



Full wwPDB EM Validation Report ⓘ

May 14, 2024 – 05:53 am BST

PDB ID : 6Z2X
EMDB ID : EMD-11051
Title : Mec1-Ddc2 (F2244L mutant) in complex with Mg AMP-PNP (State II)
Authors : Yates, L.A.; Zhang, X.
Deposited on : 2020-05-18
Resolution : 3.20 Å (reported)
Based on initial model : 6Z2W

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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

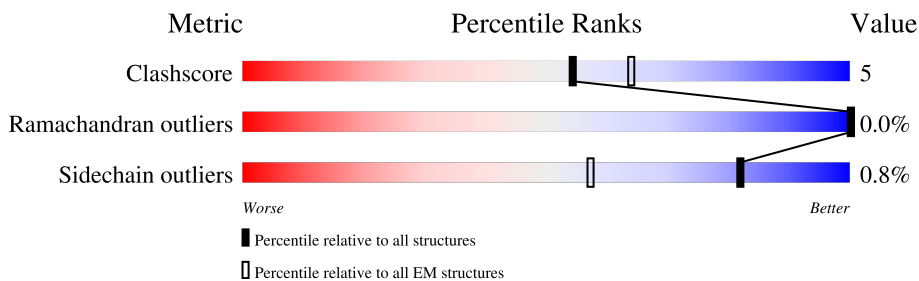
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	747	60% (green), 15% (yellow), 25% (grey)
1	D	747	59% (green), 15% (yellow), 25% (grey)
2	E	2368	83% (green), 14% (yellow), 3% (grey)
2	F	2368	83% (green), 15% (yellow), 2% (grey)

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 46604 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 DNA damage checkpoint protein LCD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	558	4576	2954	753	846	23	1	0
1	C	558	4576	2954	753	846	23	1	0

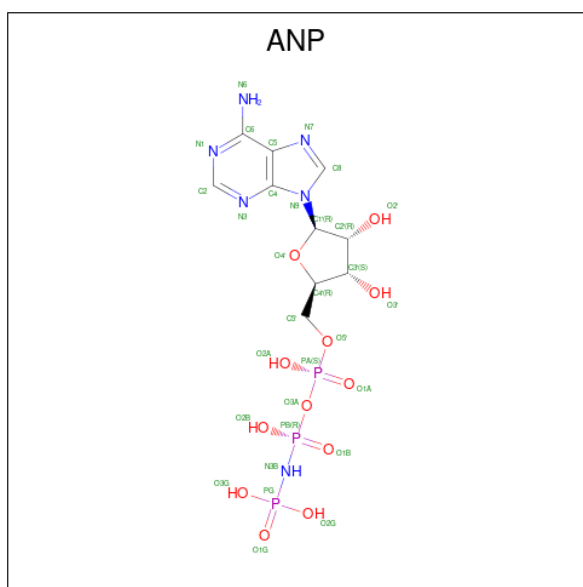
- Molecule 2 is a protein called Serine/threonine-protein kinase MEC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	2325	18692	12029	3127	3459	77	0	0
2	F	2325	18692	12029	3127	3459	77	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2244	LEU	PHE	engineered mutation	UNP P38111
F	2244	LEU	PHE	engineered mutation	UNP P38111

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



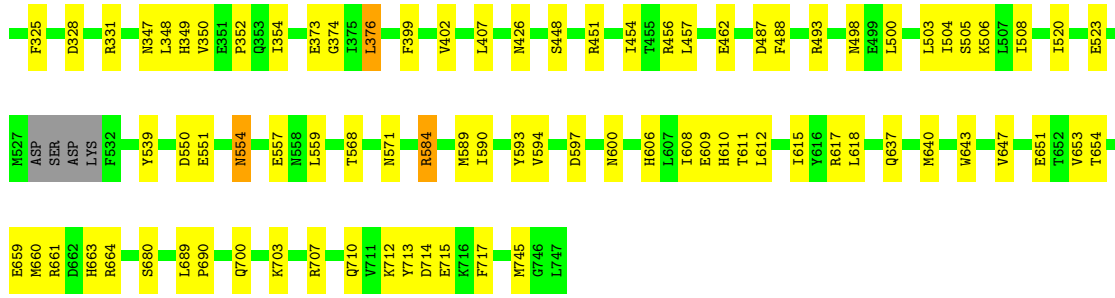
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	E	1	31	10	6	12	3	0
3	F	1	31	10	6	12	3	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

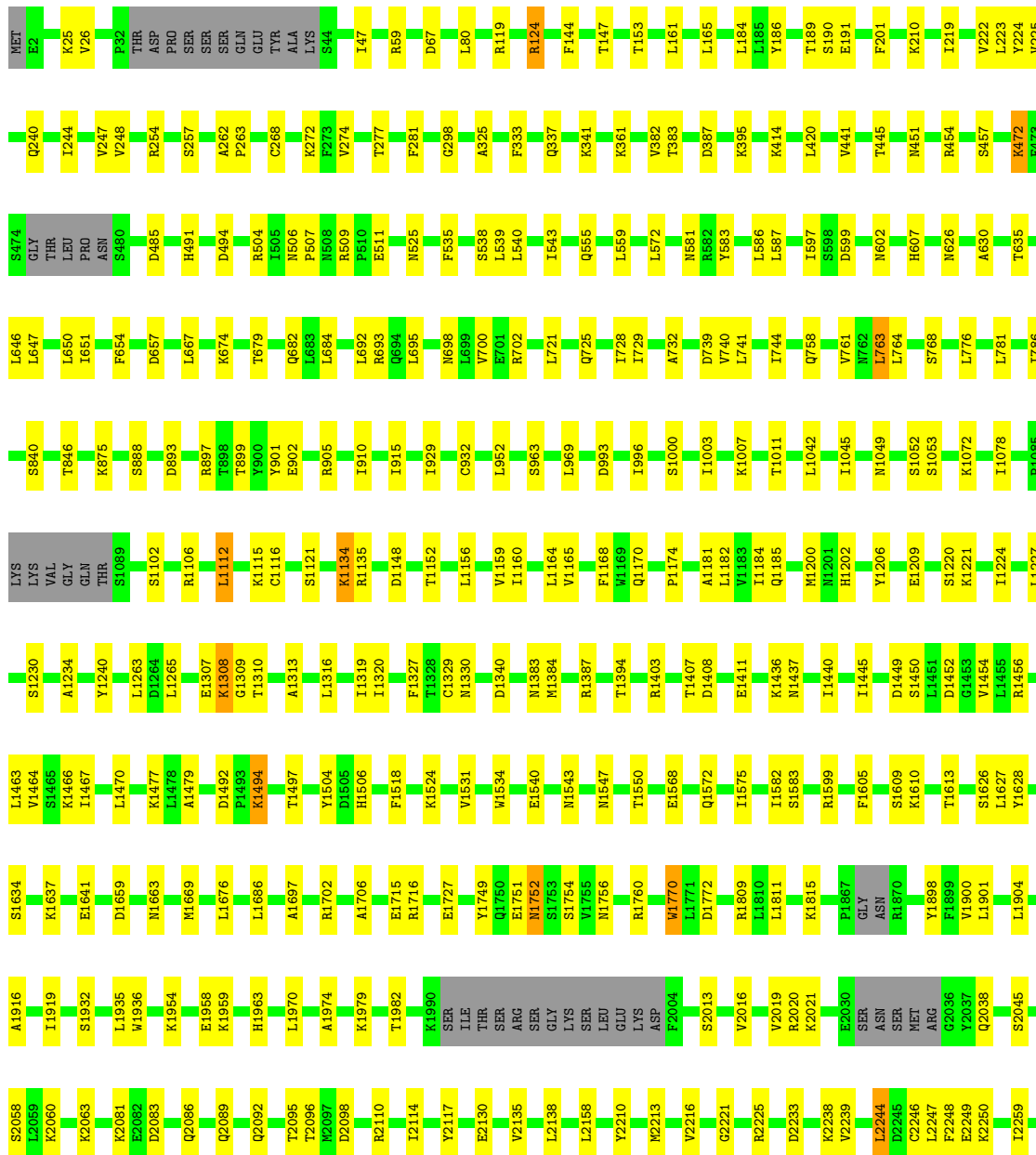
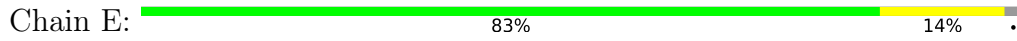
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	E	1	1	1	0
4	F	1	1	1	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	E	2	2	2	0
5	F	2	2	2	0

