1:B:174:ASP:OD1	2.38	0.53
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.42	0.53
3:D:598:LYS:HA	3:D:601:ILE:HD12	1.90	0.53
3:D:483:LEU:O	3:D:489:ASN:ND2	2.42	0.53
3:D:368:LEU:HD23	3:D:369:PRO:O	2.08	0.53
3:D:740:LEU:O	3:D:762:ASN:ND2	2.42	0.53
5:F:119:ILE:HD11	5:F:378:GLU:CD	2.30	0.53
2:C:551:HIS:CE1	2:C:553:THR:HG1	2.27	0.52
3:D:346:ARG:NH1	8:2:15:DC:OP1	2.43	0.52
3:D:863:LEU:HD11	3:D:901:ARG:HD2	1.91	0.52
2:C:1095:ASP:CB	2:C:1096:ILE:HD12	2.38	0.52
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.41	0.52
6:H:157:MET:SD	6:H:157:MET:N	2.83	0.52
2:C:339:ASN:O	2:C:342:ASP:N	2.42	0.52
3:D:368:LEU:HD22	3:D:441:LEU:CD2	2.39	0.52
3:D:478:LEU:HB2	4:E:20:VAL:HG13	1.90	0.52
2:C:251:ALA:CB	2:C:255:ILE:HD12	2.40	0.52
3:D:473:THR:HG23	3:D:476:ALA:H	1.73	0.52
1:B:85:LEU:HD23	1:B:88:LEU:HD22	1.90	0.52
1:B:14:VAL:HG21	1:B:29:GLU:CD	2.29	0.52
5:F:505:ILE:O	5:F:505:ILE:HG22	2.09	0.52
1:A:38:THR:HG23	1:B:42:ALA:HA	1.91	0.52
3:D:1036:ARG:HE	3:D:1081:VAL:HG21	1.74	0.52
3:D:602:SER:OG	3:D:603:LYS:N	2.43	0.52
6:G:39:LEU:HD23	6:G:97:ILE:HD11	1.90	0.52
2:C:929:ILE:HD12	2:C:930:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.40	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD11	1.92	0.52
1:B:191:ARG:NH2	3:D:410:ASP:OD1	2.43	0.51
2:C:598:VAL:HG22	2:C:627:GLY:O	2.10	0.51
2:C:701:GLY:O	2:C:1184:THR:N	2.41	0.51
3:D:1115:ILE:HG21	3:D:1121:LEU:HD23	1.91	0.51
5:F:515:GLU:OE1	5:F:515:GLU:N	2.43	0.51
2:C:405:PHE:CE2	2:C:409:LEU:HD11	2.46	0.51
2:C:551:HIS:O	2:C:554:HIS:ND1	2.43	0.51
3:D:1029:THR:OG1	3:D:1115:ILE:HD13	2.10	0.51
3:D:71:LEU:HD12	3:D:90:VAL:HG21	1.92	0.51
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.43	0.51
2:C:521:LEU:O	2:C:525:THR:HG22	2.11	0.51
2:C:973:SER:O	2:C:977:ALA:N	2.36	0.51
5:F:461:ASN:OD1	5:F:462:LYS:N	2.43	0.51
6:H:159:HIS:O	6:H:162:GLY:N	2.43	0.51
2:C:9:LYS:NZ	2:C:791:LEU:HD22	2.25	0.51
3:D:495:ASN:OD1	3:D:495:ASN:N	2.44	0.51
6:G:127:THR:O	6:G:131:VAL:HG23	2.10	0.51
6:H:94:VAL:HG12	6:H:95:ALA:O	2.11	0.51
2:C:1278:LEU:O	2:C:1282:GLY:N	2.41	0.51
1:A:92:VAL:HA	1:A:121:VAL:HG22	1.91	0.51
6:G:72:GLU:HG2	6:G:73:LEU:HD12	1.93	0.51
3:D:865:HIS:ND1	3:D:867:GLN:OE1	2.43	0.51
7:1:58:DT:H2'	7:1:59:DT:H72	1.92	0.50
2:C:320:ASP:OD1	2:C:321:LEU:N	2.43	0.50
2:C:367:TYR:HB2	2:C:381:ALA:HB2	1.93	0.50
4:E:60:ASN:OD1	4:E:61:ASN:N	2.44	0.50
3:D:903:LEU:O	3:D:906:GLY:N	2.45	0.50
3:D:397:ALA:O	3:D:401:VAL:HG23	2.11	0.50
3:D:481:ARG:HE	4:E:47:THR:HG21	1.76	0.50
4:E:60:ASN:ND2	4:E:62:GLN:OE1	2.44	0.50
3:D:1046:ILE:HG22	3:D:1061:VAL:HA	1.93	0.50
3:D:187:ALA:O	3:D:191:SER:N	2.45	0.50
5:F:137:TYR:O	5:F:141:ILE:N	2.45	0.50
2:C:764:CYS:SG	2:C:765:ILE:N	2.84	0.50
5:F:414:LYS:O	5:F:417:ASP:N	2.45	0.50
1:A:166:ARG:HD2	1:A:170:ARG:HE	1.76	0.50
2:C:838:CYS:HB2	2:C:918:LEU:HD21	1.93	0.50
7:1:45:DT:O4	8:2:46:DA:C6	2.64	0.50
2:C:69:GLN:OE1	2:C:101:ARG:NH2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:TYR:O	3:D:297:ARG:NH2	2.45	0.50
