



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:56 PM UTC

PDB ID : 1XQS / pdb_00001xqs
Title : Crystal structure of the HspBP1 core domain complexed with the fragment of Hsp70 ATPase domain
Authors : Shomura, Y.; Dragovic, Z.; Chang, H.C.; Tzvetkov, N.; Young, J.C.; Brodsky, J.L.; Guerriero, V.; Hartl, F.U.; Bracher, A.
Deposited on : 2004-10-13
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

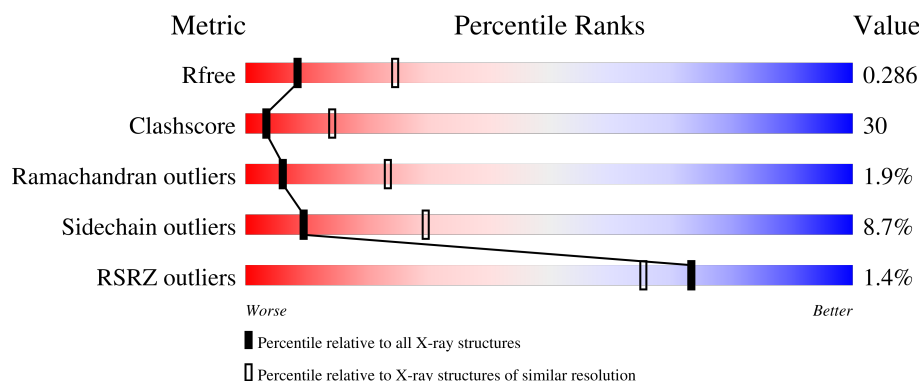
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
2	C	191	
2	D	191	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6795 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 HSPBP1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1278	368	380	20			
1	B	264	Total	C	N	O	S	0	0	0
			2022	1265	362	375	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLY	-	cloning artifact	UNP Q9NZL4
A	81	SER	-	cloning artifact	UNP Q9NZL4
A	82	HIS	-	cloning artifact	UNP Q9NZL4
A	83	MET	-	cloning artifact	UNP Q9NZL4
A	88	GLY	GLU	engineered mutation	UNP Q9NZL4
B	80	GLY	-	cloning artifact	UNP Q9NZL4
B	81	SER	-	cloning artifact	UNP Q9NZL4
B	82	HIS	-	cloning artifact	UNP Q9NZL4
B	83	MET	-	cloning artifact	UNP Q9NZL4
B	88	GLY	GLU	engineered mutation	UNP Q9NZL4

- Molecule 2 is a protein called Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	165	Total	C	N	O	S	0	0	0
			1316	825	237	252	2			
2	D	165	Total	C	N	O	S	0	0	0
			1316	825	237	252	2			

There are 6 discrepancies between the modelled and reference sequences:

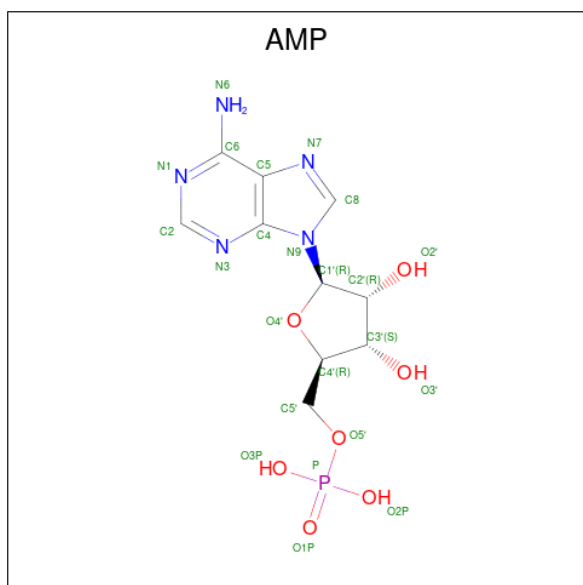
Chain	Residue	Modelled	Actual	Comment	Reference
C	181	GLY	-	cloning artifact	UNP P08107
C	182	ALA	-	cloning artifact	UNP P08107

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Chain	Residue	Modelled	Actual	Comment	Reference
C	183	MET	-	cloning artifact	UNP P08107
D	181	GLY	-	cloning artifact	UNP P08107
D	182	ALA	-	cloning artifact	UNP P08107
D	183	MET	-	cloning artifact	UNP P08107

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

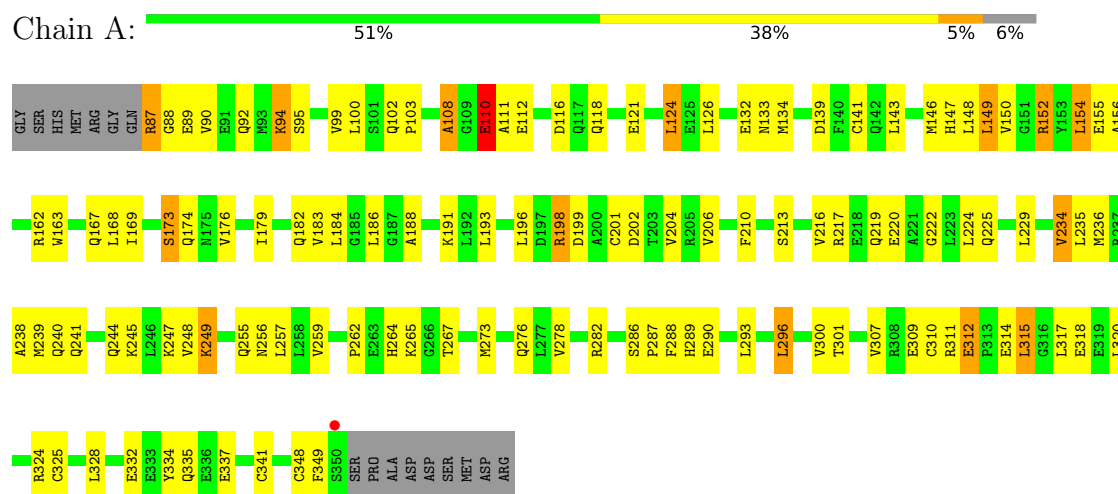
- Molecule 4 is water.

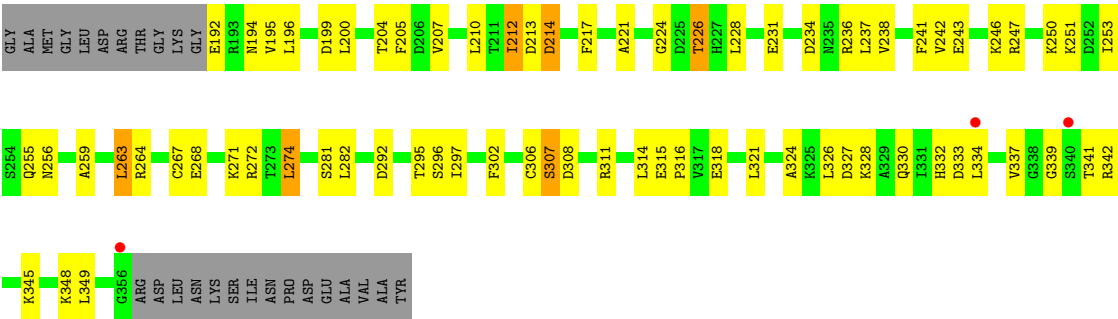
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	6	Total	O	0	0
			6	6		
4	C	18	Total	O	0	0
			18	18		
4	D	7	Total	O	0	0
			7	7		