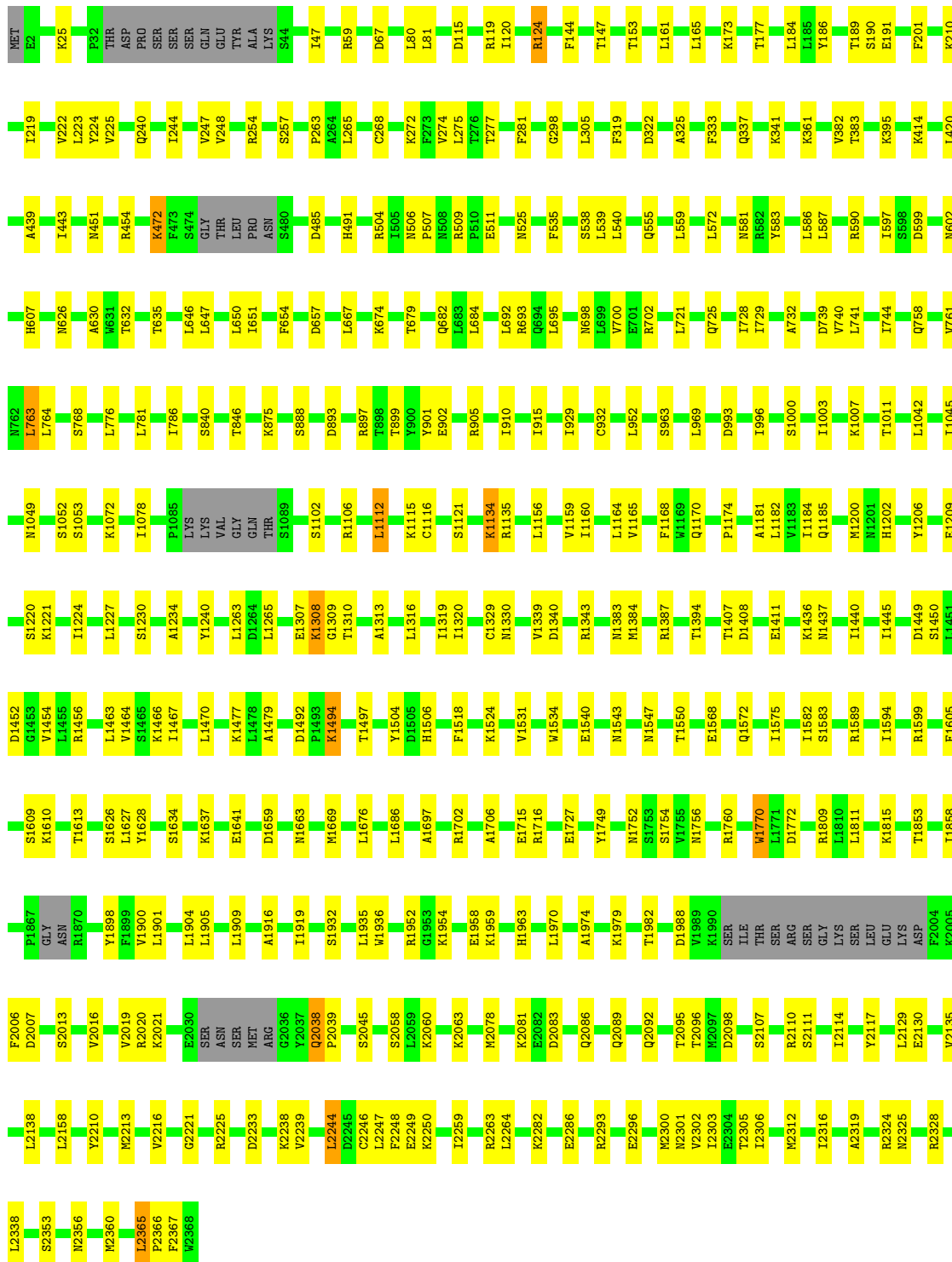
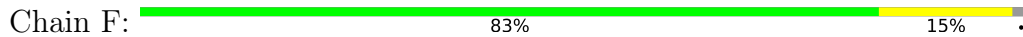


● Molecule 2: Serine/threonine-protein kinase MEC1





• Molecule 2: Serine/threonine-protein kinase MEC1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	12205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k 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: MG, ANP, ZN

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	C	0.41	0/4664	0.66	4/6303 (0.1%)
1	D	0.41	0/4664	0.66	4/6303 (0.1%)
2	E	0.35	0/19078	0.61	8/25836 (0.0%)
2	F	0.35	0/19078	0.61	8/25836 (0.0%)
All	All	0.37	0/47484	0.62	24/64278 (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
2	E	0	7
2	F	0	7
All	All	0	14

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1408	ASP	CB-CG-OD1	7.97	125.47	118.30
2	E	1408	ASP	CB-CG-OD1	7.96	125.47	118.30
1	C	376	LEU	CA-CB-CG	-6.62	100.07	115.30
1	D	376	LEU	CA-CB-CG	-6.60	100.13	115.30
2	E	657	ASP	CB-CG-OD1	6.49	124.14	118.30
2	F	657	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	231	LEU	CA-CB-CG	6.04	129.18	115.30
2	E	2138	LEU	CA-CB-CG	6.01	129.13	115.30
2	F	2138	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	231	LEU	CA-CB-CG	5.97	129.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	763	LEU	CA-CB-CG	5.96	129.02	115.30
2	F	763	LEU	CA-CB-CG	5.96	129.00	115.30
2	F	1227	LEU	CA-CB-CG	5.82	128.67	115.30
2	E	1227	LEU	CA-CB-CG	5.81	128.66	115.30
2	E	2365	LEU	CA-CB-CG	5.74	128.50	115.30
2	F	2365	LEU	CA-CB-CG	5.73	128.48	115.30
2	F	2244	LEU	CA-CB-CG	5.32	127.53	115.30
2	E	1407	THR	C-N-CA	5.32	134.99	121.70
2	F	1407	THR	C-N-CA	5.31	134.98	121.70
2	E	2244	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	597	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	597	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	212	LEU	CA-CB-CG	5.10	127.02	115.30
1	D	212	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1307	GLU	Peptide
2	E	1308	LYS	Peptide
2	E	1752	ASN	Peptide
2	E	1754	SER	Peptide
2	E	1770	TRP	Peptide
2	E	2264	LEU	Peptide
2	E	472	LYS	Peptide
2	F	1307	GLU	Peptide
2	F	1308	LYS	Peptide
2	F	1752	ASN	Peptide
2	F	1754	SER	Peptide
2	F	1770	TRP	Peptide
2	F	2264	LEU	Peptide
2	F	472	LYS	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	C	4576	0	4635	64	0
1	D	4576	0	4635	67	0
2	E	18692	0	18657	193	0
2	F	18692	0	18656	204	0
3	E	31	0	13	1	0
3	F	31	0	13	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	46604	0	46609	505	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 5.