3:D:410:ASP:O	3:D:414:GLU:N	2.41	0.50
2:C:1339:LEU:HD22	3:D:17:PHE:CE2	2.47	0.50
6:H:39:LEU:N	6:H:97:ILE:O	2.39	0.50
1:B:83:LEU:HD21	3:D:526:VAL:CG2	2.42	0.49
2:C:804:PHE:HD1	2:C:1098:LEU:HD11	1.77	0.49
2:C:845:LEU:HD22	2:C:889:PRO:O	2.12	0.49
3:D:1058:SER:OG	3:D:1109:LEU:O	2.26	0.49
3:D:107:LEU:HD12	3:D:240:THR:HA	1.93	0.49
2:C:14:ASP:OD1	2:C:15:PHE:N	2.45	0.49
2:C:658:GLN:O	2:C:661:VAL:HG22	2.12	0.49
2:C:725:GLN:NE2	2:C:734:ILE:O	2.46	0.49
3:D:384:LYS:HD3	3:D:411:ILE:HG23	1.94	0.49
5:F:305:LEU:HD11	5:F:319:ALA:HB2	1.93	0.49
5:F:452:ILE:HG23	5:F:457:ILE:HD11	1.94	0.49
6:H:55:GLU:OE1	6:H:55:GLU:N	2.45	0.49
2:C:131:THR:OG1	2:C:134:GLY:N	2.40	0.49
2:C:348:SER:HA	2:C:351:LEU:HD12	1.94	0.49
2:C:396:ASP:OD1	2:C:397:LEU:N	2.45	0.49
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.45	0.49
3:D:1371:ARG:O	3:D:1375:ALA:N	2.39	0.49
3:D:511:TYR:OH	3:D:724:MET:SD	2.57	0.49
2:C:905:ILE:HG13	5:F:595:LEU:HD22	1.94	0.49
2:C:323:ALA:O	2:C:326:SER:OG	2.21	0.49
2:C:559:CYS:SG	2:C:561:ILE:HD12	2.53	0.49
2:C:623:LEU:HD12	2:C:624:ASP:H	1.77	0.49
3:D:1164:SER:O	3:D:1176:VAL:N	2.46	0.49
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.33	0.49
5:F:514:ASP:O	5:F:516:ASP:N	2.45	0.49
5:F:607:LEU:O	5:F:610:PHE:N	2.45	0.49
2:C:60:GLN:OE1	2:C:66:SER:N	2.45	0.49
2:C:838:CYS:CB	2:C:918:LEU:HD11	2.41	0.49
3:D:282:LEU:HD11	3:D:287:ALA:CB	2.42	0.49
3:D:373:ALA:HB1	3:D:377:PHE:CE2	2.48	0.49
5:F:583:THR:HG23	5:F:586:ARG:CZ	2.42	0.49
3:D:1292:LEU:O	3:D:1295:ASN:N	2.40	0.49
3:D:812:ASP:O	3:D:897:HIS:ND1	2.44	0.49
3:D:913:GLU:OE1	3:D:913:GLU:N	2.43	0.49
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.95	0.49
3:D:1173:ARG:O	3:D:1190:ILE:N	2.45	0.49
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1166:GLY:N	3:D:1174:ARG:O	2.46	0.49
3:D:1163:VAL:HG21	3:D:1175:LEU:HD11	1.94	0.49
5:F:130:VAL:HG13	5:F:365:MET:HG2	1.95	0.49
1:B:135:ASP:OD1	1:B:136:GLU:N	2.46	0.48
2:C:936:ARG:CG	2:C:1042:LEU:HD12	2.44	0.48
2:C:1308:ILE:HG21	3:D:379:PRO:HG2	1.94	0.48
2:C:857:VAL:HG11	2:C:862:LEU:HD11	1.95	0.48
3:D:1109:LEU:HB3	3:D:1113:VAL:HG11	1.96	0.48
1:A:102:LEU:HD13	1:A:115:ILE:HA	1.95	0.48
3:D:1147:ALA:HB3	3:D:1308:GLY:HA2	1.95	0.48
3:D:1256:ILE:HD12	3:D:1257:VAL:N	2.29	0.48
3:D:884:SER:N	3:D:887:SER:OG	2.46	0.48
3:D:1220:ILE:HG22	3:D:1229:VAL:HG22	1.94	0.48
4:E:52:ARG:NH2	4:E:55:GLU:OE1	2.47	0.48
3:D:835:LEU:O	3:D:839:VAL:HG23	2.13	0.48
2:C:357:ASN:OD1	2:C:358:ASP:N	2.47	0.48
1:B:15:ASP:N	1:B:27:THR:OG1	2.46	0.48
2:C:575:LEU:O	2:C:575:LEU:HD12	2.13	0.48
3:D:968:ASN:OD1	3:D:972:LYS:N	2.47	0.48
5:F:493:LYS:O	5:F:497:VAL:HG23	2.13	0.48
7:1:29:DG:C2'	7:1:30:DT:H72	2.44	0.48
1:B:111:THR:HA	1:B:129:VAL:HG22	1.95	0.48
2:C:100:LEU:HD21	2:C:122:VAL:HG23	1.96	0.48
2:C:1230:MET:SD	2:C:1231:TYR:N	2.87	0.48
3:D:1265:THR:O	3:D:1303:SER:N	2.40	0.48
3:D:510:LEU:O	3:D:514:THR:HG22	2.13	0.48
3:D:767:LEU:HD13	3:D:772:TYR:HB2	1.96	0.48