3 Residue-property plots

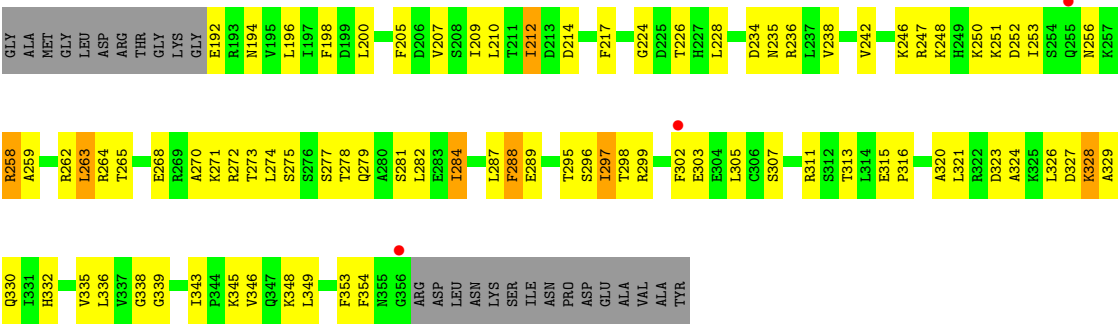
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: HSPBP1 protein





● Molecule 2: Heat shock 70 kDa protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.48Å 94.81Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 2.90 46.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.60-2.90) 99.7 (46.60-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.296 0.236 , 0.286	Depositor DCC
R_{free} test set	1258 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6795	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2073	1.03	8/2793 (0.3%)
1	B	0.45	0/2049	0.94	3/2765 (0.1%)
2	C	0.53	0/1334	0.94	2/1790 (0.1%)
2	D	0.49	0/1334	0.94	2/1790 (0.1%)
All	All	0.50	0/6790	0.97	15/9138 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLY	N-CA-C	-7.75	106.14	114.67
1	A	234	VAL	N-CA-C	-6.75	103.90	110.72
2	C	224	GLY	N-CA-C	6.55	118.79	111.85
2	D	224	GLY	N-CA-C	6.32	119.67	110.63
1	B	94	LYS	N-CA-C	-6.13	105.66	113.01
1	A	94	LYS	N-CA-C	-5.90	105.34	112.54
1	A	152	ARG	N-CA-C	5.82	118.50	111.40
1	A	173	SER	N-CA-C	5.81	118.56	111.82
1	A	121	GLU	N-CA-C	-5.62	105.06	111.07
1	B	138	ALA	N-CA-C	-5.43	105.26	111.07
1	A	150	VAL	N-CA-C	5.26	115.47	110.42
1	B	298	SER	N-CA-C	-5.25	107.04	113.50
2	C	341	THR	N-CA-C	-5.24	106.12	112.88
2	D	284	ILE	N-CA-C	5.09	114.82	106.72
1	A	220	GLU	N-CA-C	5.01	117.13	111.11

There are no chirality outliers.

There are no planarity outliers.