All (505) 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)
2:E:2135:VAL:HG21	3:E:2401:ANP:H2	1.73	0.69
2:E:1506:HIS:O	2:E:1702:ARG:NH2	2.26	0.69
2:F:2135:VAL:HG21	3:F:2401:ANP:H2	1.73	0.69
2:F:1506:HIS:O	2:F:1702:ARG:NH2	2.26	0.68
2:F:776:LEU:HD23	2:F:840:SER:HB2	1.77	0.66
2:E:776:LEU:HD23	2:E:840:SER:HB2	1.77	0.66
2:E:153:THR:HG23	2:E:184:LEU:HD21	1.80	0.63
2:F:223:LEU:HD11	2:F:277:THR:HG23	1.80	0.63
2:F:153:THR:HG23	2:F:184:LEU:HD21	1.80	0.63
1:D:426:ASN:ND2	1:D:551:GLU:OE2	2.31	0.63
1:C:241:ASN:O	1:C:260:ARG:NH1	2.32	0.63
2:E:268:CYS:SG	2:E:272:LYS:NZ	2.72	0.63
1:C:426:ASN:ND2	1:C:551:GLU:OE2	2.31	0.62
2:E:1313:ALA:O	2:E:1316:LEU:HB3	1.99	0.62
2:F:268:CYS:SG	2:F:272:LYS:NZ	2.72	0.62
1:D:241:ASN:O	1:D:260:ARG:NH1	2.32	0.62
1:D:643:TRP:NE1	1:D:745:MET:SD	2.71	0.62
1:C:643:TRP:NE1	1:C:745:MET:SD	2.72	0.62
2:F:247:VAL:HG22	2:F:274:VAL:HG22	1.82	0.62
2:F:1313:ALA:O	2:F:1316:LEU:HB3	1.99	0.62
2:E:223:LEU:HD11	2:E:277:THR:HG23	1.80	0.61
2:E:247:VAL:HG22	2:E:274:VAL:HG22	1.82	0.61
2:E:1045:ILE:O	2:E:1049:ASN:ND2	2.33	0.61
2:F:1045:ILE:O	2:F:1049:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:506:ASN:HB3	2:E:509:ARG:HB3	1.82	0.61
2:E:1135:ARG:HH12	2:E:1613:THR:HA	1.66	0.60
2:F:506:ASN:HB3	2:F:509:ARG:HB3	1.82	0.60
2:F:1135:ARG:HH12	2:F:1613:THR:HA	1.66	0.60
2:F:1182:LEU:HD22	2:F:1234:ALA:HB3	1.83	0.60
1:C:557:GLU:HG3	1:C:617:ARG:HH12	1.67	0.60
2:E:1182:LEU:HD22	2:E:1234:ALA:HB3	1.83	0.60
1:D:637:GLN:HG2	2:E:667:LEU:HD23	1.84	0.59
2:F:165:LEU:HD21	2:F:224:TYR:HE2	1.69	0.58
2:E:700:VAL:HG13	2:E:740:VAL:HG12	1.86	0.58
2:E:2092:GLN:HA	2:E:2095:THR:HG22	1.86	0.58
2:F:1449:ASP:OD2	2:F:2110:ARG:NE	2.34	0.58
2:E:1749:TYR:O	2:E:1760:ARG:NH2	2.37	0.57
2:E:165:LEU:HD21	2:E:224:TYR:HE2	1.69	0.57
2:F:1749:TYR:O	2:F:1760:ARG:NH2	2.37	0.57
1:D:210:ILE:HG23	1:D:302:LEU:HD11	1.86	0.57
1:C:210:ILE:HG23	1:C:302:LEU:HD11	1.87	0.57
1:D:550:ASP:O	1:D:554:ASN:HB2	2.04	0.57
2:F:700:VAL:HG13	2:F:740:VAL:HG12	1.86	0.57
2:E:1898:TYR:O	2:E:1901:LEU:HB2	2.05	0.57
2:F:1160:ILE:HA	2:F:1164:LEU:HB2	1.87	0.57
2:E:1329:CYS:SG	2:E:1330:ASN:N	2.78	0.56
2:F:1626:SER:HB2	2:F:1669:MET:HG3	1.87	0.56
1:D:710:GLN:OE1	1:D:713:TYR:OH	2.21	0.56
1:C:487:ASP:H	1:C:500:LEU:HD12	1.70	0.56
2:E:124:ARG:NH1	2:E:186:TYR:O	2.39	0.56
2:F:1898:TYR:O	2:F:1901:LEU:HB2	2.05	0.56
2:F:2092:GLN:HA	2:F:2095:THR:HG22	1.86	0.56
1:D:487:ASP:H	1:D:500:LEU:HD12	1.69	0.56
1:D:700:GLN:HA	1:D:703:LYS:HG2	1.86	0.56
1:C:399:PHE:HA	1:C:402:VAL:HG12	1.88	0.56
1:D:399:PHE:HA	1:D:402:VAL:HG12	1.88	0.56
1:D:557:GLU:HG3	1:D:617:ARG:HH12	1.69	0.56
1:D:590:ILE:HG23	2:E:586:LEU:HD13	1.88	0.56
2:E:1449:ASP:OD2	2:E:2110:ARG:NE	2.34	0.56
1:D:197:ARG:NH1	1:C:195:PRO:O	2.36	0.56
2:E:1959:LYS:O	2:E:1963:HIS:ND1	2.39	0.56
1:D:712:LYS:NZ	1:D:715:GLU:OE2	2.36	0.55
2:F:124:ARG:NH1	2:F:186:TYR:O	2.39	0.55
2:E:1160:ILE:HA	2:E:1164:LEU:HB2	1.87	0.55
2:E:1686:LEU:HD23	2:E:1716:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:LYS:NZ	1:C:715:GLU:OE2	2.35	0.55
1:C:700:GLN:HA	1:C:703:LYS:HG2	1.87	0.55
2:E:2158:LEU:HD21	2:E:2367:PHE:HZ	1.72	0.55
2:F:635:THR:HG22	2:F:646:LEU:HB3	1.89	0.55
2:F:729:ILE:HD13	2:F:763:LEU:HD13	1.87	0.55
1:D:195:PRO:O	1:C:197:ARG:NH1	2.37	0.55
2:E:1383:ASN:O	2:E:1387:ARG:NH1	2.40	0.55
2:E:1626:SER:HB2	2:E:1669:MET:HG3	1.87	0.55
2:F:1072:LYS:HB3	2:F:1078:ILE:HB	1.89	0.55
2:E:506:ASN:O	2:E:509:ARG:NH1	2.35	0.55
2:F:1329:CYS:SG	2:F:1330:ASN:N	2.78	0.55
2:E:1102:SER:OG	2:E:1116:CYS:SG	2.65	0.55
2:F:1102:SER:OG	2:F:1116:CYS:SG	2.65	0.55
2:F:2158:LEU:HD21	2:F:2367:PHE:HZ	1.72	0.54
2:F:2210:TYR:OH	2:F:2263:ARG:O	2.25	0.54
2:E:1200:MET:HG2	2:E:1202:HIS:H	1.73	0.54
2:E:1492:ASP:HB3	2:E:1494:LYS:HD3	1.89	0.54
2:F:1686:LEU:HD23	2:F:1716:ARG:HH21	1.71	0.54
1:C:550:ASP:O	1:C:554:ASN:HB2	2.07	0.54
1:C:637:GLN:HG2	2:F:667:LEU:HD23	1.90	0.54
2:E:729:ILE:HD13	2:E:763:LEU:HD13	1.87	0.54
2:E:679:THR:H	2:E:682:GLN:HE21	1.56	0.54
2:F:144:PHE:HA	2:F:147:THR:HG22	1.89	0.54
2:F:506:ASN:O	2:F:509:ARG:NH1	2.35	0.54
2:F:1383:ASN:O	2:F:1387:ARG:NH1	2.40	0.54
1:D:651:GLU:OE2	1:D:654:THR:OG1	2.26	0.54
1:D:568:THR:O	1:D:571:ASN:ND2	2.41	0.54
1:C:714:ASP:HB3	1:C:717:PHE:HD2	1.73	0.53
2:E:1072:LYS:HB3	2:E:1078:ILE:HB	1.89	0.53
2:E:2210:TYR:OH	2:E:2263:ARG:O	2.25	0.53
2:F:2210:TYR:HD1	2:F:2239:VAL:HG11	1.73	0.53
1:C:651:GLU:OE2	1:C:654:THR:OG1	2.26	0.53
2:E:635:THR:HG22	2:E:646:LEU:HB3	1.89	0.53
2:F:2210:TYR:HB2	2:F:2239:VAL:HG21	1.90	0.53
1:C:568:THR:O	1:C:571:ASN:ND2	2.41	0.53
2:F:679:THR:H	2:F:682:GLN:HE21	1.56	0.53
2:F:1492:ASP:HB3	2:F:1494:LYS:HD3	1.89	0.53
2:F:1185:GLN:NE2	2:F:1230:SER:O	2.42	0.53
2:F:2296:GLU:OE2	2:F:2324:ARG:NH1	2.42	0.53
1:D:373:GLU:OE2	1:D:493:ARG:NH2	2.38	0.53
1:D:714:ASP:HB3	1:D:717:PHE:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:PHE:HA	2:E:147:THR:HG22	1.89	0.53
1:D:207:LEU:HD22	1:D:262:LYS:HD2	1.91	0.53
2:E:692:LEU:HA	2:E:695:LEU:HD13	1.91	0.53
2:E:698:ASN:HB2	2:E:702:ARG:HH21	1.74	0.53
2:F:1200:MET:HG2	2:F:1202:HIS:H	1.72	0.53
2:F:1959:LYS:O	2:F:1963:HIS:ND1	2.39	0.53
2:E:2117:TYR:HB2	2:E:2130:GLU:HB3	1.90	0.53
2:E:2210:TYR:HB2	2:E:2239:VAL:HG21	1.90	0.53
2:E:2210:TYR:HD1	2:E:2239:VAL:HG11	1.73	0.53
1:D:454:ILE:HD13	1:D:457:LEU:HD12	1.92	0.52
2:E:1320:ILE:HD12	2:E:1394:THR:HG21	1.92	0.52
2:E:2306:ILE:HG22	2:E:2316:ILE:HD11	1.91	0.52
2:F:626:ASN:O	2:F:630:ALA:N	2.40	0.52
2:F:647:LEU:HD23	2:F:650:LEU:HD12	1.91	0.52
2:E:1185:GLN:NE2	2:E:1230:SER:O	2.42	0.52
1:C:207:LEU:HD22	1:C:262:LYS:HD2	1.91	0.52
1:C:454:ILE:HD13	1:C:457:LEU:HD12	1.91	0.52
2:E:2296:GLU:OE2	2:E:2324:ARG:NH1	2.42	0.52
2:F:698:ASN:HB2	2:F:702:ARG:HH21	1.74	0.52
2:E:647:LEU:HD23	2:E:650:LEU:HD12	1.91	0.52
2:F:692:LEU:HA	2:F:695:LEU:HD13	1.91	0.52
2:F:2306:ILE:HG22	2:F:2316:ILE:HD11	1.91	0.52
