Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 12:11 AM EST

PDB ID	:	2OOX
Title	:	Crystal structure of the adenylate sensor from AMP-activated protein kinase complexed with AMP
Authors	:	Townley, R.; Shapiro, L.
Deposited on	:	2007-01-26
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

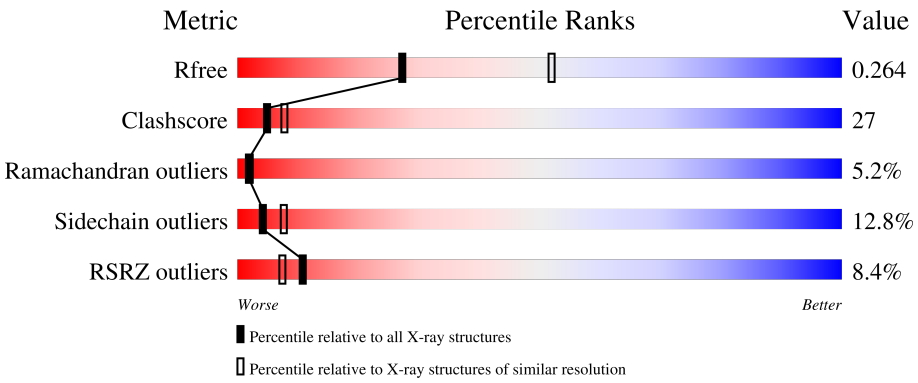
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	137	10% 53% 31% 9% • 7%
1	C	137	16% 49% 31% 12% • 7%
2	B	97	12% 52% 29% 12% • •
2	D	97	12% 45% 30% 15% 5% •
3	E	333	6% 63% 30% 6% •

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Mol	Chain	Length	Quality of chain
3	G	333	4% 57% 30% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9329 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	1025	657	178	180	10	0	0	0
1	C	128	1003	646	173	175	9	0	0	0

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	93	733	467	125	139	2	0	0	0
2	D	93	733	467	125	139	2	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	cloning artifact	UNP P78789
D	202	MET	-	cloning artifact	UNP P78789

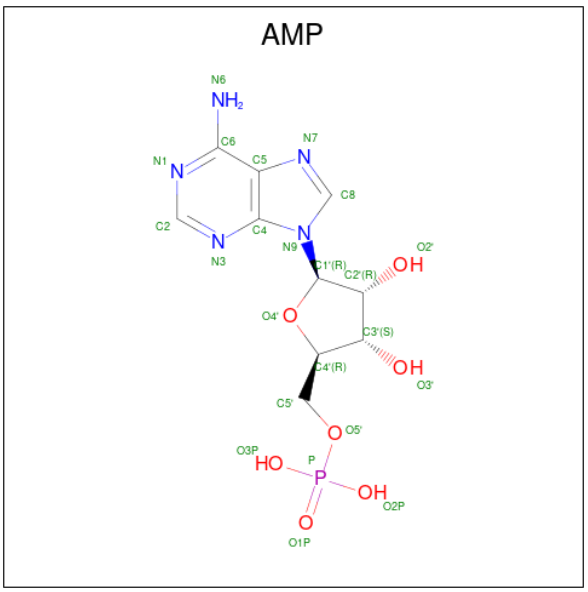
- Molecule 3 is a protein called Hypothetical protein C1556.08c in chromosome I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	324	2548	1629	426	478	15	0	1	0
3	E	333	2589	1649	433	492	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	MET	-	cloning artifact	UNP Q10343
G	2	MET	-	cloning artifact	UNP Q10343

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	G	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
4	E	1	23	10	5	7	1	0	0

- Molecule 5 is water.

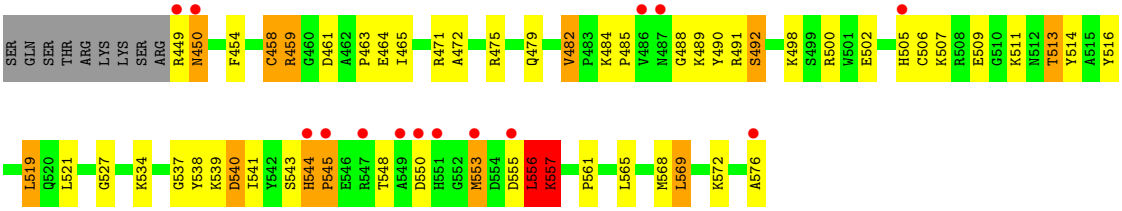
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	94	94	94	0	0
			Total	O		
5	B	78	78	78	0	0
			Total	O		
5	G	217	217	217	0	0
			Total	O		
5	C	66	66	66	0	0
			Total	O		
5	D	51	51	51	0	0
			Total	O		
5	E	146	146	146	0	0

3 Residue-property plots (i)

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.

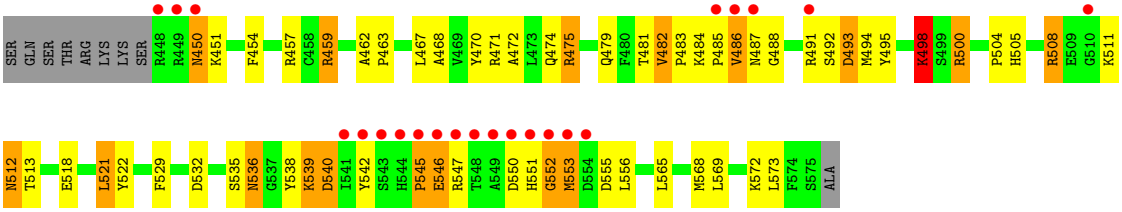
- Molecule 1: SNF1-like protein kinase ssp2

Chain A:



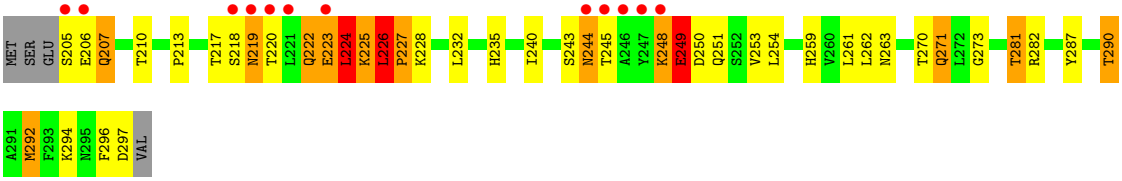
- Molecule 1: SNF1-like protein kinase ssp2

Chain C:



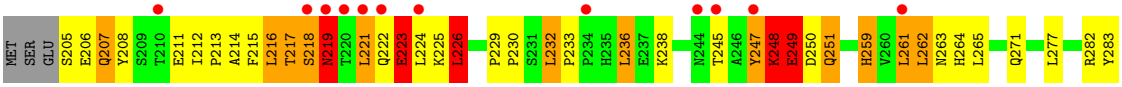
- Molecule 2: SPCC1919.03c protein

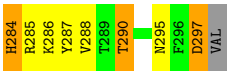
Chain B:



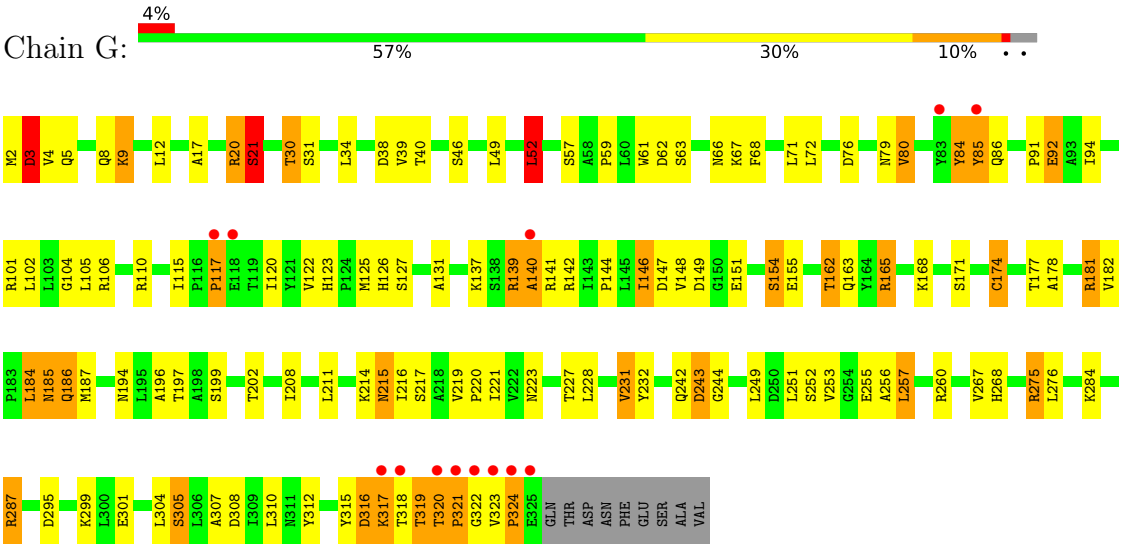
- Molecule 2: SPCC1919.03c protein

Chain D:

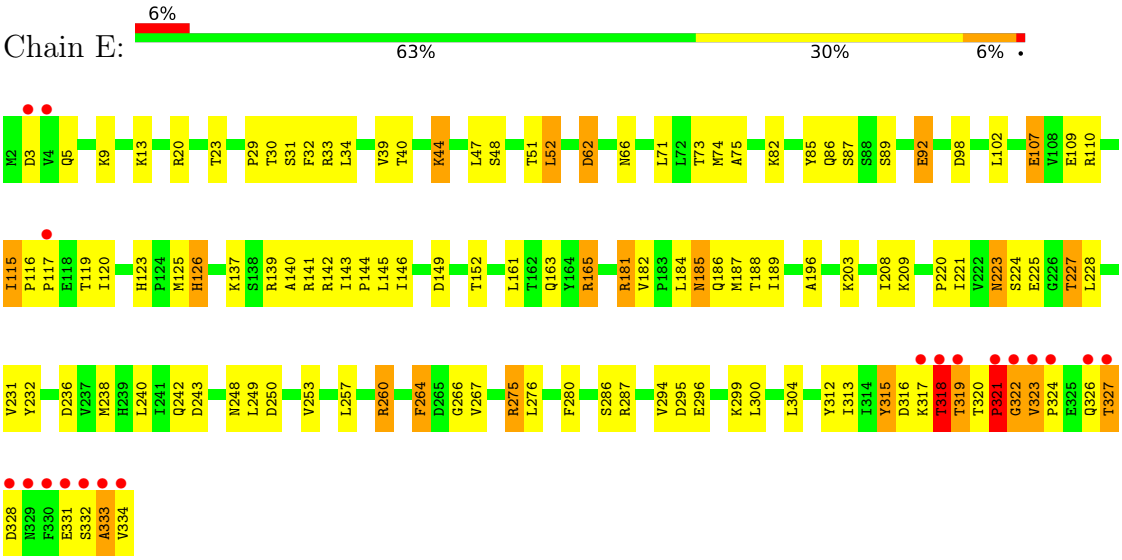




• Molecule 3: Hypothetical protein C1556.08c in chromosome I



• Molecule 3: Hypothetical protein C1556.08c in chromosome I



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.46Å 97.39Å 168.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 29.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.60) 99.9 (29.69-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.91 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.273 0.200 , 0.264	Depositor DCC
R_{free} test set	1903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9329	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.79	0/1053	0.93	4/1420 (0.3%)
1	C	0.77	2/1030 (0.2%)	0.82	1/1393 (0.1%)
2	B	0.74	0/751	0.89	1/1026 (0.1%)
2	D	1.03	3/751 (0.4%)	0.96	2/1026 (0.2%)
3	E	0.74	0/2631	0.83	3/3565 (0.1%)
3	G	0.76	1/2596 (0.0%)	0.85	2/3521 (0.1%)
All	All	0.78	6/8812 (0.1%)	0.86	13/11951 (0.1%)