3:D:198:CYS:HB2	3:D:224:LEU:HD13	1.96	0.48
2:C:256:GLU:HB3	2:C:261:VAL:HG22	1.95	0.47
2:C:624:ASP:N	2:C:628:HIS:O	2.44	0.47
3:D:606:ASN:C	3:D:610:ARG:HE	2.17	0.47
3:D:107:LEU:HD12	3:D:240:THR:CA	2.44	0.47
5:F:593:LYS:NZ	6:G:55:GLU:OE2	2.48	0.47
1:B:158:ARG:HD2	1:B:172:LEU:HD21	1.95	0.47
3:D:48:THR:O	3:D:50:LYS:N	2.48	0.47
3:D:517:CYS:SG	3:D:519:ASN:N	2.87	0.47
4:E:6:VAL:HG12	4:E:6:VAL:O	2.15	0.47
2:C:1042:LEU:HD11	2:C:1048:LYS:HA	1.96	0.47
2:C:11:ILE:HD12	2:C:12:ARG:N	2.30	0.47
2:C:835:GLU:C	2:C:836:LEU:HD22	2.34	0.47
2:C:929:ILE:HD12	2:C:930:ASP:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:310:GLU:OE2	5:F:355:ILE:HG21	2.13	0.47
5:F:397:ARG:O	8:2:23:DT:N3	2.48	0.47
2:C:564:PRO:HB3	9:3:1:GTP:O1A	2.15	0.47
2:C:483:ASP:OD1	2:C:484:LEU:N	2.47	0.47
2:C:961:SER:OG	2:C:962:GLU:N	2.48	0.47
3:D:816:THR:OG1	3:D:883:ARG:NH2	2.48	0.47
6:H:159:HIS:N	6:H:162:GLY:O	2.44	0.47
6:H:60:ILE:HD12	6:H:174:GLN:CG	2.44	0.47
6:H:50:LEU:HD12	6:H:58:GLU:OE1	2.14	0.47
1:A:32:GLU:HA	1:A:198:LEU:HD23	1.96	0.47
2:C:617:ALA:O	2:C:654:ASP:N	2.44	0.47
2:C:878:THR:HG23	2:C:925:SER:HB3	1.97	0.47
3:D:37:GLU:O	3:D:39:LYS:NZ	2.47	0.47
3:D:826:ILE:HG22	3:D:831:VAL:HG23	1.97	0.47
2:C:1084:ASP:OD1	2:C:1084:ASP:N	2.44	0.47
2:C:1247:SER:OG	2:C:1248:THR:N	2.48	0.47
2:C:739:ASP:OD1	2:C:740:GLU:N	2.48	0.47
3:D:281:ARG:NH2	3:D:284:ASP:OD2	2.47	0.47
1:A:99:ILE:HG22	1:A:145:LYS:HA	1.97	0.47
1:B:56:VAL:HG13	1:B:144:ILE:HG23	1.97	0.47
2:C:422:LYS:HA	2:C:425:ILE:HD12	1.97	0.47
3:D:1346:GLY:N	3:D:1349:GLU:OE1	2.48	0.47
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.15	0.47
3:D:623:GLN:O	3:D:627:THR:HG22	2.15	0.47
1:A:34:GLY:O	1:B:45:ARG:NH2	2.48	0.47
2:C:1034:ARG:O	2:C:1038:GLN:N	2.47	0.47
2:C:1236:ASN:OD1	2:C:1237:HIS:N	2.47	0.47
2:C:1309:VAL:HG11	3:D:394:ILE:HD11	1.97	0.47
3:D:186:GLN:O	3:D:190:LYS:N	2.36	0.47
3:D:296:LYS:HA	3:D:299:LEU:HD12	1.95	0.47
6:G:187:LEU:O	6:G:191:GLU:N	2.37	0.47
1:A:220:ALA:O	1:A:224:LEU:HD13	2.14	0.47
5:F:263:PRO:O	5:F:265:GLN:N	2.48	0.47
1:A:22:THR:OG1	1:A:207:THR:O	2.11	0.46
2:C:1219:GLU:OE1	3:D:538:ARG:NH2	2.47	0.46
5:F:262:VAL:HB	5:F:263:PRO:HD2	1.97	0.46
6:H:147:LEU:HD12	6:H:196:ILE:HD13	1.96	0.46
6:H:34:GLU:O	6:H:82:ARG:N	2.36	0.46
2:C:100:LEU:CD2	2:C:122:VAL:HG23	2.45	0.46
2:C:866:ASP:OD1	2:C:869:GLY:N	2.48	0.46
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:214:ARG:NH1	3:D:218:THR:OG1	2.49	0.46
3:D:515:ARG:O	3:D:573:THR:HG21	2.15	0.46
1:B:217:ILE:HD12	1:B:218:ARG:N	2.30	0.46
2:C:1120:ALA:HB2	2:C:1199:LEU:CD2	2.44	0.46
2:C:61:SER:HG	2:C:65:ASN:H	1.63	0.46
2:C:948:ILE:O	2:C:952:GLN:N	2.45	0.46
3:D:1319:PHE:CZ	3:D:1320:ILE:HD11	2.51	0.46
3:D:1353:VAL:HG23	3:D:1355:ARG:H	1.79	0.46
6:G:34:GLU:O	6:G:82:ARG:N	2.47	0.46
2:C:413:GLU:OE1	2:C:413:GLU:N	2.49	0.46
3:D:1313:SER:O	3:D:1316:THR:OG1	2.30	0.46
3:D:957:SER:O	3:D:985:ILE:N	2.46	0.46
6:G:84:ALA:HB3	12:G:301:CMP:H5'1	1.97	0.46