1:D:539:TYR:O	1:D:600:ASN:ND2	2.40	0.52
2:E:201:PHE:HB3	2:E:210:LYS:HE3	1.92	0.52
2:F:201:PHE:HB3	2:F:210:LYS:HE3	1.92	0.52
1:C:226:LEU:HD23	1:C:229:LEU:HD12	1.92	0.52
1:C:373:GLU:OE2	1:C:493:ARG:NH2	2.39	0.52
2:E:1106:ARG:NH1	2:E:1340:ASP:OD2	2.43	0.52
2:F:1053:SER:OG	2:F:1170:GLN:O	2.28	0.52
2:F:2117:TYR:HB2	2:F:2130:GLU:HB3	1.90	0.52
2:F:1320:ILE:HD12	2:F:1394:THR:HG21	1.92	0.51
2:E:1470:LEU:HB2	2:E:1479:ALA:HB2	1.93	0.51
2:F:2282:LYS:NZ	2:F:2286:GLU:OE2	2.42	0.51
2:F:1659:ASP:O	2:F:1663:ASN:ND2	2.44	0.51
2:E:1053:SER:OG	2:E:1170:GLN:O	2.28	0.51
2:F:1106:ARG:NH1	2:F:1340:ASP:OD2	2.43	0.51
1:D:226:LEU:HD23	1:D:229:LEU:HD12	1.92	0.51
1:D:574:MET:O	1:D:578:SER:OG	2.26	0.51
2:E:2233:ASP:OD1	2:E:2238:LYS:N	2.44	0.51
2:F:1160:ILE:HG23	2:F:1184:ILE:HD11	1.92	0.51
2:E:1160:ILE:HG23	2:E:1184:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2058:SER:OG	2:F:2060:LYS:O	2.24	0.50
2:F:2233:ASP:OD1	2:F:2238:LYS:N	2.44	0.50
2:E:1659:ASP:O	2:E:1663:ASN:ND2	2.44	0.50
2:E:1772:ASP:OD2	2:E:1809:ARG:NH1	2.44	0.50
2:E:2060:LYS:HZ3	2:E:2081:LYS:HE2	1.75	0.50
2:F:1160:ILE:HG12	2:F:1184:ILE:HG13	1.94	0.50
2:F:2060:LYS:HZ3	2:F:2081:LYS:HE2	1.75	0.50
2:E:893:ASP:OD2	2:E:897:ARG:N	2.35	0.50
2:F:1452:ASP:OD2	2:F:1456:ARG:NH2	2.45	0.50
2:F:1463:LEU:HA	2:F:1466:LYS:HE2	1.93	0.50
2:E:1452:ASP:OD2	2:E:1456:ARG:NH2	2.45	0.50
1:C:328:ASP:HA	1:C:331:ARG:HG2	1.94	0.50
1:C:660:MET:HA	1:C:663:HIS:HD1	1.77	0.50
2:F:1772:ASP:OD2	2:F:1809:ARG:NH1	2.44	0.50
1:D:328:ASP:HA	1:D:331:ARG:HG2	1.94	0.50
2:E:2019:VAL:HG12	2:E:2021:LYS:H	1.77	0.50
2:F:764:LEU:O	2:F:768:SER:OG	2.27	0.49
2:F:1568:GLU:HA	2:F:1605:PHE:HZ	1.77	0.49
2:F:1470:LEU:HB2	2:F:1479:ALA:HB2	1.93	0.49
1:C:594:VAL:O	2:F:590:ARG:NH1	2.38	0.49
2:E:1160:ILE:HG12	2:E:1184:ILE:HG13	1.94	0.49
2:E:1463:LEU:HA	2:E:1466:LYS:HE2	1.93	0.49
2:F:1543:ASN:ND2	2:F:1572:GLN:OE1	2.45	0.49
2:F:189:THR:HA	2:F:254:ARG:HH12	1.78	0.49
2:F:1042:LEU:HD12	2:F:1045:ILE:HD11	1.95	0.49
2:E:626:ASN:O	2:E:630:ALA:N	2.40	0.49
2:E:2353:SER:OG	2:E:2356:ASN:ND2	2.45	0.49
1:C:606:HIS:O	1:C:610:HIS:N	2.45	0.49
1:C:640:MET:HG2	2:F:667:LEU:HG	1.93	0.49
1:C:237:PHE:HB3	1:C:244:ILE:HB	1.95	0.49
2:E:1568:GLU:HA	2:E:1605:PHE:HZ	1.77	0.49
2:F:451:ASN:HB3	2:F:454:ARG:HB3	1.95	0.49
1:D:237:PHE:HB3	1:D:244:ILE:HB	1.95	0.49
2:F:1531:VAL:O	2:F:1534:TRP:HB2	2.13	0.49
1:C:407:LEU:O	1:C:456:ARG:NH1	2.46	0.49
2:E:1042:LEU:HD12	2:E:1045:ILE:HD11	1.95	0.49
2:E:2098:ASP:HB3	2:E:2114:ILE:HG12	1.95	0.49
2:F:2098:ASP:HB3	2:F:2114:ILE:HG12	1.95	0.49
2:F:2019:VAL:HG12	2:F:2021:LYS:H	1.77	0.48
1:C:612:LEU:O	1:C:615:ILE:HB	2.13	0.48
2:E:1583:SER:HB3	2:E:1676:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:507:PRO:O	2:F:555:GLN:NE2	2.39	0.48
1:D:612:LEU:O	1:D:615:ILE:HB	2.12	0.48
1:D:660:MET:HA	1:D:663:HIS:HD1	1.77	0.48
2:F:1583:SER:HB3	2:F:1676:LEU:HB3	1.95	0.48
2:F:244:ILE:HA	2:F:247:VAL:HG12	1.96	0.48
2:F:2089:GLN:OE1	2:F:2305:THR:OG1	2.30	0.48
2:E:451:ASN:HB3	2:E:454:ARG:HB3	1.95	0.48
2:E:2096:THR:HG21	2:E:2302:VAL:HG21	1.95	0.48
2:F:902:GLU:OE2	2:F:905:ARG:NH2	2.43	0.48
2:E:2246:CYS:HB2	2:E:2250:LYS:HB3	1.96	0.48
2:E:1206:TYR:HB3	2:E:1209:GLU:HB2	1.96	0.48
1:C:609:GLU:OE1	1:C:707:ARG:NH1	2.42	0.48
2:F:1979:LYS:HA	2:F:1982:THR:HG22	1.96	0.48
1:D:349:HIS:H	2:E:1599:ARG:NH2	2.12	0.47
2:E:189:THR:HA	2:E:254:ARG:HH12	1.78	0.47
2:E:1531:VAL:O	2:E:1534:TRP:HB2	2.13	0.47
2:E:1979:LYS:HA	2:E:1982:THR:HG22	1.96	0.47
2:F:2325:ASN:OD1	2:F:2328:ARG:NH1	2.47	0.47
2:F:1464:VAL:HA	2:F:1467:ILE:HD12	1.96	0.47
2:F:2353:SER:OG	2:F:2356:ASN:ND2	2.45	0.47
1:D:349:HIS:H	2:E:1599:ARG:HH22	1.62	0.47
1:C:219:ASP:H	1:C:505:SER:HB3	1.80	0.47
2:E:764:LEU:O	2:E:768:SER:OG	2.27	0.47
2:E:1582:ILE:HD11	2:E:1634:SER:HB2	1.96	0.47
2:F:67:ASP:OD1	2:F:119:ARG:NH2	2.47	0.47
1:D:219:ASP:H	1:D:505:SER:HB3	1.80	0.47
1:C:590:ILE:HG23	2:F:586:LEU:HD13	1.96	0.47
2:F:1206:TYR:HB3	2:F:1209:GLU:HB2	1.96	0.47
2:F:1240:TYR:OH	2:F:1263:LEU:O	2.32	0.47
1:D:615:ILE:O	1:D:618:LEU:HB3	2.14	0.47
2:E:67:ASP:OD1	2:E:119:ARG:NH2	2.47	0.47
2:F:1900:VAL:O	2:F:1904:LEU:N	2.46	0.47
2:E:1464:VAL:HA	2:E:1467:ILE:HD12	1.96	0.47
2:E:507:PRO:O	2:E:555:GLN:NE2	2.39	0.47
2:F:888:SER:HB3	2:F:1174:PRO:HB2	1.97	0.47
2:F:1504:TYR:OH	2:F:1540:GLU:OE2	2.30	0.47
2:F:2246:CYS:HB2	2:F:2250:LYS:HB3	1.96	0.47
2:F:2096:THR:HG21	2:F:2302:VAL:HG21	1.96	0.47
2:E:1727:GLU:HG3	2:E:1770:TRP:HH2	1.80	0.47
2:E:2325:ASN:OD1	2:E:2328:ARG:NH1	2.48	0.47
2:F:963:SER:HB2	2:F:1007:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:888:SER:HB3	2:E:1174:PRO:HB2	1.97	0.47
2:E:1543:ASN:ND2	2:E:1572:GLN:OE1	2.45	0.47
2:E:2020:ARG:HD2	2:E:2117:TYR:HA	1.97	0.47
2:F:846:THR:HA	2:F:875:LYS:HG3	1.97	0.47
1:C:503:LEU:HD23	1:C:506:LYS:HE3	1.97	0.46
2:E:2282:LYS:NZ	2:E:2286:GLU:OE2	2.42	0.46
1:C:615:ILE:O	1:C:618:LEU:HB3	2.15	0.46
1:C:349:HIS:H	2:F:1599:ARG:HH22	1.63	0.46
2:E:244:ILE:HA	2:E:247:VAL:HG12	1.96	0.46
2:E:846:THR:HA	2:E:875:LYS:HG3	1.97	0.46
1:D:282:ILE:HG23	1:D:296:VAL:HG13	1.97	0.46
1:C:659:GLU:O	1:C:663:HIS:ND1	2.48	0.46
2:E:1954:LYS:O	2:E:1958:GLU:N	2.43	0.46
2:F:248:VAL:HG21	2:F:298:GLY:HA2	1.98	0.46
1:C:710:GLN:OE1	1:C:713:TYR:OH	2.22	0.46
1:D:689:LEU:HA	1:D:690:PRO:HD3	1.73	0.46
2:E:1003:ILE:HG22	2:E:1011:THR:HB	1.98	0.46
2:E:1052:SER:OG	2:E:1053:SER:N	2.49	0.46
2:E:1308:LYS:O	2:E:1310:THR:N	2.49	0.46
2:E:1575:ILE:HG12	2:E:1627:LEU:HD21	1.97	0.46
2:F:1582:ILE:HD11	2:F:1634:SER:HB2	1.96	0.46
1:D:503:LEU:HD23	1:D:506:LYS:HE3	1.97	0.46
2:E:1518:PHE:HB3	2:E:1524:LYS:HD2	1.97	0.46
2:F:1518:PHE:HB3	2:F:1524:LYS:HD2	1.97	0.46
2:F:1932:SER:HA	2:F:1935:LEU:HD12	1.97	0.46
2:F:1265:LEU:HD21	2:F:1319:ILE:HG21	1.97	0.46
2:F:2365:LEU:HA	2:F:2366:PRO:HD3	1.80	0.46
1:D:407:LEU:O	1:D:456:ARG:NH1	2.46	0.46
1:C:349:HIS:H	2:F:1599:ARG:NH2	2.13	0.46