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	2046	0	2057	109	0
1	B	2022	0	2018	170	0
2	C	1316	0	1321	67	0
2	D	1316	0	1321	78	0
3	C	23	0	12	1	0
3	D	23	0	12	3	0
4	A	18	0	0	0	0
4	B	6	0	0	5	0
4	C	18	0	0	1	0
4	D	7	0	0	2	0
All	All	6795	0	6741	404	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 30.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG12	1:A:288:PHE:CG	1.85	1.11
1:A:273:MET:CE	1:A:276:GLN:HB3	1.80	1.11
1:B:239:MET:HE1	1:B:273:MET:SD	1.90	1.11
1:B:94:LYS:HG2	1:B:143:LEU:HD21	1.32	1.08
1:A:103:PRO:HA	1:A:152:ARG:HH22	1.15	1.05
1:A:273:MET:HE3	1:A:273:MET:HA	1.40	1.00
1:A:100:LEU:HD21	1:A:124:LEU:HD13	1.46	0.97
2:C:194:ASN:H	2:C:332:HIS:HD2	1.13	0.95
1:B:236:MET:HE2	1:B:273:MET:HB2	1.50	0.93
1:B:146:MET:HA	1:B:146:MET:HE2	1.48	0.92
1:B:239:MET:HE2	1:B:273:MET:HE1	1.49	0.92
1:B:94:LYS:HG2	1:B:143:LEU:CD2	2.01	0.90
1:A:248:VAL:HG12	1:A:288:PHE:CD2	2.06	0.90
1:B:100:LEU:HD21	1:B:124:LEU:HD13	1.52	0.89
1:A:273:MET:HE2	1:A:276:GLN:HB3	1.54	0.89
2:C:194:ASN:H	2:C:332:HIS:CD2	1.91	0.88
1:A:103:PRO:HA	1:A:152:ARG:NH2	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:CE	1:A:276:GLN:CB	2.55	0.83
2:C:295:THR:HG22	2:C:296:SER:N	1.93	0.83
2:C:342:ARG:HD2	3:C:401:AMP:N6	1.94	0.82
1:A:248:VAL:HG12	1:A:288:PHE:CB	2.10	0.81
1:A:262:PRO:HB3	1:A:265:LYS:HE3	1.61	0.81
1:B:262:PRO:HB3	1:B:265:LYS:HE3	1.63	0.81
1:B:90:VAL:O	1:B:94:LYS:HG3	1.80	0.80
1:A:179:ILE:O	1:A:183:VAL:HG23	1.81	0.79
1:B:123:ALA:O	1:B:127:LEU:HB2	1.81	0.79
1:B:301:THR:HA	4:B:521:HOH:O	1.83	0.78
1:A:154:LEU:HD13	1:A:169:ILE:CD1	2.14	0.78
1:B:97:LEU:HD12	1:B:143:LEU:HD22	1.66	0.78
1:B:100:LEU:HG	1:B:153:TYR:CZ	2.19	0.77
1:B:255:GLN:O	1:B:259:VAL:HG23	1.84	0.77
2:C:238:VAL:O	2:C:242:VAL:HG23	1.83	0.77
2:D:194:ASN:H	2:D:332:HIS:CD2	2.03	0.77
2:D:315:GLU:HB3	2:D:316:PRO:HD3	1.65	0.77
1:A:236:MET:HG3	1:A:273:MET:HE1	1.67	0.77
2:D:258:ARG:NH1	2:D:262:ARG:HD2	2.00	0.76
1:A:273:MET:HE3	1:A:276:GLN:HB3	1.67	0.76
1:B:220:GLU:O	1:B:224:LEU:HD13	1.86	0.76
2:D:295:THR:HG22	2:D:296:SER:H	1.51	0.76
2:D:194:ASN:H	2:D:332:HIS:HD2	1.31	0.76
2:D:256:ASN:HD22	2:D:259:ALA:HB2	1.51	0.76
2:C:295:THR:HG22	2:C:296:SER:H	1.51	0.75
1:A:100:LEU:HD21	1:A:124:LEU:CD1	2.17	0.74
2:C:307:SER:HB2	2:C:311:ARG:HH12	1.51	0.74
1:B:239:MET:CE	1:B:273:MET:HE1	2.17	0.73
2:C:315:GLU:HB3	2:C:316:PRO:HD3	1.68	0.73
1:A:92:GLN:O	1:A:95:SER:HB3	1.89	0.73
1:B:219:GLN:NE2	1:B:221:ALA:HB3	2.03	0.73
1:B:193:LEU:HD21	1:B:226:PHE:HE1	1.54	0.73
1:B:344:LEU:O	1:B:348:CYS:HB2	1.88	0.72
1:B:256:ASN:ND2	1:B:256:ASN:O	2.23	0.72
1:B:177:ALA:O	1:B:181:GLU:HG3	1.90	0.72
1:A:273:MET:HE1	1:A:276:GLN:HG2	1.71	0.72
1:B:90:VAL:HG13	1:B:94:LYS:HE3	1.73	0.71
1:B:312:GLU:HB2	1:B:315:LEU:HD13	1.72	0.70
1:B:240:GLN:HG2	1:B:276:GLN:OE1	1.90	0.70
2:C:255:GLN:HE21	2:D:323:ASP:HB3	1.56	0.70
1:B:236:MET:HE2	1:B:273:MET:HE2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:HB3	1:B:335:GLN:HE21	1.56	0.70
2:D:198:PHE:HB3	2:D:336:LEU:HD23	1.72	0.70
1:A:236:MET:O	1:A:240:GLN:HG3	1.92	0.70
1:A:262:PRO:O	1:A:265:LYS:HG3	1.91	0.70
1:B:134:MET:HE3	1:B:176:VAL:HG22	1.73	0.70
1:B:239:MET:CE	1:B:273:MET:SD	2.76	0.69
1:A:154:LEU:HD13	1:A:169:ILE:HD12	1.74	0.69
2:D:313:THR:O	2:D:316:PRO:HD2	1.93	0.69
2:C:345:LYS:O	2:C:349:LEU:HD23	1.93	0.69
1:A:307:VAL:O	1:A:311:ARG:HG3	1.93	0.69
2:D:295:THR:HG22	2:D:296:SER:N	2.07	0.68
2:D:212:ILE:HD13	2:D:212:ILE:C	2.18	0.68
2:D:238:VAL:HG13	2:D:263:LEU:HD13	1.75	0.68
1:B:142:GLN:C	1:B:144:SER:H	2.02	0.67
1:B:94:LYS:CG	1:B:143:LEU:HD21	2.17	0.67
1:A:154:LEU:CD1	1:A:169:ILE:HD12	2.23	0.67
1:B:140:PHE:HE2	1:B:146:MET:HE3	1.58	0.67
2:C:271:LYS:HG3	2:C:302:PHE:CZ	2.30	0.66
1:A:99:VAL:O	1:A:102:GLN:HG2	1.96	0.65
2:C:237:LEU:HD22	2:C:297:ILE:CD1	2.27	0.65
2:D:345:LYS:O	2:D:349:LEU:HD23	1.95	0.65
2:C:295:THR:CG2	2:C:296:SER:N	2.60	0.65
1:A:193:LEU:HD22	1:A:234:VAL:HG21	1.79	0.64
1:B:217:ARG:HH21	2:D:281:SER:CB	2.09	0.64
2:C:237:LEU:CD2	2:C:297:ILE:CD1	2.75	0.64
1:A:87:ARG:N	1:A:87:ARG:HD2	2.12	0.64
1:B:207:LYS:O	1:B:210:PHE:HB3	1.96	0.64
1:B:236:MET:CE	1:B:273:MET:HB2	2.26	0.64
2:D:234:ASP:OD2	2:D:271:LYS:HD3	1.97	0.64
1:B:248:VAL:HB	1:B:288:PHE:HB2	1.80	0.63
2:C:295:THR:CG2	2:C:296:SER:H	2.11	0.63
1:A:134:MET:HG3	4:C:511:HOH:O	1.97	0.63
1:A:273:MET:HE1	1:A:276:GLN:CG	2.29	0.63
1:B:128:ALA:HA	1:B:168:LEU:HD13	1.81	0.63
1:A:134:MET:SD	2:C:268:GLU:OE1	2.57	0.62
1:B:329:GLN:HA	1:B:329:GLN:OE1	1.99	0.62
2:C:241:PHE:CE1	2:C:295:THR:HG21	2.34	0.62
2:C:327:ASP:H	2:C:330:GLN:NE2	1.97	0.62
1:B:232:PHE:CD1	1:B:268:LEU:HD21	2.34	0.62
1:A:310:CYS:HB3	1:A:317:LEU:HD23	1.82	0.62
2:D:272:ARG:HG3	3:D:402:AMP:C6	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:CE	1:A:273:MET:HA	2.23	0.61
2:C:327:ASP:HB3	2:C:330:GLN:HE21	1.65	0.61
1:B:243:VAL:HG12	1:B:246:LEU:H	1.65	0.61
2:C:255:GLN:OE1	2:C:255:GLN:HA	2.00	0.61
2:D:238:VAL:O	2:D:242:VAL:HG23	2.00	0.61
1:A:154:LEU:O	1:A:162:ARG:HG2	2.00	0.61
1:A:108:ALA:HB1	1:A:112:GLU:CD	2.25	0.61
1:B:175:ASN:HB3	2:D:273:THR:OG1	2.00	0.61
1:B:256:ASN:C	1:B:256:ASN:HD22	2.01	0.61
2:C:221:ALA:HB2	2:C:324:ALA:HB2	1.83	0.61
2:D:256:ASN:HD22	2:D:259:ALA:CB	2.14	0.60
2:C:237:LEU:CD2	2:C:297:ILE:HD13	2.32	0.60
2:D:252:ASP:HB2	4:D:529:HOH:O	2.02	0.60
1:A:134:MET:HE1	2:C:272:ARG:CZ	2.31	0.60
2:C:212:ILE:C	2:C:212:ILE:HD13	2.25	0.60
1:B:294:GLY:HA2	1:B:340:PHE:CD1	2.37	0.60
2:D:209:ILE:CD1	2:D:321:LEU:HD23	2.32	0.60
1:A:154:LEU:HD13	1:A:169:ILE:HD11	1.84	0.59
1:A:248:VAL:CG1	1:A:288:PHE:CD2	2.85	0.59
1:B:256:ASN:ND2	1:B:256:ASN:C	2.60	0.59
2:C:241:PHE:HE1	2:C:295:THR:HG21	1.67	0.59
2:D:256:ASN:ND2	2:D:259:ALA:H	1.99	0.59
1:A:248:VAL:HG12	1:A:288:PHE:HB3	1.85	0.59
1:A:318:GLU:HB2	1:A:349:PHE:CE2	2.38	0.59
1:B:146:MET:O	1:B:150:VAL:HG23	2.03	0.58
1:B:116:ASP:O	1:B:120:ARG:HG3	2.03	0.58
2:C:221:ALA:CB	2:C:324:ALA:HB2	2.33	0.58
1:B:236:MET:O	1:B:240:GLN:HG3	2.03	0.58
2:D:209:ILE:HD11	2:D:321:LEU:HD23	1.85	0.58
2:C:250:LYS:O	2:C:251:LYS:HG3	2.04	0.58
1:B:239:MET:CE	1:B:273:MET:CE	2.82	0.57
2:D:353:PHE:HD2	2:D:354:PHE:CE1	2.22	0.57
1:B:262:PRO:CB	1:B:265:LYS:HE3	2.33	0.57
2:C:315:GLU:CB	2:C:316:PRO:HD3	2.34	0.57
1:A:236:MET:HG3	1:A:273:MET:CE	2.34	0.57