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	2
1	C	0	1
2	D	0	2
3	E	0	2
3	G	0	2
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	218	SER	CB-OG	16.16	1.63	1.42
2	D	284	HIS	CA-CB	-10.79	1.30	1.53
1	C	481	THR	C-N	-10.41	1.10	1.34
2	D	286	LYS	C-N	-8.59	1.14	1.34
1	C	482	VAL	C-N	6.38	1.46	1.34
3	G	174	CYS	CB-SG	-5.72	1.72	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	285	ARG	O-C-N	-8.71	108.77	122.70
3	E	321	PRO	N-CA-CB	7.76	112.61	103.30
1	A	519	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	459	ARG	NE-CZ-NH1	-6.07	117.27	120.30
3	G	52	LEU	CA-CB-CG	6.04	129.19	115.30
2	D	285	ARG	CA-C-N	6.00	130.40	117.20
3	E	324	PRO	N-CA-CB	5.85	110.32	103.30
3	E	260	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	B	292	MET	CG-SD-CE	-5.34	91.65	100.20
1	A	540	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	481	THR	O-C-N	5.20	131.02	122.70
1	A	556	LEU	CA-CB-CG	5.17	127.20	115.30
3	G	260	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	PRO	Peptide
1	A	553	MET	Peptide
1	C	487	ASN	Peptide
2	D	223	GLU	Peptide
2	D	249	GLU	Peptide
3	E	315	TYR	Peptide
3	E	62	ASP	Peptide
3	G	243	ASP	Peptide
3	G	323	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1025	0	997	60	0
1	C	1003	0	964	77	0
2	B	733	0	735	66	0
2	D	733	0	733	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2589	0	2608	109	0
3	G	2548	0	2601	139	1
4	E	23	0	12	2	0
4	G	23	0	12	0	0
5	A	94	0	0	27	0
5	B	78	0	0	20	0
5	C	66	0	0	25	0
5	D	51	0	0	13	0
5	E	146	0	0	28	3
5	G	217	0	0	56	2
All	All	9329	0	8662	476	3

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 27.