1:C:454:ILE:HD11	1:C:559:LEU:HD21	1.98	0.46
2:E:963:SER:HB2	2:E:1007:LYS:HE3	1.97	0.46
2:E:1265:LEU:HD21	2:E:1319:ILE:HG21	1.97	0.46
2:F:728:ILE:O	2:F:732:ALA:N	2.44	0.46
2:F:1308:LYS:O	2:F:1310:THR:N	2.49	0.46
1:C:689:LEU:HA	1:C:690:PRO:HD3	1.73	0.46
2:F:1575:ILE:HG12	2:F:1627:LEU:HD21	1.97	0.46
2:F:1727:GLU:HG3	2:F:1770:TRP:HH2	1.80	0.46
2:F:2020:ARG:HD2	2:F:2117:TYR:HA	1.97	0.46
1:D:606:HIS:O	1:D:610:HIS:N	2.46	0.45
1:C:608:ILE:HA	1:C:611:THR:HG22	1.98	0.45
2:E:1494:LYS:HA	2:E:1497:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1052:SER:OG	2:F:1053:SER:N	2.49	0.45
1:D:608:ILE:HA	1:D:611:THR:HG22	1.98	0.45
1:C:462:GLU:HA	1:C:584:ARG:HH22	1.80	0.45
2:F:758:GLN:HA	2:F:761:VAL:HG12	1.99	0.45
2:F:1411:GLU:HG3	2:F:1445:ILE:HD11	1.98	0.45
2:E:1134:LYS:HE3	2:E:1610:LYS:HB2	1.98	0.45
2:F:1494:LYS:HA	2:F:1497:THR:HG22	1.98	0.45
1:D:462:GLU:HA	1:D:584:ARG:HH22	1.80	0.45
1:D:651:GLU:HG3	1:D:712:LYS:HD3	1.99	0.45
2:E:414:LYS:HD2	2:E:485:ASP:HA	1.99	0.45
2:E:1900:VAL:O	2:E:1904:LEU:N	2.46	0.45
2:F:173:LYS:O	2:F:177:THR:OG1	2.33	0.45
2:F:651:ILE:HD11	2:F:684:LEU:HD22	1.99	0.45
2:F:1756:ASN:HA	2:F:1760:ARG:HD2	1.99	0.45
1:D:719:GLU:HB2	2:E:26:VAL:HG21	1.98	0.45
1:C:304:TYR:HE1	1:C:374:GLY:HA3	1.82	0.45
1:C:488:PHE:HA	1:C:498:ASN:HA	1.98	0.45
2:E:1715:GLU:OE1	2:E:1716:ARG:NH1	2.50	0.45
1:D:640:MET:HG2	2:E:667:LEU:HG	1.98	0.45
2:E:248:VAL:HG21	2:E:298:GLY:HA2	1.97	0.45
2:F:414:LYS:HD2	2:F:485:ASP:HA	1.99	0.45
2:F:993:ASP:HA	2:F:996:ILE:HG12	1.98	0.45
1:D:304:TYR:HE1	1:D:374:GLY:HA3	1.82	0.45
1:D:589:MET:HA	1:D:593:TYR:HD2	1.81	0.45
1:D:659:GLU:O	1:D:663:HIS:ND1	2.49	0.45
2:E:2300:MET:HA	2:E:2303:ILE:HG22	1.98	0.45
2:F:781:LEU:HD22	2:F:786:ILE:HG21	1.99	0.45
1:C:282:ILE:HG23	1:C:296:VAL:HG13	1.98	0.45
2:E:728:ILE:O	2:E:732:ALA:N	2.44	0.45
2:E:758:GLN:HA	2:E:761:VAL:HG12	1.99	0.45
2:E:1411:GLU:HG3	2:E:1445:ILE:HD11	1.98	0.45
2:E:1932:SER:HA	2:E:1935:LEU:HD12	1.97	0.45
2:F:2300:MET:HA	2:F:2303:ILE:HG22	1.98	0.45
2:E:2089:GLN:OE1	2:E:2305:THR:OG1	2.30	0.45
2:E:161:LEU:HG	2:E:225:VAL:HG21	1.99	0.44
2:E:325:ALA:HA	2:E:333:PHE:HE1	1.82	0.44
2:F:632:THR:O	2:F:635:THR:OG1	2.30	0.44
2:F:1003:ILE:HG22	2:F:1011:THR:HB	1.98	0.44
2:F:1134:LYS:HE3	2:F:1610:LYS:HB2	1.98	0.44
2:F:910:ILE:HD12	2:F:929:ILE:HG22	1.98	0.44
2:F:1156:LEU:HA	2:F:1159:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:TYR:O	1:C:600:ASN:ND2	2.39	0.44
2:E:910:ILE:HD12	2:E:929:ILE:HG22	1.98	0.44
2:E:721:LEU:HD21	2:E:744:ILE:HG13	2.00	0.44
2:E:993:ASP:HA	2:E:996:ILE:HG12	1.98	0.44
1:D:680:SER:HB2	2:E:395:LYS:HD2	1.99	0.44
2:F:161:LEU:HG	2:F:225:VAL:HG21	1.99	0.44
2:F:420:LEU:HD11	2:F:454:ARG:HG3	2.00	0.44
1:D:454:ILE:HD11	1:D:559:LEU:HD21	2.00	0.44
1:C:376:LEU:HA	1:C:376:LEU:HD23	1.75	0.44
1:C:285:ILE:O	1:C:293:LYS:NZ	2.48	0.44
2:E:996:ILE:O	2:E:1000:SER:OG	2.36	0.44
2:F:1112:LEU:HA	2:F:1115:LYS:HG2	1.99	0.44
2:E:1637:LYS:N	2:E:1641:GLU:OE2	2.51	0.44
2:F:1936:TRP:NE1	2:F:2016:VAL:O	2.43	0.44
2:F:1637:LYS:N	2:F:1641:GLU:OE2	2.51	0.44
1:C:680:SER:HB2	2:F:395:LYS:HD2	2.00	0.43
2:E:420:LEU:HD11	2:E:454:ARG:HG3	2.00	0.43
2:E:511:GLU:HA	2:E:555:GLN:HB2	2.00	0.43
2:E:651:ILE:HD11	2:E:684:LEU:HD22	1.99	0.43
2:E:899:THR:HG23	2:E:901:TYR:H	1.83	0.43
2:E:929:ILE:HA	2:E:932:CYS:HB2	2.00	0.43
2:F:325:ALA:HA	2:F:333:PHE:HE1	1.83	0.43
2:F:1715:GLU:OE1	2:F:1716:ARG:NH1	2.50	0.43
2:F:2083:ASP:OD1	2:F:2083:ASP:N	2.50	0.43
1:D:596:GLN:NE2	2:E:494:ASP:O	2.50	0.43
2:E:781:LEU:HD22	2:E:786:ILE:HG21	1.99	0.43
2:E:902:GLU:OE2	2:E:905:ARG:NH2	2.43	0.43
2:E:1936:TRP:NE1	2:E:2016:VAL:O	2.43	0.43
2:E:1970:LEU:O	2:E:1974:ALA:HB2	2.18	0.43
2:F:1609:SER:OG	2:F:1610:LYS:N	2.51	0.43
2:F:1970:LEU:O	2:F:1974:ALA:HB2	2.18	0.43
2:E:725:GLN:HB2	2:E:729:ILE:HD12	2.00	0.43
2:E:1156:LEU:HA	2:E:1159:VAL:HG12	1.99	0.43
2:E:1756:ASN:HA	2:E:1760:ARG:HD2	1.99	0.43
2:E:2086:GLN:HE21	2:E:2247:LEU:HB2	1.83	0.43
2:F:1858:ILE:H	2:F:1858:ILE:HG13	1.64	0.43
2:E:1112:LEU:HA	2:E:1115:LYS:HG2	1.99	0.43
2:E:1609:SER:OG	2:E:1610:LYS:N	2.51	0.43
2:F:899:THR:HG23	2:F:901:TYR:H	1.83	0.43
1:D:285:ILE:O	1:D:293:LYS:NZ	2.51	0.43
1:D:488:PHE:HA	1:D:498:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:VAL:HG22	2:F:581:ASN:HB2	2.00	0.43
2:E:491:HIS:O	2:E:504:ARG:NH1	2.51	0.43
2:F:2259:ILE:N	2:F:2360:MET:SD	2.91	0.43
2:F:2086:GLN:HE21	2:F:2247:LEU:HB2	1.83	0.43
2:E:1240:TYR:OH	2:E:1263:LEU:O	2.32	0.43
2:E:1811:LEU:O	2:E:1815:LYS:HB2	2.18	0.43
2:E:2058:SER:OG	2:E:2060:LYS:O	2.24	0.43
2:F:511:GLU:HA	2:F:555:GLN:HB2	2.00	0.43
2:E:382:VAL:HG13	2:E:383:THR:HG22	2.01	0.43
2:F:491:HIS:O	2:F:504:ARG:NH1	2.51	0.43
2:F:2225:ARG:HH22	2:F:2244:LEU:H	1.67	0.43
2:F:721:LEU:HD21	2:F:744:ILE:HG13	2.00	0.43
2:F:1811:LEU:O	2:F:1815:LYS:HB2	2.18	0.43
1:C:647:VAL:HA	1:C:745:MET:HG2	2.00	0.43
2:E:219:ILE:HA	2:E:222:VAL:HG12	2.01	0.43
2:E:441:VAL:O	2:E:445:THR:OG1	2.27	0.43
2:E:1497:THR:HB	2:E:1534:TRP:HE1	1.84	0.43
2:F:382:VAL:HG13	2:F:383:THR:HG22	2.01	0.43
1:D:348:LEU:HB3	1:D:350:VAL:HG22	2.01	0.42
1:D:352:PRO:HB2	1:D:354:ILE:HG23	2.01	0.42
2:F:996:ILE:O	2:F:1000:SER:OG	2.36	0.42
2:F:2213:MET:HA	2:F:2216:VAL:HB	2.00	0.42
2:E:387:ASP:OD1	2:E:387:ASP:N	2.51	0.42
2:E:454:ARG:O	2:E:457:SER:OG	2.31	0.42
2:E:915:ILE:HG13	2:E:952:LEU:HD21	2.02	0.42
2:E:1751:GLU:HB3	2:E:1752:ASN:H	1.72	0.42
2:F:725:GLN:HB2	2:F:729:ILE:HD12	2.00	0.42
1:C:283:LYS:HD3	1:C:325:PHE:HE1	1.84	0.42
2:F:555:GLN:NE2	2:F:599:ASP:OD1	2.49	0.42
1:D:264:THR:OG1	1:D:265:LEU:N	2.53	0.42
2:E:2225:ARG:HH22	2:E:2244:LEU:H	1.67	0.42
2:F:741:LEU:HA	2:F:744:ILE:HG22	2.01	0.42
2:E:651:ILE:HA	2:E:654:PHE:HB3	2.00	0.42
2:E:741:LEU:HA	2:E:744:ILE:HG22	2.01	0.42
2:F:507:PRO:HG3	2:F:597:ILE:HD11	2.01	0.42
2:F:1221:LYS:HA	2:F:1224:ILE:HG22	2.02	0.42
1:D:653:VAL:HG22	2:E:581:ASN:HB2	2.02	0.42