1:B:236:MET:HE1	1:B:271:MET:HG2	1.86	0.57
2:C:195:VAL:HG22	2:C:333:ASP:HB2	1.86	0.57
1:A:273:MET:CE	1:A:276:GLN:CG	2.83	0.57
2:C:199:ASP:HA	2:C:337:VAL:O	2.05	0.57
1:B:162:ARG:HD2	1:B:199:ASP:OD2	2.05	0.57
2:D:192:GLU:OE2	2:D:192:GLU:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD21	1:B:226:PHE:CE1	2.36	0.57
1:A:210:PHE:HB2	1:A:249:LYS:HE3	1.86	0.56
1:B:87:ARG:HG3	1:B:90:VAL:HG23	1.87	0.56
2:D:270:ALA:O	2:D:274:LEU:HD13	2.05	0.56
2:D:246:LYS:O	2:D:250:LYS:HA	2.05	0.56
1:B:218:GLU:OE1	2:D:277:SER:HB3	2.05	0.56
1:B:244:GLN:O	1:B:248:VAL:HG13	2.05	0.56
1:B:317:LEU:HG	1:B:321:LEU:HD11	1.87	0.56
1:B:146:MET:HA	1:B:146:MET:CE	2.28	0.55
1:B:300:VAL:HG12	4:B:521:HOH:O	2.05	0.55
1:B:273:MET:O	1:B:277:LEU:HG	2.07	0.55
1:A:188:ALA:O	1:A:191:LYS:N	2.39	0.55
1:A:217:ARG:HG2	1:A:256:ASN:OD1	2.06	0.55
2:D:196:LEU:C	2:D:196:LEU:HD23	2.32	0.55
1:A:241:GLN:O	1:A:247:LYS:NZ	2.38	0.55
2:C:200:LEU:HD13	2:C:205:PHE:CD1	2.41	0.55
2:D:287:LEU:O	2:D:288:PHE:HB2	2.07	0.55
1:B:188:ALA:C	1:B:190:ARG:N	2.63	0.54
2:D:251:LYS:HE3	2:D:289:GLU:OE2	2.07	0.54
1:B:118:GLN:O	1:B:121:GLU:HB2	2.06	0.54
1:B:312:GLU:CB	1:B:315:LEU:HD13	2.37	0.54
2:C:236:ARG:NH2	2:C:308:ASP:OD2	2.41	0.54
1:A:248:VAL:HG23	1:A:249:LYS:N	2.23	0.54
1:A:110:GLU:C	1:A:112:GLU:H	2.15	0.54
1:B:153:TYR:O	1:B:155:GLU:N	2.40	0.54
2:D:274:LEU:O	2:D:299:ARG:NE	2.41	0.54
1:B:102:GLN:HA	1:B:102:GLN:NE2	2.22	0.54
1:B:330:GLN:O	1:B:330:GLN:HG2	2.07	0.54
1:B:296:LEU:O	1:B:344:LEU:HD21	2.08	0.54
2:D:327:ASP:HB3	2:D:330:GLN:NE2	2.22	0.54
1:A:282:ARG:HG2	1:A:320:LEU:HD11	1.91	0.53
1:B:110:GLU:O	1:B:114:ALA:HB2	2.09	0.53
1:B:269:CYS:C	1:B:271:MET:H	2.16	0.53
2:C:196:LEU:HB3	2:C:334:LEU:HD23	1.90	0.53
2:D:315:GLU:CB	2:D:316:PRO:HD3	2.34	0.53
1:B:243:VAL:HG11	1:B:246:LEU:HG	1.90	0.53
2:C:237:LEU:HD22	2:C:297:ILE:HD13	1.88	0.53
1:B:100:LEU:HG	1:B:153:TYR:OH	2.09	0.53
1:A:134:MET:HE1	2:C:272:ARG:NE	2.24	0.53
1:A:162:ARG:NH1	1:A:199:ASP:OD2	2.42	0.53
2:D:209:ILE:HD12	2:D:320:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:CG1	1:B:94:LYS:HE3	2.39	0.53
2:D:253:ILE:HG12	4:D:504:HOH:O	2.08	0.53
1:B:248:VAL:HA	1:B:288:PHE:CD1	2.44	0.52
1:A:134:MET:HE3	1:A:176:VAL:HG22	1.91	0.52
1:A:182:GLN:O	1:A:186:LEU:HG	2.09	0.52
1:B:143:LEU:HD12	1:B:143:LEU:H	1.74	0.52
1:B:146:MET:SD	1:B:183:VAL:HG22	2.50	0.52
2:D:345:LYS:HE3	2:D:349:LEU:HD21	1.92	0.52
1:A:289:HIS:HD2	1:A:324:ARG:HH12	1.57	0.52
1:B:188:ALA:O	1:B:190:ARG:N	2.43	0.52
1:B:321:LEU:HB2	1:B:345:LEU:HD21	1.91	0.52
1:B:97:LEU:CD1	1:B:143:LEU:HD22	2.38	0.52
1:B:217:ARG:C	1:B:219:GLN:N	2.65	0.52
2:C:231:GLU:OE2	2:C:264:ARG:HD2	2.10	0.52
1:B:201:CYS:SG	1:B:204:VAL:HG23	2.50	0.52
2:C:194:ASN:N	2:C:332:HIS:HD2	1.95	0.52
1:B:262:PRO:O	1:B:265:LYS:HG3	2.10	0.51
1:B:100:LEU:HD13	1:B:123:ALA:HB3	1.92	0.51
1:B:268:LEU:O	1:B:271:MET:HB3	2.10	0.51
1:B:301:THR:CA	4:B:521:HOH:O	2.48	0.51
2:D:299:ARG:O	2:D:303:GLU:HG3	2.10	0.51
1:A:265:LYS:NZ	1:A:301:THR:O	2.43	0.51
1:A:245:LYS:O	1:A:249:LYS:HB2	2.11	0.51
1:A:293:LEU:HD23	1:A:341:CYS:HB2	1.93	0.51
1:B:220:GLU:OE1	1:B:220:GLU:HA	2.10	0.51
1:A:255:GLN:O	1:A:259:VAL:HG23	2.11	0.50
1:B:236:MET:HE2	1:B:273:MET:CB	2.33	0.50
2:D:198:PHE:CB	2:D:336:LEU:HD23	2.39	0.50
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.11	0.50
2:C:212:ILE:HG13	2:C:217:PHE:CE2	2.47	0.50
1:B:300:VAL:C	4:B:521:HOH:O	2.55	0.50
2:D:271:LYS:HG3	2:D:302:PHE:CZ	2.46	0.50
2:D:279:GLN:O	2:D:279:GLN:HG2	2.12	0.50
1:B:202:ASP:O	1:B:206:VAL:HG23	2.11	0.50
2:D:212:ILE:HG13	2:D:217:PHE:CE2	2.47	0.50
2:D:236:ARG:HD2	2:D:305:LEU:O	2.11	0.50
1:B:261:HIS:N	1:B:262:PRO:HD3	2.27	0.49
1:B:266:GLY:O	1:B:268:LEU:N	2.45	0.49
1:B:97:LEU:HD21	1:B:140:PHE:CE1	2.47	0.49
1:B:219:GLN:HE22	1:B:221:ALA:HB3	1.78	0.49
1:A:87:ARG:NH1	1:A:139:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:O	1:B:226:PHE:HB3	2.12	0.49
2:D:272:ARG:HG3	3:D:402:AMP:N6	2.27	0.49
1:B:93:MET:HB3	1:B:130:LEU:HD12	1.94	0.49
1:B:142:GLN:C	1:B:144:SER:N	2.70	0.49
1:B:197:ASP:OD2	1:B:234:VAL:HG13	2.13	0.49
2:C:318:GLU:O	2:C:321:LEU:HB2	2.13	0.49
2:D:200:LEU:CD1	2:D:205:PHE:HB2	2.42	0.49
2:D:282:LEU:N	2:D:282:LEU:HD12	2.28	0.49
1:A:236:MET:HA	1:A:239:MET:HG3	1.93	0.49
1:B:132:GLU:O	2:D:265:THR:HB	2.12	0.49
1:B:134:MET:HE1	2:D:272:ARG:HD2	1.95	0.49
1:B:212:ILE:O	1:B:216:VAL:HG22	2.12	0.49
2:C:243:GLU:HA	2:C:246:LYS:HE3	1.94	0.49
2:C:250:LYS:C	2:C:251:LYS:HG3	2.38	0.49
1:B:192:LEU:HD13	1:B:211:ALA:HB3	1.95	0.48
1:B:332:GLU:HA	1:B:335:GLN:HG3	1.95	0.48
2:C:204:THR:HG22	2:C:226:THR:HA	1.94	0.48
2:D:338:GLY:HA2	3:D:402:AMP:O1P	2.14	0.48
1:B:213:SER:O	1:B:217:ARG:HD3	2.14	0.48
2:D:299:ARG:HG2	2:D:299:ARG:HH11	1.78	0.48
1:B:132:GLU:CD	2:D:262:ARG:HG2	2.39	0.48
1:B:188:ALA:C	1:B:190:ARG:H	2.21	0.48
2:D:307:SER:HB2	2:D:311:ARG:HH12	1.79	0.48
1:B:295:ALA:C	1:B:297:CYS:H	2.22	0.48
1:A:245:LYS:NZ	2:C:292:ASP:OD2	2.43	0.48
2:C:314:LEU:O	2:C:315:GLU:C	2.57	0.48
2:D:295:THR:CG2	2:D:296:SER:H	2.24	0.48
1:B:217:ARG:O	1:B:218:GLU:C	2.57	0.47
1:A:94:LYS:HE2	1:A:143:LEU:HD21	1.96	0.47
2:D:284:ILE:HD12	2:D:287:LEU:HD22	1.95	0.47
2:D:297:ILE:HG13	2:D:298:THR:N	2.29	0.47
1:B:236:MET:CE	1:B:273:MET:HE2	2.43	0.47
1:B:264:HIS:O	1:B:265:LYS:C	2.56	0.47
1:B:340:PHE:N	1:B:340:PHE:CD2	2.79	0.47
1:A:201:CYS:HB3	1:A:204:VAL:HG23	1.95	0.47
1:B:118:GLN:HA	1:B:121:GLU:OE2	2.14	0.47
2:C:274:LEU:HD21	2:C:297:ILE:HG23	1.95	0.47
2:D:328:LYS:HG3	2:D:329:ALA:N	2.29	0.47
1:A:335:GLN:NE2	2:C:247:ARG:HD2	2.29	0.47
2:D:343:ILE:HB	2:D:346:VAL:HG23	1.95	0.47
1:B:124:LEU:HD11	1:B:149:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLN:HE21	1:B:221:ALA:HB3	1.80	0.47
1:A:240:GLN:HE21	1:A:276:GLN:NE2	2.13	0.47
1:B:100:LEU:HD13	1:B:123:ALA:CB	2.44	0.47
1:B:102:GLN:CD	1:B:103:PRO:HD2	2.39	0.47
1:A:245:LYS:HA	1:A:248:VAL:HG22	1.97	0.47
2:C:234:ASP:OD1	2:C:268:GLU:HG3	2.15	0.47
1:B:210:PHE:O	1:B:213:SER:HB3	2.15	0.46
2:C:212:ILE:HG13	2:C:217:PHE:CZ	2.50	0.46
1:A:146:MET:HG2	1:A:183:VAL:HG22	1.98	0.46
1:A:225:GLN:O	1:A:229:LEU:HD12	2.15	0.46
1:A:332:GLU:O	1:A:335:GLN:HG3	2.15	0.46
1:B:317:LEU:HG	1:B:321:LEU:CD1	2.46	0.46
2:D:212:ILE:HD13	2:D:212:ILE:O	2.15	0.46
1:B:94:LYS:O	1:B:98:ARG:HG3	2.15	0.46
2:C:238:VAL:HG13	2:C:263:LEU:HD13	1.98	0.46