All (476) 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)
3:G:79:ASN:HB2	5:G:569:HOH:O	1.32	1.24
3:G:46:SER:HB2	5:G:440:HOH:O	1.37	1.22
3:E:30:THR:O	5:E:526:HOH:O	1.53	1.20
5:C:593:HOH:O	3:E:152:THR:HB	1.43	1.16
1:C:474:GLN:HB3	5:C:615:HOH:O	1.47	1.11
1:C:522:TYR:HA	5:C:637:HOH:O	1.50	1.08
3:E:23:THR:HG22	5:E:525:HOH:O	1.53	1.08
3:G:308:ASP:OD2	5:G:536:HOH:O	1.71	1.07
3:G:165:ARG:HG2	3:G:165:ARG:HH11	1.17	1.07
3:G:320:THR:HB	3:G:321:PRO:CD	1.86	1.05
3:G:199:SER:OG	5:G:595:HOH:O	1.76	1.04
3:G:63:SER:HA	5:G:566:HOH:O	1.54	1.03
3:G:216:ILE:HG12	5:G:599:HOH:O	1.57	1.03
3:G:320:THR:HB	3:G:321:PRO:HD2	1.40	1.03
1:C:474:GLN:HE22	2:D:211:GLU:HB2	1.22	1.02
3:E:51:THR:HG21	3:E:242:GLN:NE2	1.74	1.02
1:C:500:ARG:HG2	1:C:500:ARG:HH11	1.24	1.02
3:G:20:ARG:O	3:G:21:SER:HB3	1.61	0.98
2:D:284:HIS:N	5:D:332:HOH:O	1.70	0.98
2:B:224:LEU:O	2:B:226:LEU:N	1.97	0.97
2:D:287:TYR:N	5:E:526:HOH:O	1.97	0.96
3:E:224:SER:O	3:E:225:GLU:HG2	1.64	0.96
2:B:223:GLU:C	2:B:225:LYS:H	1.68	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:155:GLU:CD	5:G:567:HOH:O	2.05	0.94
1:C:450:ASN:O	5:C:627:HOH:O	1.83	0.94
3:G:162:THR:HG22	3:G:165:ARG:H	1.33	0.93
1:C:471:ARG:HA	5:C:615:HOH:O	1.69	0.93
3:G:155:GLU:OE1	5:G:567:HOH:O	1.85	0.92
3:G:211:LEU:O	3:G:215:ASN:HA	1.70	0.92
3:E:51:THR:HG21	3:E:242:GLN:HE22	1.35	0.91
3:G:76:ASP:O	5:G:569:HOH:O	1.89	0.90
3:G:317:LYS:HD2	3:G:318:THR:HG23	1.55	0.89
1:C:538:TYR:HD2	1:C:553:MET:CB	1.86	0.88
1:C:486:VAL:HG21	1:C:491:ARG:HH11	1.40	0.87
3:G:8:GLN:HB2	5:G:589:HOH:O	1.75	0.87
3:G:123:HIS:HD2	3:G:125:MET:H	1.22	0.86
3:E:115:ILE:HD12	3:E:116:PRO:HD2	1.58	0.86
3:G:139:ARG:HH22	3:G:307:ALA:CB	1.89	0.85
3:E:260:ARG:NH1	5:E:539:HOH:O	2.05	0.85
1:A:489:LYS:CB	5:A:654:HOH:O	2.24	0.85
2:B:248:LYS:HG3	3:G:287:ARG:NH2	1.91	0.85
3:G:251:LEU:HB3	5:G:608:HOH:O	1.76	0.85
3:G:2:MET:O	3:G:3:ASP:HB3	1.74	0.85
1:C:482:VAL:HG13	2:D:213:PRO:HG3	1.58	0.84
1:C:512:ASN:HA	5:C:635:HOH:O	1.75	0.84
2:D:290:THR:HG22	5:D:331:HOH:O	1.77	0.84
3:E:109:GLU:HB3	3:E:115:ILE:HG22	1.60	0.84
3:G:17:ALA:O	3:G:20:ARG:O	1.96	0.83
1:A:479:GLN:HG2	2:B:210:THR:HG22	1.61	0.83
3:G:80:VAL:HG11	3:G:105:LEU:HD11	1.61	0.83
3:G:106:ARG:HD2	5:G:568:HOH:O	1.79	0.83
3:G:199:SER:HB2	5:G:402:HOH:O	1.79	0.83
2:D:297:ASP:OD2	5:D:325:HOH:O	1.95	0.82
1:C:454:PHE:CE2	2:D:261:LEU:HD12	2.14	0.82
1:C:500:ARG:HH11	1:C:500:ARG:CG	1.92	0.82
3:G:315:TYR:O	3:G:316:ASP:O	1.97	0.81
3:E:223:ASN:HD22	3:E:223:ASN:C	1.83	0.81
3:E:71:LEU:HD21	3:E:142:ARG:HG3	1.63	0.80
1:A:555:ASP:HA	5:A:662:HOH:O	1.81	0.80
1:C:532:ASP:OD1	2:D:264:HIS:HD2	1.65	0.80
3:G:252:SER:O	5:G:608:HOH:O	1.99	0.80
1:A:491:ARG:C	2:B:227:PRO:HG2	2.03	0.78
3:E:31:SER:HA	5:E:526:HOH:O	1.83	0.78
2:D:221:LEU:HB2	2:D:223:GLU:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:HIS:O	5:G:561:HOH:O	2.01	0.78
3:G:162:THR:HG21	5:G:520:HOH:O	1.84	0.77
2:D:261:LEU:HD13	2:D:264:HIS:HB2	1.66	0.77
1:C:500:ARG:HG2	1:C:500:ARG:NH1	1.98	0.77
1:C:467:LEU:O	5:C:616:HOH:O	2.01	0.77
1:A:482:VAL:HG22	2:B:213:PRO:HG3	1.66	0.76
2:B:219:ASN:CB	5:B:335:HOH:O	2.32	0.76
2:B:249:GLU:HG2	2:B:250:ASP:H	1.50	0.76
3:E:240:LEU:HG	3:E:248:ASN:HB3	1.66	0.76
1:A:505:HIS:NE2	5:A:670:HOH:O	1.91	0.75
1:A:572:LYS:HB2	5:A:665:HOH:O	1.86	0.75
3:G:255:GLU:HB2	5:G:608:HOH:O	1.85	0.75