2:E:559:LEU:HD13	2:E:607:HIS:CD2	2.55	0.42
2:E:1121:SER:HB2	2:E:1628:TYR:HB2	2.02	0.42
2:F:1450:SER:O	2:F:1454:VAL:N	2.49	0.42
1:C:589:MET:HA	1:C:593:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2083:ASP:OD1	2:E:2083:ASP:N	2.50	0.42
2:E:2213:MET:HA	2:E:2216:VAL:HB	2.00	0.42
2:E:2259:ILE:N	2:E:2360:MET:SD	2.91	0.42
2:F:535:PHE:HB3	2:F:539:LEU:HD23	2.02	0.42
2:F:1121:SER:HB2	2:F:1628:TYR:HB2	2.02	0.42
2:F:2013:SER:O	2:F:2045:SER:OG	2.38	0.42
2:F:651:ILE:HA	2:F:654:PHE:HB3	2.00	0.42
2:F:929:ILE:HA	2:F:932:CYS:HB2	2.00	0.42
2:F:2293:ARG:NH1	2:F:2338:LEU:O	2.53	0.42
1:C:448:SER:HA	1:C:451:ARG:HG2	2.02	0.42
2:E:507:PRO:HG3	2:E:597:ILE:HD11	2.01	0.42
2:E:1547:ASN:HB3	2:E:1550:THR:HG22	2.02	0.42
1:D:448:SER:HA	1:D:451:ARG:HG2	2.01	0.42
2:E:1916:ALA:HA	2:E:1919:ILE:HG22	2.01	0.42
2:F:559:LEU:HD13	2:F:607:HIS:CD2	2.55	0.42
2:F:739:ASP:HB3	2:F:741:LEU:H	1.85	0.42
2:F:1224:ILE:HD12	2:F:1224:ILE:HA	1.91	0.42
2:F:1497:THR:HB	2:F:1534:TRP:HE1	1.84	0.42
2:F:1697:ALA:HB3	2:F:1706:ALA:HB2	2.01	0.42
1:D:241:ASN:ND2	2:F:322:ASP:OD2	2.53	0.41
2:E:47:ILE:HD13	2:E:80:LEU:HD11	2.01	0.41
2:E:535:PHE:HB3	2:E:539:LEU:HD23	2.02	0.41
1:D:647:VAL:HG23	1:D:745:MET:HG3	2.02	0.41
1:D:689:LEU:HD23	1:D:694:GLU:HB3	2.02	0.41
1:C:278:ILE:HG23	1:C:299:LEU:HD22	2.02	0.41
2:F:1954:LYS:O	2:F:1958:GLU:N	2.43	0.41
1:D:283:LYS:HD3	1:D:325:PHE:HE1	1.85	0.41
1:D:661:ARG:HA	1:D:664:ARG:HG2	2.02	0.41
1:C:225:ILE:HG23	1:C:508:ILE:HD13	2.02	0.41
2:E:693:ARG:HA	2:E:728:ILE:HG22	2.03	0.41
2:F:219:ILE:HA	2:F:222:VAL:HG12	2.01	0.41
2:F:693:ARG:HA	2:F:728:ILE:HG22	2.03	0.41
2:F:2006:PHE:HB3	2:F:2007:ASP:H	1.70	0.41
2:F:1916:ALA:HA	2:F:1919:ILE:HG22	2.01	0.41
2:F:2016:VAL:HA	2:F:2045:SER:HA	2.03	0.41
1:D:206:PHE:HZ	1:D:306:ILE:HG23	1.86	0.41
1:C:661:ARG:HA	1:C:664:ARG:HG2	2.02	0.41
2:E:583:TYR:O	2:E:587:LEU:HB2	2.21	0.41
2:E:1697:ALA:HB3	2:E:1706:ALA:HB2	2.01	0.41
2:F:583:TYR:O	2:F:587:LEU:HB2	2.20	0.41
2:E:1168:PHE:HE1	2:E:1181:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2013:SER:O	2:E:2045:SER:OG	2.38	0.41
2:E:2263:ARG:HA	2:E:2364:TRP:HZ2	1.86	0.41
2:F:81:LEU:HD13	2:F:81:LEU:HA	1.92	0.41
2:F:337:GLN:O	2:F:341:LYS:HB2	2.20	0.41
2:F:915:ILE:HG13	2:F:952:LEU:HD21	2.02	0.41
1:D:225:ILE:HG23	1:D:508:ILE:HD13	2.02	0.41
1:D:675:ILE:HD13	1:D:701:LEU:HD11	2.03	0.41
2:E:240:GLN:HG2	2:E:281:PHE:HE1	1.85	0.41
2:E:555:GLN:NE2	2:E:599:ASP:OD1	2.49	0.41
2:E:1450:SER:O	2:E:1454:VAL:N	2.49	0.41
2:E:2248:PHE:HB3	2:E:2319:ALA:HB1	2.02	0.41
2:F:2038:GLN:HA	2:F:2039:PRO:HD3	1.85	0.41
1:D:503:LEU:HB3	1:D:520:ILE:HD13	2.01	0.41
2:E:190:SER:OG	2:E:191:GLU:N	2.53	0.41
2:E:1221:LYS:HA	2:E:1224:ILE:HG22	2.02	0.41
2:E:1224:ILE:HD12	2:E:1224:ILE:HA	1.91	0.41
2:E:2221:GLY:HA3	2:E:2249:GLU:H	1.85	0.41
2:E:2264:LEU:HD12	2:E:2264:LEU:HA	1.89	0.41
2:F:47:ILE:HD13	2:F:80:LEU:HD11	2.01	0.41
2:F:1168:PHE:HE1	2:F:1181:ALA:HB2	1.86	0.41
2:F:2078:MET:HB3	2:F:2129:LEU:HG	2.03	0.41
1:C:503:LEU:HB3	1:C:520:ILE:HD13	2.02	0.41
1:C:659:GLU:HB2	2:F:538:SER:HB3	2.03	0.41
2:E:262:ALA:HA	2:E:263:PRO:HD3	1.92	0.41
2:E:337:GLN:O	2:E:341:LYS:HB2	2.20	0.41
2:E:540:LEU:HD22	2:E:572:LEU:HD11	2.03	0.41
2:E:1165:VAL:HG21	2:E:1220:SER:HB2	2.02	0.41
2:F:190:SER:OG	2:F:191:GLU:N	2.53	0.41
2:F:257:SER:HA	2:F:263:PRO:HB3	2.03	0.41
2:F:1901:LEU:O	2:F:1905:LEU:N	2.51	0.41
1:D:659:GLU:HB2	2:E:538:SER:HB3	2.03	0.41
1:C:206:PHE:HZ	1:C:306:ILE:HG23	1.86	0.41
1:C:523:GLU:OE2	2:F:1589:ARG:NH1	2.54	0.41
2:E:739:ASP:HB3	2:E:741:LEU:H	1.85	0.41
2:E:1148:ASP:O	2:E:1152:THR:OG1	2.36	0.41
2:F:1165:VAL:HG21	2:F:1220:SER:HB2	2.02	0.41
2:F:2248:PHE:HB3	2:F:2319:ALA:HB1	2.02	0.41
1:C:348:LEU:HB3	1:C:350:VAL:HG22	2.03	0.40
1:C:352:PRO:HB2	1:C:354:ILE:HG23	2.03	0.40
2:F:115:ASP:OD1	2:F:115:ASP:N	2.54	0.40
2:F:1547:ASN:HB3	2:F:1550:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:TYR:HE1	1:D:490:GLY:HA2	1.85	0.40
2:E:543:ILE:HD12	2:E:543:ILE:HA	1.90	0.40
2:E:1156:LEU:HA	2:E:1156:LEU:HD23	1.93	0.40
2:E:1265:LEU:HA	2:E:1265:LEU:HD23	1.90	0.40
2:E:1327:PHE:HD1	2:E:1403:ARG:HG3	1.87	0.40
2:E:1437:ASN:HA	2:E:1440:ILE:HD12	2.04	0.40
2:E:1504:TYR:OH	2:E:1540:GLU:OE2	2.30	0.40
2:F:240:GLN:HG2	2:F:281:PHE:HE1	1.85	0.40
2:F:265:LEU:HD11	2:F:305:LEU:HD13	2.04	0.40
2:F:540:LEU:HD22	2:F:572:LEU:HD11	2.03	0.40
2:F:1437:ASN:HA	2:F:1440:ILE:HD12	2.03	0.40
2:F:1853:THR:HG21	2:F:2301:ASN:HD21	1.87	0.40
2:F:1988:ASP:OD1	2:F:1988:ASP:N	2.51	0.40
1:C:215:ILE:HD11	1:C:504:ILE:HG21	2.02	0.40
1:C:264:THR:OG1	1:C:265:LEU:N	2.54	0.40
2:F:893:ASP:OD2	2:F:897:ARG:N	2.35	0.40
2:F:1339:VAL:O	2:F:1343:ARG:HG2	2.22	0.40
2:F:1909:LEU:HD23	2:F:1952:ARG:HH22	1.86	0.40
2:F:2107:SER:O	2:F:2111:SER:N	2.55	0.40
2:F:2221:GLY:HA3	2:F:2249:GLU:H	1.84	0.40
2:E:247:VAL:HG13	2:E:274:VAL:HG13	2.04	0.40
2:E:257:SER:HA	2:E:263:PRO:HB3	2.03	0.40
2:F:120:ILE:H	2:F:120:ILE:HG13	1.72	0.40
2:F:439:ALA:O	2:F:443:ILE:HB	2.22	0.40
2:F:1156:LEU:HA	2:F:1156:LEU:HD23	1.93	0.40
2:F:1594:ILE:HG23	2:F:1627:LEU:HD22	2.03	0.40
1:D:294:LEU:HD12	1:D:517:PRO:HG3	2.03	0.40
2:E:2016:VAL:HA	2:E:2045:SER:HA	2.03	0.40
2:F:275:LEU:HD22	2:F:319:PHE:HB2	2.04	0.40
2:F:2019:VAL:HA	2:F:2130:GLU:HG3	2.03	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	C	555/747 (74%)	511 (92%)	44 (8%)	0	100	100
1	D	555/747 (74%)	511 (92%)	44 (8%)	0	100	100
2	E	2311/2368 (98%)	2119 (92%)	191 (8%)	1 (0%)	100	100
2	F	2311/2368 (98%)	2119 (92%)	191 (8%)	1 (0%)	100	100
All	All	5732/6230 (92%)	5260 (92%)	470 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1309	GLY
2	F	1309	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	517/698 (74%)	514 (99%)	3 (1%)	86	94
1	D	517/698 (74%)	514 (99%)	3 (1%)	86	94
2	E	2068/2174 (95%)	2050 (99%)	18 (1%)	78	91
2	F	2068/2174 (95%)	2050 (99%)	18 (1%)	78	91
All	All	5170/5744 (90%)	5128 (99%)	42 (1%)	82	93