1:A:110:GLU:C	1:A:112:GLU:N	2.74	0.46
1:B:105:PRO:O	1:B:106:PRO:C	2.59	0.46
1:A:278:VAL:HG11	1:A:315:LEU:HG	1.98	0.46
1:A:290:GLU:HA	1:A:337:GLU:HG3	1.98	0.46
1:A:108:ALA:HB1	1:A:112:GLU:HB3	1.96	0.45
1:B:260:GLY:C	1:B:261:HIS:ND1	2.74	0.45
1:B:125:GLU:O	1:B:126:LEU:C	2.60	0.45
1:A:202:ASP:O	1:A:206:VAL:HG23	2.16	0.45
1:B:121:GLU:HG2	1:B:164:ARG:HD2	1.97	0.45
1:B:260:GLY:O	1:B:261:HIS:ND1	2.49	0.45
1:A:213:SER:OG	1:A:217:ARG:HD3	2.16	0.45
2:D:295:THR:CG2	2:D:296:SER:N	2.76	0.45
2:C:243:GLU:HA	2:C:246:LYS:CE	2.46	0.45
2:C:339:GLY:O	2:C:342:ARG:HG3	2.17	0.45
1:A:198:ARG:CB	1:A:198:ARG:HH11	2.30	0.45
2:D:256:ASN:ND2	2:D:259:ALA:N	2.64	0.45
1:A:87:ARG:C	1:A:89:GLU:H	2.23	0.45
1:B:132:GLU:CD	2:D:262:ARG:HE	2.24	0.45
2:C:281:SER:C	2:C:282:LEU:HD12	2.42	0.45
2:D:234:ASP:OD1	2:D:268:GLU:HG3	2.17	0.45
1:B:263:GLU:HG2	1:B:264:HIS:N	2.31	0.45
1:B:288:PHE:CD1	1:B:288:PHE:O	2.70	0.45
1:A:248:VAL:CG1	1:A:288:PHE:HB3	2.46	0.44
1:A:286:SER:HB2	1:A:287:PRO:CD	2.47	0.44
1:B:281:VAL:HG12	1:B:281:VAL:O	2.16	0.44
1:B:317:LEU:O	1:B:321:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:ARG:HG2	2:D:299:ARG:NH1	2.32	0.44
2:C:306:CYS:O	2:C:307:SER:C	2.60	0.44
1:B:184:LEU:C	1:B:186:LEU:H	2.25	0.44
1:B:217:ARG:O	1:B:219:GLN:N	2.50	0.44
1:A:134:MET:HE1	2:C:272:ARG:HD2	1.99	0.44
1:A:244:GLN:O	1:A:247:LYS:N	2.51	0.44
1:B:269:CYS:HB2	1:B:305:GLN:NE2	2.32	0.44
2:C:256:ASN:ND2	2:C:259:ALA:HB2	2.31	0.44
2:C:263:LEU:HD22	2:C:267:CYS:SG	2.58	0.44
1:A:147:HIS:N	1:A:147:HIS:CD2	2.84	0.44
1:B:153:TYR:O	1:B:154:LEU:C	2.60	0.44
1:A:163:TRP:HB3	1:A:204:VAL:HA	2.00	0.44
1:A:100:LEU:HB3	1:A:148:LEU:HD21	2.00	0.43
2:D:196:LEU:HD21	2:D:207:VAL:HG23	2.00	0.43
1:A:149:LEU:HD21	1:A:168:LEU:HG	2.00	0.43
2:D:264:ARG:O	2:D:265:THR:C	2.58	0.43
1:B:140:PHE:CZ	1:B:145:GLY:HA3	2.54	0.43
1:B:248:VAL:HG12	1:B:288:PHE:CG	2.53	0.43
1:B:248:VAL:CG2	1:B:249:LYS:N	2.80	0.43
2:C:199:ASP:HB2	2:C:337:VAL:CG2	2.48	0.43
1:A:311:ARG:O	1:A:312:GLU:C	2.61	0.43
1:A:235:LEU:O	1:A:238:ALA:HB3	2.18	0.43
1:B:303:PHE:CE2	1:B:305:GLN:HB3	2.53	0.43
2:D:234:ASP:O	2:D:238:VAL:HG23	2.18	0.43
2:C:199:ASP:CB	2:C:337:VAL:HG23	2.48	0.43
1:B:161:LEU:O	1:B:165:ALA:HB2	2.19	0.43
1:A:124:LEU:HD12	1:A:168:LEU:CD2	2.49	0.43
1:B:111:ALA:O	1:B:114:ALA:HB3	2.19	0.43
1:B:333:GLU:HB3	2:D:247:ARG:O	2.19	0.43
1:A:324:ARG:O	1:A:325:CYS:C	2.62	0.42
1:B:237:ARG:HG3	1:B:237:ARG:HH11	1.84	0.42
1:B:266:GLY:C	1:B:268:LEU:N	2.76	0.42
1:B:301:THR:N	4:B:521:HOH:O	2.51	0.42
1:A:87:ARG:C	1:A:89:GLU:N	2.75	0.42
1:A:328:LEU:HD22	1:A:334:TYR:HB3	2.01	0.42
1:A:219:GLN:HE21	1:A:222:GLY:H	1.67	0.42
1:B:136:ASN:O	1:B:139:ASP:HB2	2.19	0.42
2:C:255:GLN:NE2	2:D:323:ASP:HB3	2.30	0.42
2:D:272:ARG:O	2:D:275:SER:HB2	2.19	0.42
1:A:139:ASP:O	1:A:143:LEU:HD12	2.20	0.42
1:A:110:GLU:O	1:A:112:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:HB2	1:B:108:ALA:HB2	2.00	0.42
1:B:230:ASP:O	1:B:234:VAL:HG23	2.20	0.42
1:B:317:LEU:HG	1:B:321:LEU:CG	2.49	0.42
1:B:329:GLN:C	1:B:331:HIS:H	2.27	0.42
1:A:154:LEU:HD11	1:A:169:ILE:HD12	1.99	0.42
1:B:87:ARG:HE	1:B:90:VAL:CG2	2.32	0.42
1:A:173:SER:O	1:A:174:GLN:C	2.62	0.42
1:A:236:MET:HE2	1:A:273:MET:SD	2.60	0.42
1:A:133:ASN:O	1:A:134:MET:C	2.63	0.42
1:B:100:LEU:CD1	1:B:123:ALA:HB3	2.49	0.42
2:D:209:ILE:HD13	2:D:321:LEU:HD23	2.02	0.42
1:A:134:MET:CE	2:C:272:ARG:CZ	2.97	0.42
1:A:141:CYS:HB3	1:A:182:GLN:HE22	1.85	0.42
2:D:324:ALA:O	2:D:326:LEU:HD13	2.20	0.42
1:B:93:MET:C	1:B:95:SER:N	2.78	0.42
1:B:180:GLN:O	1:B:184:LEU:HG	2.20	0.42
1:B:332:GLU:C	1:B:334:TYR:N	2.78	0.42
1:B:126:LEU:C	1:B:126:LEU:HD23	2.45	0.41
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.88	0.41
1:A:348:CYS:C	1:A:349:PHE:CG	2.97	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.86	0.41
1:B:248:VAL:HG12	1:B:288:PHE:CD2	2.55	0.41
2:D:343:ILE:HB	2:D:346:VAL:CG2	2.50	0.41
1:A:286:SER:HB2	1:A:287:PRO:HD2	2.02	0.41
1:B:128:ALA:CA	1:B:168:LEU:HD13	2.49	0.41
1:B:236:MET:CE	1:B:271:MET:HG2	2.50	0.41
1:B:262:PRO:CA	1:B:265:LYS:HE3	2.50	0.41
1:B:269:CYS:C	1:B:271:MET:N	2.73	0.41
1:B:324:ARG:C	1:B:326:GLN:N	2.79	0.41
1:B:333:GLU:CB	2:D:248:LYS:HA	2.50	0.41
2:C:242:VAL:HG13	2:C:253:ILE:HG12	2.02	0.41
2:D:207:VAL:HG11	2:D:316:PRO:HB2	2.01	0.41
1:A:134:MET:HE1	2:C:272:ARG:CD	2.51	0.41
1:B:188:ALA:O	1:B:189:LEU:C	2.62	0.41
1:B:193:LEU:HD12	1:B:229:LEU:HD13	2.02	0.41
1:B:146:MET:HE1	1:B:149:LEU:HD23	2.01	0.41
2:C:345:LYS:HE3	2:C:349:LEU:HD21	2.03	0.41
1:B:120:ARG:O	1:B:124:LEU:HB2	2.20	0.41
1:B:332:GLU:C	1:B:334:TYR:H	2.28	0.41
1:A:236:MET:HE2	1:A:273:MET:HE3	2.03	0.41
1:A:307:VAL:HG13	1:A:348:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HH21	2:D:281:SER:HB2	1.85	0.41
1:B:266:GLY:C	1:B:268:LEU:H	2.29	0.41
2:C:213:ASP:OD1	2:C:214:ASP:HB2	2.21	0.41
2:C:327:ASP:O	2:C:328:LYS:C	2.63	0.41
2:D:196:LEU:C	2:D:196:LEU:CD2	2.94	0.41
2:D:212:ILE:HG13	2:D:217:PHE:CZ	2.56	0.41
1:A:87:ARG:HH11	1:A:90:VAL:CG2	2.34	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.87	0.41
2:D:200:LEU:HD13	2:D:205:PHE:HB2	2.02	0.41
1:A:314:GLU:H	1:A:314:GLU:HG3	1.56	0.40
1:B:115:ALA:O	1:B:116:ASP:C	2.64	0.40
1:B:139:ASP:O	1:B:142:GLN:HB2	2.20	0.40
2:C:237:LEU:HD21	2:C:297:ILE:HD13	2.01	0.40
1:B:87:ARG:CG	1:B:90:VAL:HG23	2.48	0.40
1:B:142:GLN:OE1	1:B:142:GLN:HA	2.21	0.40
1:A:264:HIS:O	1:A:265:LYS:C	2.63	0.40
1:B:219:GLN:O	1:B:219:GLN:HG3	2.20	0.40
2:C:200:LEU:HD12	2:C:200:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	262/280 (94%)	234 (89%)	24 (9%)	4 (2%)	8	28
1	B	262/280 (94%)	218 (83%)	36 (14%)	8 (3%)	3	14
2	C	163/191 (85%)	149 (91%)	13 (8%)	1 (1%)	21	51
2	D	163/191 (85%)	147 (90%)	13 (8%)	3 (2%)	6	25
All	All	850/942 (90%)	748 (88%)	86 (10%)	16 (2%)	6	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	B	154	LEU
1	B	267	THR
2	D	328	LYS
1	A	156	ALA
1	B	143	LEU
1	B	296	LEU
2	D	288	PHE
1	A	108	ALA
1	A	110	GLU
1	B	189	LEU
1	B	116	ASP
2	C	307	SER
1	B	225	GLN
1	B	333	GLU
2	D	339	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/235 (93%)	197 (90%)	22 (10%)	7	24
1	B	214/235 (91%)	196 (92%)	18 (8%)	10	31
2	C	144/163 (88%)	133 (92%)	11 (8%)	12	36
2	D	144/163 (88%)	132 (92%)	12 (8%)	10	32
All	All	721/796 (91%)	658 (91%)	63 (9%)	9	30