2:B:223:GLU:C	2:B:225:LYS:N	2.39	0.75
2:B:235:HIS:HD2	2:B:261:LEU:HD21	1.51	0.74
3:G:221:ILE:HD11	3:G:232:TYR:HB2	1.68	0.74
2:D:259:HIS:CE1	2:D:282:ARG:HH22	2.05	0.74
3:E:140:ALA:HB2	3:E:332:SER:HB3	1.69	0.73
2:B:225:LYS:O	2:B:226:LEU:C	2.27	0.73
1:A:472:ALA:HB1	5:A:665:HOH:O	1.89	0.72
2:B:219:ASN:HB2	5:B:335:HOH:O	1.89	0.72
2:B:297:ASP:OD2	5:B:347:HOH:O	2.07	0.72
3:E:9:LYS:HD2	5:E:546:HOH:O	1.89	0.72
3:G:165:ARG:HG2	3:G:165:ARG:NH1	1.93	0.72
2:B:249:GLU:CG	2:B:250:ASP:H	2.02	0.72
1:C:454:PHE:CE2	2:D:261:LEU:CD1	2.72	0.72
3:G:165:ARG:HH11	3:G:165:ARG:CG	1.99	0.72
2:B:244:ASN:O	5:B:321:HOH:O	2.08	0.72
3:E:165:ARG:CG	3:E:165:ARG:HH11	2.03	0.71
2:D:238:LYS:O	5:D:317:HOH:O	2.07	0.71
4:E:401:AMP:O3P	5:E:433:HOH:O	2.08	0.71
1:C:486:VAL:HG21	1:C:491:ARG:NH1	2.04	0.71
3:G:67:LYS:HB3	5:G:567:HOH:O	1.90	0.70
3:E:188:THR:HA	5:E:502:HOH:O	1.91	0.70
2:B:245:THR:HG21	5:B:371:HOH:O	1.91	0.70
2:B:205:SER:HB2	5:B:313:HOH:O	1.89	0.70
1:A:491:ARG:CA	2:B:227:PRO:HG2	2.22	0.70
3:E:141:ARG:HD2	3:E:334:VAL:HA	1.74	0.70
3:G:187:MET:HE3	3:G:312:TYR:CZ	2.27	0.69
3:E:236:ASP:OD1	3:E:260:ARG:HD2	1.93	0.69
1:C:470:TYR:O	5:C:615:HOH:O	2.10	0.69
2:B:222:GLN:HG3	2:B:224:LEU:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:203:LYS:HE3	5:E:537:HOH:O	1.91	0.69
5:A:603:HOH:O	3:E:89:SER:HB3	1.93	0.69
3:E:141:ARG:HH11	3:E:334:VAL:HA	1.58	0.69
2:B:240:ILE:O	5:B:372:HOH:O	2.09	0.68
3:G:319:THR:HG22	3:G:320:THR:HG23	1.76	0.68
1:C:521:LEU:O	5:C:637:HOH:O	2.09	0.68
2:B:243:SER:O	2:B:245:THR:N	2.26	0.68
3:E:223:ASN:ND2	3:E:224:SER:O	2.27	0.68
1:A:513:THR:HB	1:A:540:ASP:HA	1.76	0.68
3:G:140:ALA:O	5:G:444:HOH:O	2.11	0.68
1:A:502:GLU:OE1	5:A:584:HOH:O	2.12	0.68
1:C:491:ARG:HB2	1:C:493:ASP:OD1	1.94	0.68
3:G:123:HIS:CD2	3:G:125:MET:H	2.07	0.67
3:G:320:THR:CB	3:G:321:PRO:CD	2.70	0.67
3:E:75:ALA:HB2	3:E:334:VAL:CG2	2.24	0.67
3:G:275:ARG:NH2	5:G:464:HOH:O	2.27	0.67
3:E:221:ILE:HD11	3:E:232:TYR:HB2	1.77	0.67
1:A:491:ARG:HA	2:B:227:PRO:HG2	1.76	0.66
3:G:40:THR:O	3:G:101:ARG:NH1	2.28	0.66
1:C:498:LYS:HA	1:C:518:GLU:HA	1.76	0.66
3:E:119:THR:HA	5:E:499:HOH:O	1.94	0.66
2:D:223:GLU:HA	2:D:226:LEU:HD22	1.77	0.66
2:B:297:ASP:HA	5:B:347:HOH:O	1.96	0.66
3:E:23:THR:CG2	5:E:525:HOH:O	2.25	0.66
3:E:82:LYS:HE2	3:E:86:GLN:OE1	1.94	0.66
3:G:182:VAL:HG23	5:G:589:HOH:O	1.95	0.66
3:E:115:ILE:HB	3:E:331:GLU:HB2	1.78	0.66
1:A:500:ARG:HD3	1:A:516:TYR:CE1	2.31	0.66
5:A:659:HOH:O	2:B:290:THR:HG23	1.96	0.66
1:C:468:ALA:C	5:C:616:HOH:O	2.34	0.66
3:G:57:SER:HB2	3:G:72:LEU:O	1.95	0.65
3:G:76:ASP:O	3:G:80:VAL:HG12	1.95	0.65
1:C:505:HIS:CE1	5:C:593:HOH:O	2.50	0.65
3:E:320:THR:HA	3:E:321:PRO:CB	2.27	0.65
5:G:575:HOH:O	1:C:457:ARG:HD2	1.95	0.65
2:B:282:ARG:NH1	2:B:287:TYR:OH	2.29	0.65
1:C:505:HIS:NE2	5:C:593:HOH:O	2.30	0.64
2:B:290:THR:HG21	5:G:546:HOH:O	1.98	0.64
3:G:117:PRO:HA	5:G:580:HOH:O	1.96	0.64
1:C:450:ASN:CG	5:C:625:HOH:O	2.36	0.64
3:E:140:ALA:HB2	3:E:332:SER:CB	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:139:ARG:O	3:G:141:ARG:N	2.27	0.64
1:A:506:CYS:HB3	1:A:513:THR:HG23	1.80	0.64
3:G:139:ARG:HH22	3:G:307:ALA:HB2	1.61	0.64
3:G:199:SER:HB3	5:G:403:HOH:O	1.97	0.64
3:G:185:ASN:C	3:G:185:ASN:HD22	2.01	0.64
3:E:224:SER:O	3:E:225:GLU:CG	2.42	0.64
3:G:38:ASP:CG	5:G:441:HOH:O	2.36	0.63