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	347	ASN
1	D	554	ASN
1	D	584	ARG
1	C	347	ASN
1	C	554	ASN
1	C	584	ARG

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Mol	Chain	Res	Type
2	E	25	LYS
2	E	59	ARG
2	E	124	ARG
2	E	361	LYS
2	E	472	LYS
2	E	525	ASN
2	E	602	ASN
2	E	674	LYS
2	E	969	LEU
2	E	1112	LEU
2	E	1134	LYS
2	E	1384	MET
2	E	1436	LYS
2	E	1477	LYS
2	E	1494	LYS
2	E	2038	GLN
2	E	2063	LYS
2	E	2312	MET
2	F	25	LYS
2	F	59	ARG
2	F	124	ARG
2	F	361	LYS
2	F	472	LYS
2	F	525	ASN
2	F	602	ASN
2	F	674	LYS
2	F	969	LEU
2	F	1112	LEU
2	F	1134	LYS
2	F	1384	MET
2	F	1436	LYS
2	F	1477	LYS
2	F	1494	LYS
2	F	2038	GLN
2	F	2063	LYS
2	F	2312	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	353	GLN
1	D	554	ASN

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Mol	Chain	Res	Type
1	C	353	GLN
1	C	554	ASN
2	E	602	ASN
2	E	682	GLN
2	E	986	ASN
2	E	1274	HIS
2	E	1439	GLN
2	E	1840	ASN
2	E	1847	ASN
2	E	1943	ASN
2	E	2086	GLN
2	E	2317	GLN
2	E	2356	ASN
2	F	602	ASN
2	F	682	GLN
2	F	986	ASN
2	F	1274	HIS
2	F	1439	GLN
2	F	1840	ASN
2	F	1847	ASN
2	F	1943	ASN
2	F	2086	GLN
2	F	2317	GLN
2	F	2356	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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
3	ANP	E	2401	5	29,33,33	1.09	4 (13%)	31,52,52	1.27	3 (9%)
3	ANP	F	2401	5	29,33,33	1.09	4 (13%)	31,52,52	1.27	3 (9%)