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	110	GLU
1	A	116	ASP
1	A	118	GLN
1	A	124	LEU
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	149	LEU
1	A	154	LEU
1	A	155	GLU
1	A	167	GLN
1	A	196	LEU
1	A	198	ARG
1	A	216	VAL
1	A	224	LEU
1	A	249	LYS
1	A	257	LEU
1	A	267	THR
1	A	296	LEU
1	A	300	VAL
1	A	312	GLU
1	A	315	LEU
1	B	106	PRO
1	B	124	LEU
1	B	127	LEU
1	B	132	GLU
1	B	149	LEU
1	B	152	ARG
1	B	174	GLN
1	B	196	LEU
1	B	229	LEU
1	B	244	GLN
1	B	248	VAL
1	B	249	LYS
1	B	256	ASN
1	B	257	LEU
1	B	263	GLU
1	B	288	PHE
1	B	328	LEU
1	B	330	GLN
2	C	192	GLU
2	C	207	VAL
2	C	210	LEU
2	C	212	ILE
2	C	214	ASP
2	C	226	THR
2	C	228	LEU
2	C	263	LEU

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Mol	Chain	Res	Type
2	C	274	LEU
2	C	326	LEU
2	C	348	LYS
2	D	210	LEU
2	D	212	ILE
2	D	214	ASP
2	D	226	THR
2	D	228	LEU
2	D	235	ASN
2	D	258	ARG
2	D	263	LEU
2	D	278	THR
2	D	297	ILE
2	D	335	VAL
2	D	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	118	GLN
1	A	136	ASN
1	A	182	GLN
1	A	219	GLN
1	A	244	GLN
1	A	255	GLN
1	A	276	GLN
1	A	289	HIS
1	A	335	GLN
1	B	102	GLN
1	B	117	GLN
1	B	136	ASN
1	B	147	HIS
1	B	219	GLN
1	B	225	GLN
1	B	255	GLN
1	B	276	GLN
1	B	289	HIS
1	B	305	GLN
1	B	331	HIS
1	B	335	GLN
2	C	239	ASN