1:A:569:LEU:HD23	5:A:665:HOH:O	1.99	0.63
1:A:485:PRO:HG3	1:A:490:TYR:CZ	2.34	0.63
2:B:248:LYS:HA	2:B:248:LYS:HE3	1.80	0.62
3:G:91:PRO:HG3	1:C:459:ARG:HD2	1.80	0.62
2:B:250:ASP:O	2:B:253:VAL:HG12	2.00	0.62
3:E:71:LEU:CD2	3:E:142:ARG:HG3	2.28	0.62
2:B:225:LYS:NZ	5:B:351:HOH:O	2.30	0.62
1:C:457:ARG:NH1	5:C:580:HOH:O	1.95	0.62
2:D:250:ASP:O	2:D:251:GLN:CB	2.47	0.62
1:A:454:PHE:CZ	2:B:261:LEU:HD13	2.35	0.61
3:G:66:ASN:ND2	3:G:154:SER:OG	2.21	0.61
2:D:218:SER:HA	2:D:219:ASN:CB	2.30	0.61
3:G:67:LYS:CB	5:G:567:HOH:O	2.47	0.61
3:G:92:GLU:HG2	5:C:630:HOH:O	2.01	0.61
3:E:142:ARG:NH1	5:E:493:HOH:O	2.34	0.61
1:A:492:SER:OG	2:B:228:LYS:O	2.18	0.61
3:G:30:THR:O	5:G:555:HOH:O	2.16	0.61
1:C:538:TYR:CD2	1:C:553:MET:CB	2.76	0.60
1:C:482:VAL:CG1	1:C:483:PRO:CD	2.79	0.60
2:D:218:SER:HA	2:D:219:ASN:HB2	1.83	0.60
2:B:292:MET:HE1	3:G:61:TRP:HD1	1.66	0.60
1:C:482:VAL:HG12	1:C:483:PRO:CD	2.32	0.59
1:A:509:GLU:HG3	5:A:586:HOH:O	2.02	0.59
1:A:545:PRO:HD2	1:A:548:THR:H	1.67	0.59
3:E:107:GLU:HA	3:E:107:GLU:OE2	2.02	0.59
2:D:248:LYS:H	2:D:248:LYS:CD	2.16	0.59
3:E:109:GLU:CB	3:E:115:ILE:HG22	2.30	0.59
2:D:283:TYR:CA	5:D:332:HOH:O	2.49	0.59
2:B:223:GLU:O	2:B:225:LYS:N	2.32	0.59
1:A:461:ASP:OD1	2:B:225:LYS:NZ	2.36	0.59
1:A:540:ASP:N	3:G:151:GLU:OE1	2.35	0.59
3:G:320:THR:CB	3:G:321:PRO:HD2	2.25	0.59
1:C:539:LYS:NZ	5:C:596:HOH:O	2.13	0.59
3:E:141:ARG:NH2	4:E:401:AMP:O2P	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:LYS:CA	5:G:567:HOH:O	2.51	0.59
3:E:264:PHE:O	3:E:266:GLY:N	2.35	0.59
3:G:305:SER:N	5:G:536:HOH:O	2.05	0.58
1:C:535:SER:HB3	2:D:263:ASN:HB3	1.85	0.58
3:E:51:THR:HG21	3:E:242:GLN:HE21	1.68	0.58
3:E:62:ASP:OD2	3:E:62:ASP:C	2.41	0.58
3:E:317:LYS:HE2	3:E:317:LYS:HA	1.84	0.58
1:A:465:ILE:HG12	5:A:603:HOH:O	2.02	0.58
3:G:5:GLN:NE2	5:G:484:HOH:O	2.33	0.58
2:D:245:THR:OG1	5:D:336:HOH:O	2.17	0.58
1:A:491:ARG:HA	2:B:227:PRO:CG	2.33	0.58
3:G:184:LEU:HD13	3:G:275:ARG:HA	1.86	0.58
1:C:536:ASN:HB3	5:C:592:HOH:O	2.03	0.58
2:B:226:LEU:O	2:B:227:PRO:O	2.21	0.57
1:C:483:PRO:HG2	2:D:215:PHE:HZ	1.69	0.57
5:A:631:HOH:O	3:E:92:GLU:HG2	2.04	0.57
2:B:282:ARG:HD2	5:B:376:HOH:O	2.04	0.57
3:E:137:LYS:NZ	3:E:315:TYR:OH	2.37	0.57
3:G:144:PRO:HB2	3:G:146:ILE:HD11	1.87	0.57
2:D:213:PRO:HB3	2:D:215:PHE:HE2	1.68	0.57
2:D:215:PHE:O	2:D:216:LEU:HB2	2.04	0.57
3:E:223:ASN:C	3:E:223:ASN:ND2	2.53	0.57
2:D:213:PRO:HB3	2:D:215:PHE:CE2	2.39	0.57
3:E:29:PRO:HG2	3:E:32:PHE:HB3	1.85	0.57
1:A:576:ALA:HA	5:A:647:HOH:O	2.03	0.57
2:D:261:LEU:CD1	2:D:264:HIS:HB2	2.32	0.57
2:B:225:LYS:O	2:B:226:LEU:O	2.23	0.56
5:C:640:HOH:O	2:D:263:ASN:ND2	2.38	0.56
5:G:576:HOH:O	2:D:271:GLN:HG2	2.05	0.56
2:B:207:GLN:HA	5:B:356:HOH:O	2.06	0.56
3:G:181:ARG:HA	3:G:275:ARG:HG3	1.87	0.56
2:D:288:VAL:HG22	3:E:32:PHE:CZ	2.40	0.56
3:E:145:LEU:HD21	3:E:161:LEU:HD22	1.86	0.56
2:B:225:LYS:C	2:B:226:LEU:O	2.44	0.56
1:C:471:ARG:N	5:C:616:HOH:O	1.85	0.56
1:C:568:MET:O	1:C:572:LYS:HG2	2.06	0.56
1:A:557:LYS:O	2:B:281:THR:OG1	2.23	0.55
3:G:20:ARG:NE	5:G:558:HOH:O	2.29	0.55
1:C:486:VAL:CG1	1:C:491:ARG:HD2	2.36	0.55
1:A:507:LYS:HG2	5:A:584:HOH:O	2.05	0.55
1:C:474:GLN:HE22	2:D:211:GLU:CB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:MET:CE	3:E:238:MET:HB2	2.36	0.55
1:C:482:VAL:HG12	1:C:483:PRO:HD2	1.89	0.55