1:A:17:GLU:OE2	1:A:27:THR:N	2.48	0.46
2:C:758:ARG:CZ	2:C:833:ILE:HB	2.46	0.46
3:D:481:ARG:NE	4:E:47:THR:HG21	2.31	0.46
3:D:738:ARG:O	3:D:742:GLY:N	2.47	0.46
5:F:271:ASN:OD1	5:F:274:ARG:NH1	2.49	0.46
5:F:353:LEU:HD23	5:F:354:THR:N	2.31	0.46
2:C:235:ASN:OD1	2:C:236:LYS:N	2.48	0.46
3:D:1330:ARG:O	3:D:1333:THR:OG1	2.32	0.46
2:C:638:SER:O	2:C:640:GLY:N	2.49	0.46
2:C:839:VAL:O	2:C:886:LYS:NZ	2.44	0.46
3:D:479:GLU:HG3	4:E:20:VAL:HG11	1.97	0.46
2:C:258:ASN:OD1	2:C:259:GLY:N	2.45	0.46
2:C:725:GLN:O	2:C:773:LEU:HD11	2.16	0.46
6:G:22:LYS:NZ	6:G:91:ALA:HB1	2.31	0.46
2:C:138:ILE:O	2:C:141:THR:OG1	2.08	0.45
2:C:1336:ASN:O	3:D:23:ALA:N	2.49	0.45
3:D:105:ILE:O	3:D:241:VAL:HG13	2.16	0.45
5:F:320:ILE:HD12	5:F:327:SER:CB	2.46	0.45
2:C:1146:GLN:OE1	2:C:1161:LEU:HD22	2.16	0.45
2:C:1324:ASN:OD1	2:C:1325:VAL:N	2.50	0.45
2:C:866:ASP:OD2	2:C:944:ARG:NH1	2.49	0.45
3:D:646:ILE:HD11	3:D:762:ASN:HD21	1.82	0.45
5:F:149:ASP:O	5:F:153:ALA:N	2.50	0.45
7:1:13:DC:H2'	7:1:14:DT:H72	1.98	0.45
2:C:805:MET:N	2:C:805:MET:SD	2.89	0.45
1:A:15:ASP:OD1	1:A:16:ILE:N	2.49	0.45
5:F:605:GLU:N	5:F:605:GLU:OE1	2.49	0.45
6:G:73:LEU:HD13	12:G:301:CMP:O3'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:166:LYS:O	6:H:167:ILE:HD13	2.16	0.45
3:D:1328:THR:HG22	3:D:1332:LEU:HD11	1.98	0.45
5:F:449:THR:HG21	5:F:504:PRO:HG3	1.97	0.45
1:B:11:PRO:HG3	1:B:31:LEU:HD21	1.99	0.45
2:C:20:GLN:OE1	2:C:21:VAL:N	2.50	0.45
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.97	0.45
2:C:1129:ASN:O	2:C:1133:LYS:NZ	2.46	0.45
2:C:399:ALA:HA	2:C:402:ARG:HB3	1.99	0.45
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.99	0.45
3:D:678:ARG:O	3:D:682:VAL:HG23	2.16	0.45
5:F:122:ARG:HB3	5:F:371:LYS:HD2	1.99	0.45
6:G:195:LEU:O	6:G:196:ILE:HD13	2.17	0.45
2:C:386:GLU:N	2:C:386:GLU:OE1	2.50	0.45
3:D:1306:LEU:C	3:D:1307:LEU:HD22	2.37	0.45
2:C:237:LEU:CD1	2:C:292:ILE:HD11	2.47	0.45
2:C:453:ILE:HD12	2:C:454:ARG:N	2.32	0.45
2:C:155:VAL:HG23	2:C:176:ILE:HG13	1.98	0.45
2:C:732:ILE:HD11	2:C:751:TYR:HD2	1.82	0.45
5:F:554:ARG:O	5:F:558:VAL:HG23	2.17	0.45
3:D:474:LEU:HD21	4:E:27:ALA:HB3	1.99	0.44
6:G:113:LEU:HD23	6:H:113:LEU:HD23	1.99	0.44
1:B:84:ASN:HB2	1:B:130:ILE:HG23	1.98	0.44
2:C:12:ARG:NH1	2:C:699:LEU:O	2.50	0.44
2:C:1330:ILE:HG22	2:C:1335:ILE:HB	1.99	0.44
3:D:152:THR:HG22	3:D:152:THR:O	2.18	0.44
6:G:199:HIS:ND1	6:G:199:HIS:O	2.50	0.44
1:A:218:ARG:NE	1:B:233:ASP:O	2.33	0.44
5:F:460:ILE:HA	5:F:463:LEU:HD12	1.99	0.44
3:D:452:LEU:HD13	3:D:500:ILE:HG22	1.99	0.44
3:D:848:VAL:O	3:D:848:VAL:HG23	2.18	0.44
6:H:144:ALA:O	6:H:147:LEU:HD23	2.18	0.44
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.44	0.44
2:C:675:ASP:OD1	2:C:676:ALA:N	2.48	0.44
5:F:320:ILE:HD12	5:F:327:SER:HB2	2.00	0.44
1:B:210:THR:O	1:B:211:ILE:HD13	2.18	0.44
3:D:135:ILE:HG22	3:D:139:LEU:HD12	1.99	0.44
5:F:270:VAL:O	5:F:274:ARG:N	2.49	0.44
1:B:102:LEU:HD13	1:B:103:ASN:N	2.32	0.44
2:C:1120:ALA:O	2:C:1124:ILE:HD12	2.18	0.44