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Mol	Chain	Res	Type
2	C	255	GLN
2	C	256	ASN
2	C	330	GLN
2	C	332	HIS
2	D	239	ASN
2	D	249	HIS
2	D	256	ASN
2	D	330	GLN
2	D	332	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AMP	D	402	-	25,25,25	1.98	6 (24%)	37,38,38	1.03	2 (5%)
3	AMP	C	401	-	25,25,25	2.02	7 (28%)	37,38,38	1.02	1 (2%)

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	AMP	D	402	-	-	0/10/26/26	0/3/3/3
3	AMP	C	401	-	-	0/10/26/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	AMP	C4-N3	5.53	1.44	1.34
3	D	402	AMP	C4-N3	5.24	1.44	1.34
3	C	401	AMP	P-O3P	3.98	1.69	1.54
3	D	402	AMP	P-O3P	3.95	1.69	1.54
3	C	401	AMP	C6-N1	3.48	1.45	1.35
3	D	402	AMP	C6-N1	3.44	1.45	1.35
3	C	401	AMP	C2-N1	2.97	1.39	1.33
3	D	402	AMP	C2-N1	2.90	1.39	1.33
3	D	402	AMP	C2-N3	2.72	1.38	1.33
3	C	401	AMP	C8-N7	-2.25	1.27	1.31
3	C	401	AMP	C2-N3	2.23	1.37	1.33
3	D	402	AMP	C8-N7	-2.20	1.27	1.31
3	C	401	AMP	C5-C6	2.20	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	AMP	N3-C2-N1	-2.76	124.40	128.58
3	D	402	AMP	N3-C2-N1	-2.66	124.55	128.58
3	D	402	AMP	O3P-P-O5'	-2.02	101.39	106.67

There are no chirality outliers.

There are no torsion outliers.

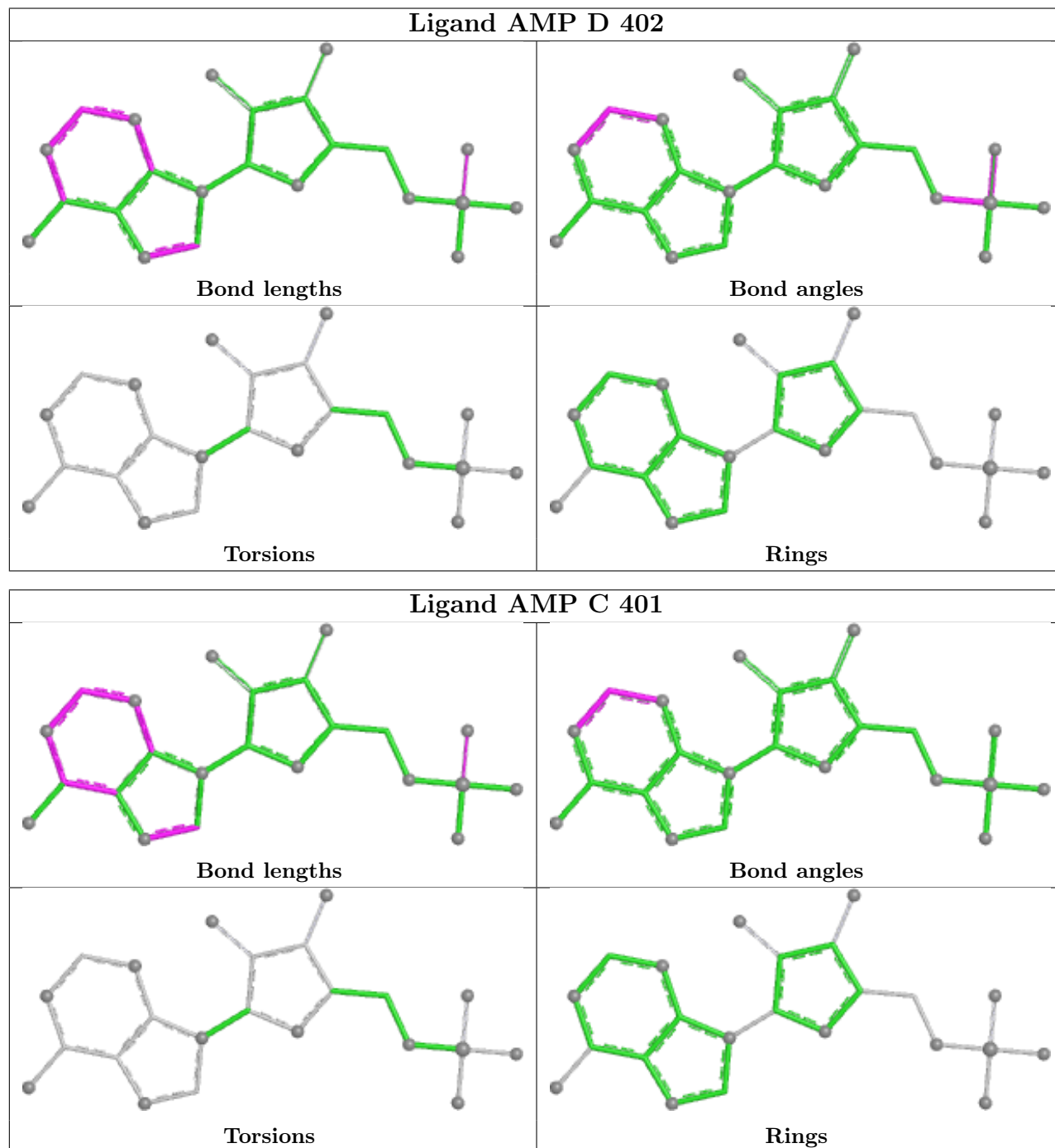
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	AMP	3	0
3	C	401	AMP	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/280 (94%)	-0.21	1 (0%) 88 85	31, 54, 88, 116	0
1	B	264/280 (94%)	0.34	5 (1%) 66 58	53, 85, 114, 143	0
2	C	165/191 (86%)	-0.19	3 (1%) 67 59	29, 62, 79, 83	0
2	D	165/191 (86%)	0.02	3 (1%) 67 59	50, 67, 83, 93	0
All	All	858/942 (91%)	0.01	12 (1%) 73 65	29, 67, 102, 143	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	340	SER	3.2
2	D	356	GLY	3.2
1	B	106	PRO	2.8
2	D	302	PHE	2.4
1	A	350	SER	2.4
1	B	222	GLY	2.3
2	D	255	GLN	2.2
1	B	274	VAL	2.2
1	B	341	CYS	2.2
1	B	88	GLY	2.1
2	C	334	LEU	2.1
2	C	356	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