3:G:139:ARG:HH22	3:G:307:ALA:HB3	1.70	0.55
5:C:637:HOH:O	2:D:230:PRO:O	2.18	0.55
2:B:235:HIS:O	2:B:261:LEU:HD11	2.07	0.55
3:G:84:TYR:HB3	3:G:94:ILE:HD12	1.89	0.55
3:E:318:THR:HB	5:E:497:HOH:O	2.05	0.55
1:C:498:LYS:NZ	2:D:205:SER:OG	2.38	0.54
2:D:212:ILE:HD12	2:D:212:ILE:H	1.70	0.54
1:A:459:ARG:NH1	3:E:250:ASP:OD1	2.35	0.54
1:A:537:GLY:HA3	5:A:589:HOH:O	2.07	0.54
3:G:80:VAL:HG11	3:G:105:LEU:CD1	2.34	0.54
3:G:305:SER:HB2	5:G:538:HOH:O	2.08	0.54
3:E:334:VAL:OXT	3:E:334:VAL:HG12	2.08	0.54
3:E:203:LYS:NZ	5:E:440:HOH:O	2.41	0.54
1:C:472:ALA:HB2	1:C:573:LEU:HD23	1.89	0.53
3:E:242:GLN:HB2	5:E:529:HOH:O	2.08	0.53
1:C:454:PHE:CZ	2:D:261:LEU:HD12	2.43	0.53
1:A:500:ARG:NE	5:A:614:HOH:O	2.42	0.53
1:C:545:PRO:HA	1:C:546:GLU:CB	2.38	0.53
3:G:149:ASP:OD1	5:G:549:HOH:O	2.19	0.53
2:B:282:ARG:NH1	5:B:341:HOH:O	2.41	0.53
3:E:185:ASN:HD22	3:E:186:GLN:H	1.56	0.53
3:E:73:THR:HG21	3:E:333:ALA:O	2.09	0.53
3:G:196:ALA:O	3:G:219:VAL:HG13	2.09	0.53
2:D:259:HIS:O	2:D:262:LEU:HD22	2.08	0.52
3:G:4:VAL:N	5:G:556:HOH:O	2.43	0.52
3:G:295:ASP:HB3	3:G:301:GLU:OE1	2.09	0.52
1:C:468:ALA:O	5:C:616:HOH:O	2.19	0.52
2:B:292:MET:CE	3:G:61:TRP:CD1	2.93	0.52
2:D:248:LYS:H	2:D:248:LYS:HD3	1.74	0.52
3:E:165:ARG:HH11	3:E:165:ARG:HG2	1.74	0.52
3:G:110:ARG:HA	3:G:115:ILE:HG22	1.91	0.52
3:E:185:ASN:HD22	3:E:186:GLN:N	2.08	0.52
3:E:149:ASP:OD1	3:E:149:ASP:C	2.48	0.52
2:D:236:LEU:O	2:D:238:LYS:N	2.38	0.52
2:D:247:TYR:HB3	2:D:248:LYS:HD2	1.90	0.52
2:D:264:HIS:HE1	5:D:345:HOH:O	1.93	0.52
3:E:221:ILE:HG12	3:E:253:VAL:HG11	1.92	0.52
1:A:557:LYS:HE3	5:A:578:HOH:O	2.10	0.52
3:E:295:ASP:OD2	3:E:299:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:144:PRO:HB2	3:E:146:ILE:HD11	1.91	0.51
2:B:292:MET:CE	3:G:61:TRP:HD1	2.22	0.51
2:D:265:LEU:HD11	2:D:277:LEU:HD22	1.91	0.51
1:C:462:ALA:HB3	1:C:463:PRO:HD3	1.92	0.51
1:C:482:VAL:CG1	1:C:483:PRO:HD2	2.40	0.51
1:C:556:LEU:HD23	3:E:149:ASP:HB2	1.91	0.51
2:D:283:TYR:HB3	5:D:332:HOH:O	2.11	0.51
1:A:458:CYS:HB2	5:A:603:HOH:O	2.09	0.51
3:G:197:THR:HG22	3:G:220:PRO:HG2	1.91	0.51
1:A:488:GLY:N	5:A:623:HOH:O	2.30	0.51
2:B:263:ASN:HA	5:B:360:HOH:O	2.09	0.51
3:G:104:GLY:HA3	5:G:578:HOH:O	2.11	0.51
3:G:187:MET:CE	3:G:312:TYR:CZ	2.93	0.51
3:E:322:GLY:H	3:E:323:VAL:CA	2.24	0.51
2:B:259:HIS:CE1	2:B:282:ARG:HH22	2.29	0.50
2:B:292:MET:HE1	3:G:61:TRP:CD1	2.45	0.50
3:E:110:ARG:HG2	3:E:115:ILE:HG23	1.93	0.50
3:G:304:LEU:HA	5:G:536:HOH:O	2.11	0.50
1:C:459:ARG:NH1	5:C:595:HOH:O	2.45	0.50
3:E:331:GLU:HG2	5:E:423:HOH:O	2.12	0.50
2:B:248:LYS:HG3	3:G:287:ARG:HH22	1.75	0.50
3:G:324:PRO:HG2	5:G:591:HOH:O	2.12	0.50
1:A:458:CYS:O	1:A:459:ARG:HG2	2.12	0.50
2:B:249:GLU:HB3	5:G:517:HOH:O	2.11	0.50
3:E:48:SER:O	3:E:52:LEU:HB2	2.12	0.50
3:E:227:THR:HG21	5:E:504:HOH:O	2.12	0.50
1:C:552:GLY:O	1:C:553:MET:CB	2.59	0.49
2:D:218:SER:CA	2:D:219:ASN:HB2	2.42	0.49
1:A:463:PRO:HB2	5:B:350:HOH:O	2.13	0.49
3:G:231:VAL:CG1	3:G:267:VAL:HG22	2.41	0.49
1:A:538:TYR:CZ	1:A:561:PRO:HD2	2.47	0.49
3:G:168:LYS:NZ	5:G:613:HOH:O	2.41	0.49
3:G:194:ASN:ND2	3:G:214:LYS:NZ	2.61	0.49
2:D:215:PHE:O	2:D:216:LEU:CB	2.61	0.49
3:E:82:LYS:HG3	3:E:209:LYS:HA	1.94	0.49
3:E:87:SER:OG	5:E:514:HOH:O	2.20	0.49
1:C:451:LYS:HB2	5:C:628:HOH:O	2.13	0.49
2:B:226:LEU:O	5:B:365:HOH:O	2.18	0.49
1:A:459:ARG:HA	1:A:527:GLY:O	2.12	0.48