2:C:1253:LEU:H	2:C:1253:LEU:HD23	1.83	0.44
2:C:251:ALA:HB1	2:C:255:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:663:VAL:HG23	2:C:664:GLY:N	2.33	0.44
2:C:1003:THR:HG22	2:C:1004:ASP:H	1.81	0.44
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.43	0.44
3:D:1344:LEU:HD23	3:D:1349:GLU:HB3	1.99	0.44
3:D:747:MET:C	3:D:755:ILE:HD12	2.38	0.44
3:D:478:LEU:HD12	4:E:24:ALA:HB2	1.99	0.44
5:F:166:VAL:HG13	5:F:259:PHE:HA	1.99	0.44
5:F:322:MET:HG3	5:F:323:ASN:H	1.82	0.44
2:C:839:VAL:CG2	2:C:1046:VAL:HG13	2.48	0.44
2:C:1054:LEU:HD23	2:C:1054:LEU:H	1.83	0.44
2:C:346:TYR:OH	2:C:436:ARG:NH1	2.50	0.44
3:D:514:THR:HG23	3:D:514:THR:O	2.17	0.44
2:C:209:ILE:HA	2:C:212:ALA:HB3	1.98	0.43
2:C:1333:LEU:HD21	3:D:327:LEU:HD13	2.00	0.43
3:D:44:ILE:HG22	3:D:50:LYS:O	2.18	0.43
3:D:844:THR:OG1	3:D:858:VAL:HG21	2.18	0.43
6:H:30:ILE:HG23	6:H:82:ARG:HD3	2.00	0.43
2:C:546:GLU:OE1	2:C:546:GLU:N	2.50	0.43
5:F:428:SER:O	5:F:432:THR:OG1	2.19	0.43
5:F:449:THR:HG21	5:F:504:PRO:CG	2.48	0.43
6:G:18:CYS:SG	6:G:97:ILE:HG23	2.59	0.43
2:C:998:LEU:HD11	2:C:1014:LEU:HD23	2.01	0.43
2:C:191:LYS:O	2:C:193:ASN:ND2	2.51	0.43
2:C:782:VAL:HG22	2:C:783:LEU:N	2.33	0.43
3:D:973:LEU:HD23	3:D:1005:LYS:O	2.18	0.43
3:D:874:GLU:OE1	3:D:875:ASN:ND2	2.52	0.43
2:C:145:ILE:HG12	2:C:512:SER:HA	2.00	0.43
2:C:230:PHE:HB3	2:C:237:LEU:HD11	2.00	0.43
2:C:52:ALA:HB2	2:C:461:GLU:HG3	2.00	0.43
2:C:490:GLN:HA	2:C:493:ILE:HD12	1.99	0.43
2:C:732:ILE:C	2:C:732:ILE:HD12	2.39	0.43
3:D:1338:ALA:HB3	3:D:1340:LYS:NZ	2.33	0.43
5:F:127:ILE:HG23	5:F:261:LEU:HD22	2.01	0.43
6:H:72:GLU:OE1	6:H:72:GLU:N	2.41	0.43
2:C:389:PHE:HB3	2:C:420:LEU:HD13	2.01	0.43
2:C:768:MET:O	2:C:784:ALA:HB1	2.19	0.43
3:D:888:CYS:O	3:D:1258:ARG:NH2	2.51	0.43
3:D:320:ASN:OD1	3:D:321:LYS:N	2.52	0.43
3:D:492:SER:OG	3:D:494:ALA:N	2.50	0.43
5:F:320:ILE:HD12	5:F:327:SER:OG	2.18	0.43
2:C:790:ASP:N	2:C:793:GLU:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:835:GLU:O	2:C:836:LEU:HD22	2.18	0.43
3:D:747:MET:HG2	3:D:774:ILE:HG22	2.00	0.43
2:C:143:ARG:NH2	2:C:512:SER:O	2.51	0.43
2:C:1033:ARG:O	2:C:1037:THR:OG1	2.20	0.43
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.01	0.43
3:D:900:GLY:O	3:D:909:ILE:HG22	2.19	0.43
1:A:40:GLY:HA2	1:A:201:LEU:HD21	2.01	0.43
2:C:1099:ASN:HD21	2:C:1101:LEU:HD12	1.84	0.43
3:D:706:VAL:O	3:D:706:VAL:HG23	2.19	0.43
5:F:421:TYR:O	5:F:424:GLY:N	2.47	0.43
6:G:41:TYR:HB3	6:G:95:ALA:HB3	2.01	0.43
2:C:1120:ALA:HB2	2:C:1199:LEU:HD21	2.00	0.42
2:C:253:PHE:HZ	2:C:287:VAL:HG12	1.83	0.42
2:C:623:LEU:HD12	2:C:628:HIS:O	2.18	0.42
3:D:863:LEU:HD21	3:D:901:ARG:HH11	1.84	0.42
3:D:474:LEU:HD23	4:E:28:ARG:HG2	2.00	0.42
5:F:141:ILE:HG21	5:F:252:LEU:HD21	2.00	0.42
2:C:537:GLY:C	2:C:538:LEU:HD22	2.40	0.42
3:D:205:LEU:HD11	3:D:214:ARG:HG2	2.01	0.42
5:F:108:VAL:HG11	5:F:381:GLU:HB3	2.01	0.42
5:F:436:ARG:O	5:F:440:THR:OG1	2.22	0.42
5:F:600:HIS:NE2	6:G:54:GLU:O	2.52	0.42