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
3	ANP	E	2401	5	-	7/14/38/38	0/3/3/3
3	ANP	F	2401	5	-	7/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2401	ANP	PB-O3A	-2.89	1.55	1.59
3	F	2401	ANP	PB-O3A	-2.87	1.55	1.59
3	F	2401	ANP	PG-O1G	2.28	1.49	1.46
3	E	2401	ANP	PG-O1G	2.27	1.49	1.46
3	F	2401	ANP	PG-N3B	2.23	1.69	1.63
3	E	2401	ANP	PG-N3B	2.21	1.69	1.63
3	E	2401	ANP	PB-O1B	2.08	1.49	1.46
3	F	2401	ANP	PB-O1B	2.05	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2401	ANP	PB-O3A-PA	-4.71	116.02	132.62
3	E	2401	ANP	PB-O3A-PA	-4.71	116.03	132.62
3	F	2401	ANP	O1G-PG-N3B	-2.28	108.41	111.77
3	E	2401	ANP	O1G-PG-N3B	-2.28	108.41	111.77
3	E	2401	ANP	C5-C6-N6	2.26	123.78	120.35
3	F	2401	ANP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

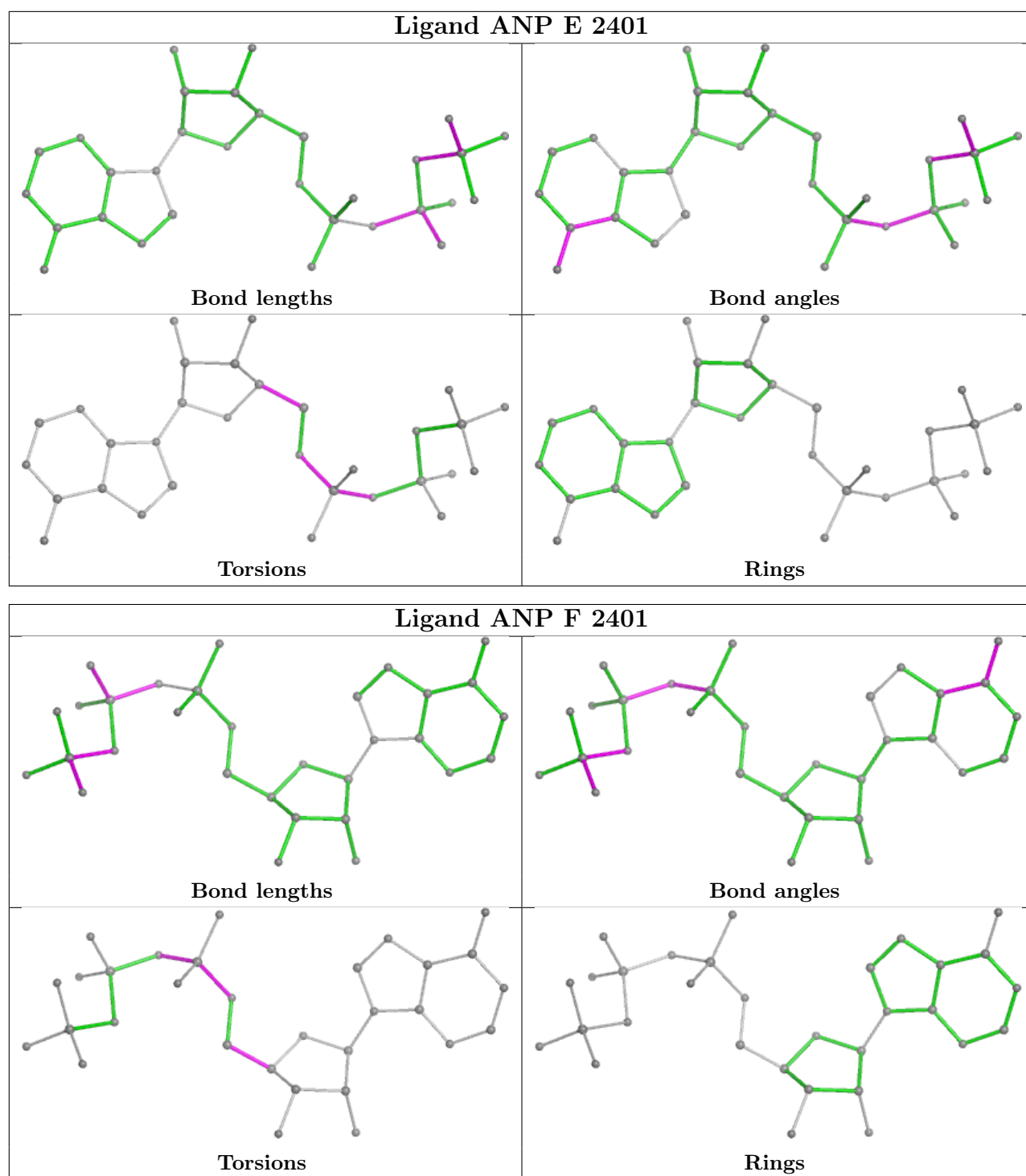
Mol	Chain	Res	Type	Atoms
3	E	2401	ANP	C5'-O5'-PA-O1A
3	E	2401	ANP	O4'-C4'-C5'-O5'
3	E	2401	ANP	C3'-C4'-C5'-O5'
3	F	2401	ANP	C5'-O5'-PA-O1A
3	F	2401	ANP	O4'-C4'-C5'-O5'
3	F	2401	ANP	C3'-C4'-C5'-O5'
3	E	2401	ANP	PB-O3A-PA-O1A
3	F	2401	ANP	PB-O3A-PA-O1A
3	E	2401	ANP	C5'-O5'-PA-O3A
3	F	2401	ANP	C5'-O5'-PA-O3A
3	E	2401	ANP	C5'-O5'-PA-O2A
3	F	2401	ANP	C5'-O5'-PA-O2A
3	E	2401	ANP	PB-O3A-PA-O2A
3	F	2401	ANP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2401	ANP	1	0
3	F	2401	ANP	1	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

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11051. 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.