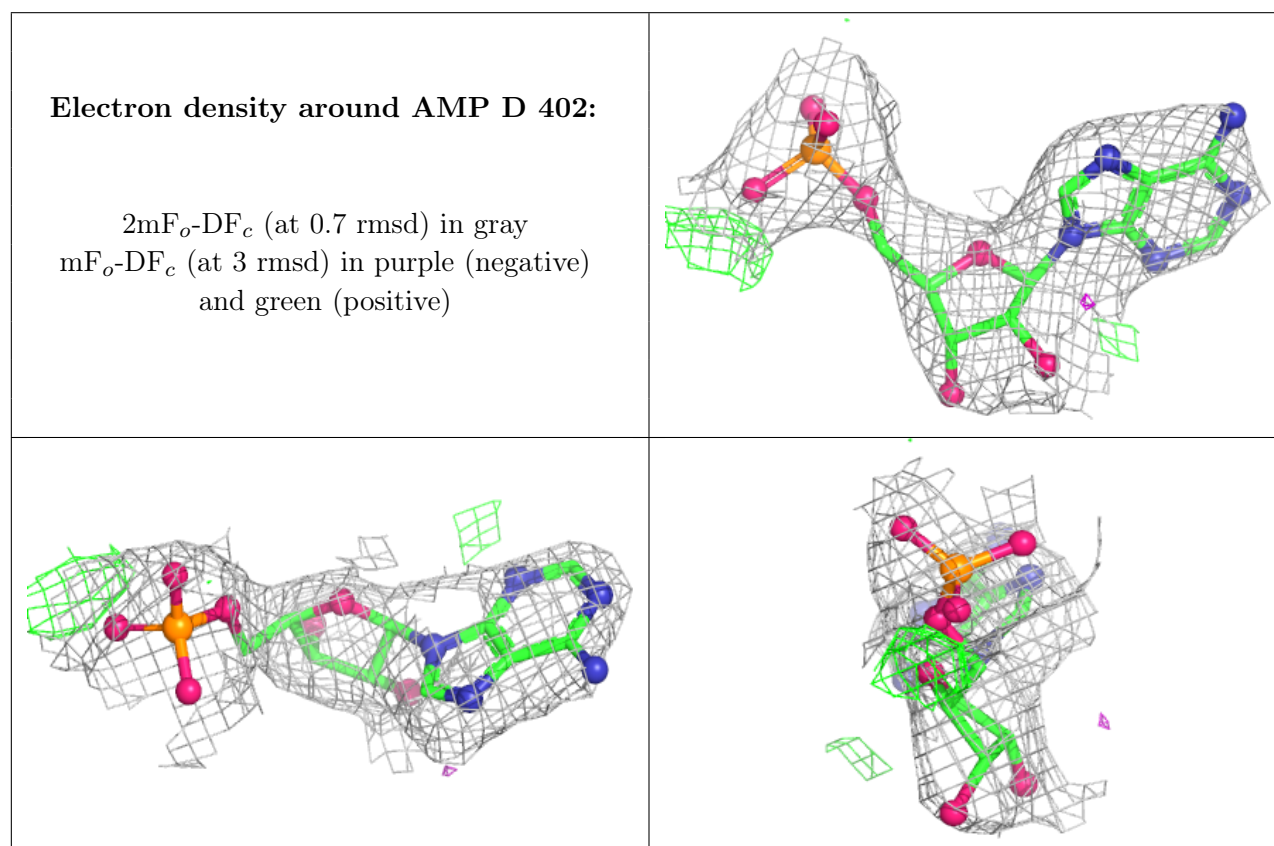
There are no oligosaccharides in this entry.

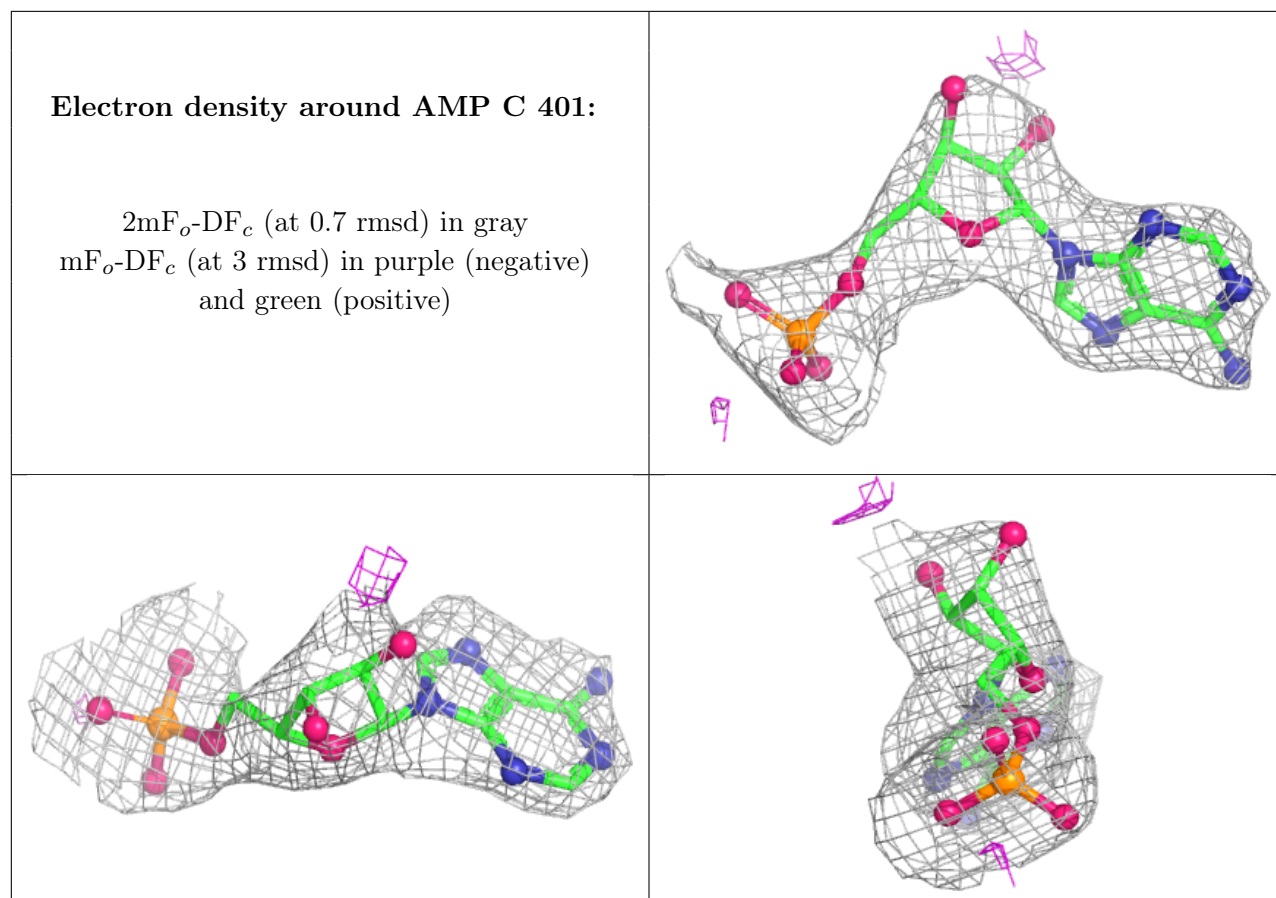
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	D	402	23/23	0.85	0.11	76,81,88,90	0
3	AMP	C	401	23/23	0.88	0.10	77,85,99,100	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers ⓘ

There are no such residues in this entry.