2:C:829:THR:HG23	2:C:1059:ARG:HG2	2.01	0.42
2:C:577:VAL:HG23	2:C:661:VAL:O	2.20	0.42
3:D:1088:VAL:O	3:D:1097:ALA:HB3	2.19	0.42
5:F:154:GLU:OE1	5:F:157:ARG:NE	2.52	0.42
6:G:63:TYR:C	6:G:64:LEU:HD22	2.39	0.42
1:A:22:THR:OG1	1:A:207:THR:N	2.49	0.42
2:C:1288:GLN:O	2:C:1292:THR:HG23	2.20	0.42
3:D:1197:ASN:N	3:D:1210:ILE:O	2.45	0.42
3:D:788:LEU:HD21	3:D:791:ALA:HB3	2.02	0.42
3:D:955:LYS:O	3:D:992:LYS:NZ	2.46	0.42
5:F:107:THR:OG1	5:F:108:VAL:HG23	2.19	0.42
5:F:123:ILE:HG22	5:F:127:ILE:HD12	2.01	0.42
2:C:1002:LEU:CD1	2:C:1011:LEU:HD11	2.49	0.42
2:C:818:VAL:HG22	2:C:819:SER:N	2.34	0.42
3:D:1040:MET:SD	3:D:1078:LEU:N	2.92	0.42
3:D:132:LEU:HD23	3:D:133:ARG:HE	1.84	0.42
3:D:198:CYS:CB	3:D:224:LEU:HD13	2.49	0.42
3:D:707:ILE:HD12	3:D:719:PHE:CE2	2.54	0.42
3:D:478:LEU:CB	4:E:20:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1028:ILE:HG23	3:D:1120:THR:HG23	2.01	0.42
5:F:393:LYS:HZ2	5:F:394:TYR:HE1	1.66	0.42
5:F:596:ARG:HD3	6:G:52:LYS:HE3	2.01	0.42
2:C:229:ILE:HD11	2:C:332:ARG:NH1	2.34	0.42
2:C:32:LEU:HD23	2:C:130:MET:SD	2.59	0.42
2:C:857:VAL:HG11	2:C:862:LEU:CG	2.50	0.42
5:F:336:GLU:OE1	5:F:339:ARG:NH2	2.49	0.42
5:F:538:GLU:OE1	5:F:541:ARG:NH2	2.49	0.42
5:F:585:GLU:O	5:F:588:ARG:HB3	2.20	0.42
1:A:47:LEU:O	1:A:180:VAL:HG21	2.20	0.42
1:A:79:LEU:O	1:A:83:LEU:HD23	2.20	0.42
2:C:101:ARG:HG2	2:C:117:ILE:HG23	2.01	0.42
2:C:1214:ASP:OD1	2:C:1215:GLY:N	2.52	0.42
3:D:747:MET:O	3:D:755:ILE:HD12	2.20	0.42
2:C:1112:ILE:HG22	2:C:1116:HIS:CD2	2.55	0.42
2:C:1220:GLN:HG2	2:C:1221:PHE:N	2.35	0.42
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.49	0.42
3:D:262:THR:O	5:F:507:MET:N	2.45	0.42
3:D:608:CYS:SG	3:D:617:THR:OG1	2.52	0.42
9:3:2:A:N6	9:3:3:G:O6	2.53	0.42
2:C:755:LYS:NZ	2:C:767:GLN:O	2.50	0.42
2:C:9:LYS:HE3	2:C:791:LEU:HD22	2.01	0.42
2:C:840:SER:OG	2:C:1048:LYS:N	2.53	0.42
3:D:114:ILE:HG22	3:D:307:LEU:CD1	2.48	0.42
3:D:1371:ARG:HA	3:D:1374:ALA:HB3	2.01	0.42
3:D:825:VAL:HG22	3:D:833:GLU:CB	2.49	0.42
2:C:42:ASP:OD2	2:C:45:GLY:N	2.52	0.41
2:C:854:ILE:HG23	2:C:855:PRO:HD2	2.00	0.41
3:D:242:LEU:HD23	3:D:243:PRO:O	2.20	0.41
3:D:597:GLY:O	3:D:600:ALA:N	2.52	0.41
3:D:756:GLU:OE1	3:D:756:GLU:N	2.52	0.41
2:C:1068:GLY:N	2:C:1072:ASN:OD1	2.46	0.41
2:C:528:ARG:HB3	2:C:575:LEU:HD21	2.02	0.41
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.51	0.41
3:D:1145:PHE:HE1	3:D:1256:ILE:HD13	1.85	0.41
5:F:223:GLU:N	5:F:223:GLU:OE1	2.43	0.41
6:H:63:TYR:C	6:H:64:LEU:HD12	2.40	0.41
2:C:1161:LEU:H	2:C:1161:LEU:HD23	1.84	0.41
2:C:595:THR:OG1	2:C:600:THR:OG1	2.29	0.41
2:C:758:ARG:NH2	2:C:762:ASN:O	2.54	0.41
3:D:545:HIS:O	3:D:545:HIS:ND1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:553:THR:HG21	2:C:608:ALA:HB1	2.02	0.41
3:D:846:GLU:O	3:D:848:VAL:HG13	2.20	0.41
5:F:353:LEU:HD22	5:F:358:VAL:HG23	2.03	0.41
6:H:157:MET:O	6:H:164:GLN:N	2.53	0.41
2:C:60:GLN:OE1	2:C:65:ASN:N	2.53	0.41
3:D:191:SER:OG	3:D:192:MET:N	2.52	0.41
3:D:825:VAL:HG22	3:D:833:GLU:HB3	2.02	0.41
5:F:583:THR:HG23	5:F:586:ARG:NH2	2.35	0.41
6:H:118:ALA:O	6:H:121:ALA:HB3	2.20	0.41
2:C:1065:LYS:HB3	2:C:1235:LEU:HD12	2.02	0.41
2:C:797:GLY:N	2:C:1231:TYR:OH	2.41	0.41
2:C:866:ASP:N	2:C:870:ILE:O	2.44	0.41
2:C:871:VAL:HG12	2:C:872:TYR:O	2.20	0.41
3:D:1027:VAL:H	3:D:1120:THR:HG22	1.85	0.41
2:C:1333:LEU:CD2	3:D:327:LEU:HD13	2.51	0.41
3:D:950:ILE:HG21	3:D:982:LEU:HD23	2.02	0.41
2:C:902:LEU:HD21	5:F:610:PHE:O	2.21	0.41
6:H:137:LEU:HD13	6:H:141:GLY:C	2.41	0.41
2:C:1253:LEU:HD23	2:C:1253:LEU:N	2.35	0.41
2:C:237:LEU:HD22	2:C:289:VAL:HA	2.01	0.41
2:C:419:ILE:HG22	2:C:420:LEU:N	2.36	0.41
2:C:842:ASP:OD1	2:C:843:THR:N	2.51	0.41
3:D:384:LYS:CD	3:D:411:ILE:HG23	2.51	0.41
3:D:950:ILE:HB	3:D:1018:ALA:HB3	2.02	0.41
2:C:247:ARG:HA	2:C:274:ILE:HD11	2.03	0.41
2:C:746:ALA:HB2	2:C:971:LEU:HD21	2.02	0.41
6:G:75:LEU:HD11	6:G:102:PHE:HD2	1.84	0.41
1:A:210:THR:HG22	1:A:210:THR:O	2.21	0.41
3:D:600:ALA:O	3:D:604:MET:HB2	2.21	0.41
5:F:471:LEU:O	5:F:475:GLY:N	2.51	0.41
1:B:56:VAL:HG13	1:B:144:ILE:CG2	2.50	0.41
2:C:1103:VAL:O	2:C:1107:MET:N	2.46	0.41
3:D:530:PRO:O	3:D:533:ALA:HB3	2.21	0.41
3:D:80:HIS:HB3	3:D:83:VAL:HG21	2.03	0.41
5:F:305:LEU:HD13	5:F:319:ALA:HB2	2.03	0.41
6:G:188:LYS:HZ2	6:G:188:LYS:HB2	1.86	0.41
7:1:17:DT:H2'	7:1:18:DT:H71	2.03	0.41
1:A:28:LEU:HD13	1:A:29:GLU:N	2.36	0.41
2:C:1279:GLU:CD	3:D:917:VAL:HG21	2.41	0.41
2:C:520:PRO:O	2:C:524:ILE:HG22	2.21	0.41
2:C:838:CYS:SG	2:C:839:VAL:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:395:LYS:HE3	5:F:536:THR:HG23	2.02	0.41
3:D:71:LEU:CD1	3:D:90:VAL:HG21	2.50	0.41
6:H:104:GLN:O	6:H:108:VAL:HG23	2.20	0.41
7:1:29:DG:N2	8:2:62:DC:O2	2.46	0.40
1:A:229:GLU:O	1:A:233:ASP:N	2.50	0.40
3:D:949:SER:HB3	3:D:1016:THR:HG23	2.04	0.40
5:F:152:GLU:OE2	5:F:218:ARG:NH1	2.54	0.40
3:D:624:ILE:HA	3:D:627:THR:HG22	2.03	0.40
5:F:154:GLU:OE1	5:F:157:ARG:NH2	2.54	0.40
2:C:15:PHE:CG	2:C:1190:ALA:HB2	2.56	0.40
2:C:1292:THR:O	2:C:1296:ASP:N	2.48	0.40
2:C:935:THR:HG23	2:C:1048:LYS:HE3	2.04	0.40
3:D:720:ASN:O	3:D:722:ILE:HD12	2.21	0.40
5:F:262:VAL:HB	5:F:263:PRO:CD	2.51	0.40
3:D:395:LYS:NZ	5:F:613:ASP:OD1	2.36	0.40
2:C:230:PHE:CD1	2:C:237:LEU:HD11	2.57	0.40
2:C:758:ARG:HD3	2:C:833:ILE:HB	2.04	0.40
2:C:884:VAL:HB	2:C:918:LEU:HD12	2.04	0.40
2:C:905:ILE:HD11	5:F:599:ARG:HB2	2.03	0.40
2:C:995:ASP:OD1	2:C:996:ARG:N	2.54	0.40
3:D:1028:ILE:CG2	3:D:1120:THR:HG23	2.52	0.40
6:H:201:LYS:HG3	6:H:203:ILE:HD11	2.04	0.40
6:H:83:SER:OG	12:H:301:CMP:O5'	2.39	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	228/329 (69%)	201 (88%)	27 (12%)	0	100	100
1	B	226/329 (69%)	203 (90%)	23 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1338/1342 (100%)	1180 (88%)	154 (12%)	4 (0%)	43	80
3	D	1331/1407 (95%)	1160 (87%)	169 (13%)	2 (0%)	49	84
4	E	77/91 (85%)	69 (90%)	8 (10%)	0	100	100
5	F	479/628 (76%)	414 (86%)	57 (12%)	8 (2%)	10	48
6	G	195/210 (93%)	178 (91%)	15 (8%)	2 (1%)	17	58
6	H	195/210 (93%)	181 (93%)	13 (7%)	1 (0%)	31	73
All	All	4069/4546 (90%)	3586 (88%)	466 (12%)	17 (0%)	40	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA
5	F	264	LYS
6	G	100	LYS
5	F	295	CYS
5	F	507	MET
3	D	96	LYS
5	F	323	ASN
6	H	168	THR
2	C	1004	ASP
5	F	298	PRO
5	F	580	PHE
6	G	99	TYR
2	C	808	ASN
2	C	1136	GLN
3	D	121	PRO
5	F	263	PRO
5	F	166	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/286 (69%)	197 (100%)	1 (0%)	90	95
1	B	196/286 (68%)	196 (100%)	0	100	100
2	C	1155/1157 (100%)	1147 (99%)	8 (1%)	85	92
3	D	1120/1168 (96%)	1107 (99%)	13 (1%)	74	87
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	429/554 (77%)	419 (98%)	10 (2%)	53	76
6	G	170/181 (94%)	170 (100%)	0	100	100
6	H	170/181 (94%)	166 (98%)	4 (2%)	52	75
All	All	3505/3888 (90%)	3469 (99%)	36 (1%)	80	89

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
2	C	768	MET
2	C	903	ARG
2	C	976	ARG
2	C	1022	LYS
2	C	1147	ARG
2	C	1230	MET
2	C	1234	LYS
2	C	1246	ARG
3	D	50	LYS
3	D	76	LYS
3	D	133	ARG
3	D	214	ARG
3	D	276	ASN
3	D	280	LYS
3	D	424	ASN
3	D	610	ARG
3	D	644	MET
3	D	720	ASN
3	D	954	ASN
3	D	1151	LYS
3	D	1197	ASN
5	F	93	ARG
5	F	105	MET

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Mol	Chain	Res	Type
5	F	309	ASN
5	F	329	LYS
5	F	374	ARG
5	F	451	ARG
5	F	499	LYS
5	F	554	ARG
5	F	557	LYS
5	F	586	ARG
6	H	52	LYS
6	H	87	ARG
6	H	147	LEU
6	H	194	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	165	HIS
2	C	799	ASN
3	D	424	ASN
3	D	450	HIS
3	D	954	ASN
3	D	1279	GLN
6	G	159	HIS
6	H	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	3	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	3	3	G

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
12	CMP	G	301	-	20,25,25	1.43	2 (10%)	21,39,39	1.53	5 (23%)
12	CMP	H	301	-	20,25,25	1.41	4 (20%)	21,39,39	1.62	6 (28%)

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
12	CMP	G	301	-	-	0/0/31/31	0/4/4/4
12	CMP	H	301	-	-	0/0/31/31	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	301	CMP	P-O3'	3.72	1.64	1.58
12	H	301	CMP	P-O3'	3.01	1.63	1.58
12	H	301	CMP	C5-C4	3.01	1.47	1.40
12	G	301	CMP	C5-C4	3.00	1.47	1.40
12	H	301	CMP	O5'-C5'	-2.24	1.42	1.46
12	H	301	CMP	O3'-C3'	-2.01	1.41	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	301	CMP	N3-C2-N1	-3.63	122.83	128.68
12	H	301	CMP	C4-C5-N7	-3.13	106.13	109.40
12	G	301	CMP	C4-C5-N7	-3.04	106.23	109.40
12	G	301	CMP	N3-C2-N1	-2.90	124.01	128.68
12	H	301	CMP	O2P-P-O1P	2.89	117.75	108.62
12	G	301	CMP	O2P-P-O1P	2.81	117.49	108.62
12	H	301	CMP	O3'-C3'-C2'	2.30	117.86	115.61
12	G	301	CMP	O5'-P-O3'	2.22	108.86	105.72
12	H	301	CMP	O5'-P-O3'	2.15	108.77	105.72
12	H	301	CMP	C2-N1-C6	2.06	122.34	118.77
12	G	301	CMP	O5'-C5'-C4'	2.05	110.50	105.71

There are no chirality outliers.

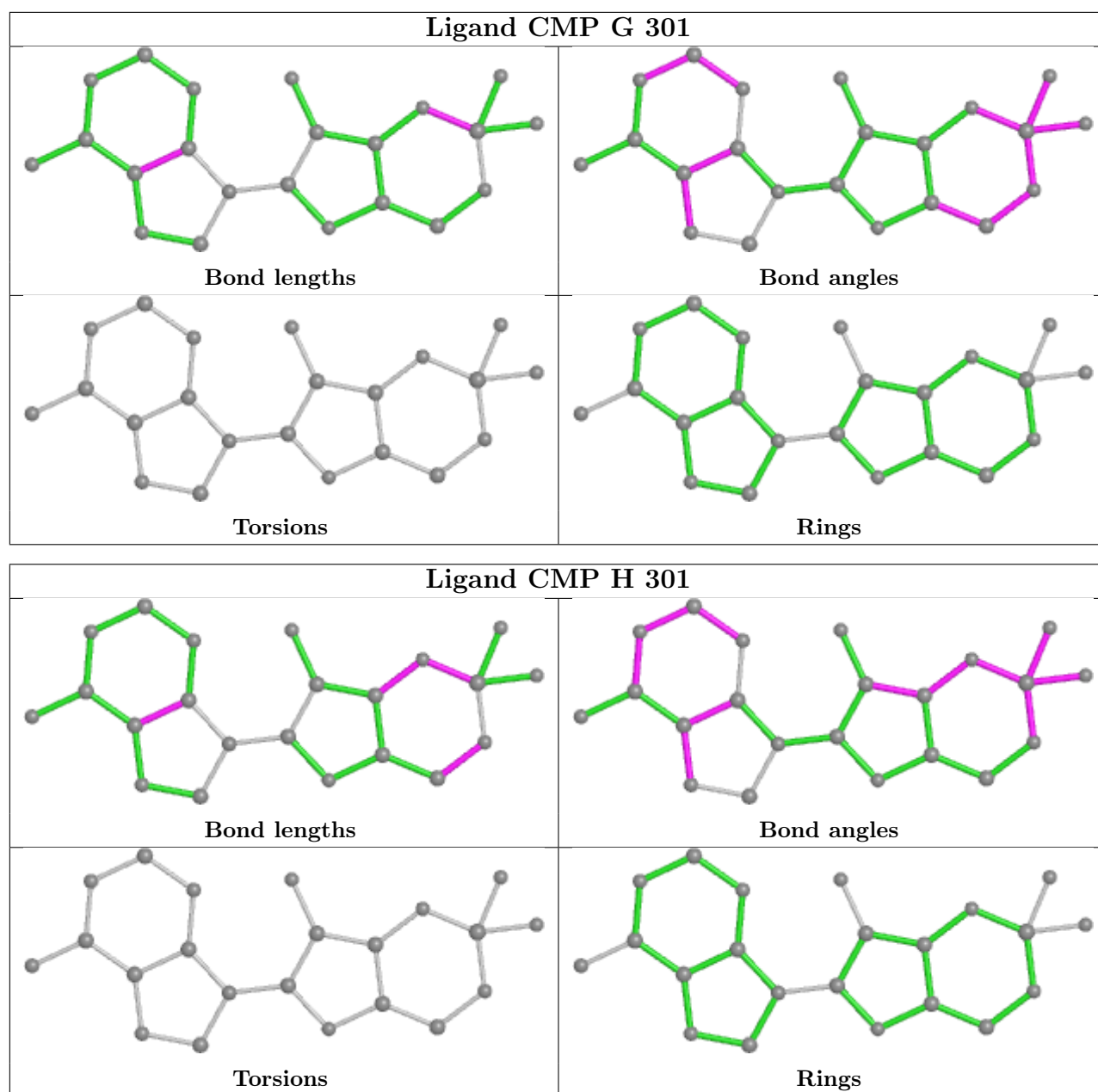
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	301	CMP	3	0
12	H	301	CMP	2	0

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.