1:A:511:LYS:HG2	5:A:587:HOH:O	2.12	0.48
2:B:219:ASN:HB3	5:B:335:HOH:O	2.04	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:185:ASN:HD22	3:G:186:GLN:N	2.11	0.48
1:A:500:ARG:HD2	1:A:514:TYR:CD1	2.48	0.48
3:G:67:LYS:HE3	5:G:618:HOH:O	2.12	0.48
3:G:12:LEU:HD12	3:G:317:LYS:HB3	1.94	0.48
3:G:231:VAL:HG12	3:G:267:VAL:HG22	1.95	0.48
1:A:459:ARG:NH1	3:E:85:TYR:OH	2.45	0.48
2:D:251:GLN:N	5:D:342:HOH:O	2.42	0.48
3:G:123:HIS:HD2	3:G:125:MET:N	2.02	0.48
1:C:454:PHE:CE2	2:D:261:LEU:HD11	2.49	0.47
3:G:110:ARG:HD2	5:G:580:HOH:O	2.13	0.47
3:G:12:LEU:CD1	3:G:317:LYS:HB3	2.44	0.47
3:G:256:ALA:N	5:G:608:HOH:O	2.47	0.47
2:B:249:GLU:CG	2:B:250:ASP:N	2.73	0.47
3:G:275:ARG:NH1	5:G:463:HOH:O	2.46	0.47
1:A:490:TYR:OH	5:A:595:HOH:O	2.15	0.47
1:A:545:PRO:HD2	1:A:548:THR:N	2.28	0.47
2:B:251:GLN:HB2	5:B:373:HOH:O	2.13	0.47
3:E:208:ILE:CD1	3:E:249:LEU:HD22	2.45	0.47
2:B:273:GLY:HA2	5:E:419:HOH:O	2.15	0.47
1:A:538:TYR:CE1	1:A:561:PRO:HD2	2.50	0.47
3:G:9:LYS:HG2	3:G:317:LYS:HG2	1.97	0.47
3:G:214:LYS:HB2	5:G:599:HOH:O	2.15	0.47
5:G:448:HOH:O	1:C:459:ARG:HD3	2.15	0.47
1:C:484:LYS:HA	1:C:485:PRO:HD3	1.77	0.47
1:A:449:ARG:O	1:A:450:ASN:ND2	2.47	0.47
3:E:75:ALA:HB2	3:E:334:VAL:HG21	1.97	0.47
3:G:231:VAL:HG12	3:G:267:VAL:CG2	2.44	0.46
3:E:44:LYS:HB2	3:E:98:ASP:CG	2.35	0.46
3:G:67:LYS:HA	5:G:567:HOH:O	2.14	0.46
1:C:495:TYR:CZ	2:D:229:PRO:HD3	2.51	0.46
1:A:500:ARG:HD3	1:A:516:TYR:HE1	1.77	0.46
1:C:451:LYS:CB	5:C:628:HOH:O	2.64	0.46
1:C:474:GLN:NE2	2:D:211:GLU:HB2	2.07	0.46
1:C:486:VAL:HG11	1:C:491:ARG:HD2	1.96	0.46
1:C:488:GLY:N	5:C:586:HOH:O	2.48	0.46
1:A:506:CYS:O	1:A:511:LYS:HB2	2.15	0.46
1:A:539:LYS:NZ	5:A:617:HOH:O	2.47	0.46
1:C:486:VAL:HG13	1:C:491:ARG:HD2	1.98	0.46
2:B:254:LEU:O	3:G:31:SER:HB3	2.15	0.46
3:E:141:ARG:HB2	3:E:334:VAL:O	2.16	0.46
3:E:125:MET:C	5:E:525:HOH:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:59:PRO:HA	3:G:71:LEU:HD12	1.97	0.46
3:G:253:VAL:HG12	3:G:257:LEU:HD22	1.98	0.46
2:D:251:GLN:HA	5:D:342:HOH:O	2.15	0.46
3:G:140:ALA:C	3:G:142:ARG:H	2.19	0.45
2:D:233:PRO:HG2	2:D:236:LEU:HD12	1.97	0.45
1:A:557:LYS:NZ	5:A:662:HOH:O	2.49	0.45
1:C:482:VAL:HG13	1:C:483:PRO:CD	2.45	0.45
2:D:232:LEU:HD22	2:D:233:PRO:HD2	1.99	0.45
1:C:482:VAL:HG12	1:C:483:PRO:N	2.30	0.45
3:E:196:ALA:O	3:E:220:PRO:HD2	2.17	0.45
3:G:86:GLN:NE2	5:G:492:HOH:O	2.48	0.45
2:D:222:GLN:C	2:D:223:GLU:HG2	2.37	0.45
3:G:171:SER:OG	3:G:284:LYS:HB2	2.16	0.45
3:G:287:ARG:H	3:G:287:ARG:HD2	1.81	0.45
3:E:9:LYS:NZ	5:E:497:HOH:O	2.49	0.45
3:E:74:MET:HE3	3:E:74:MET:HA	1.98	0.45
2:D:287:TYR:CA	5:E:526:HOH:O	2.55	0.45
3:E:142:ARG:HH21	3:E:334:VAL:C	2.20	0.45
1:A:544:HIS:NE2	3:G:151:GLU:OE2	2.50	0.45
3:G:320:THR:HB	3:G:321:PRO:HD3	1.86	0.45
1:A:464:GLU:HG2	5:A:606:HOH:O	2.17	0.45
2:B:224:LEU:O	2:B:225:LYS:C	2.54	0.45
1:A:471:ARG:O	1:A:475:ARG:HG2	2.17	0.44
2:B:235:HIS:CD2	2:B:261:LEU:HD21	2.42	0.44
3:G:223:ASN:C	3:G:223:ASN:OD1	2.55	0.44
2:D:224:LEU:H	2:D:226:LEU:HD13	1.80	0.44
3:G:174:CYS:O	3:G:177:THR:HG23	2.17	0.44
3:G:315:TYR:HB3	3:G:319:THR:CG2	2.47	0.44
1:A:459:ARG:N	5:A:603:HOH:O	2.44	0.44
3:E:73:THR:HB	3:E:334:VAL:HB	2.00	0.44
3:E:186:GLN:HB2	5:E:496:HOH:O	2.17	0.44
2:B:251:GLN:HG2	5:B:368:HOH:O	2.16	0.44
1:C:492:SER:C	1:C:494:MET:N	2.70	0.44
2:D:290:THR:HA	3:E:34:LEU:O	2.18	0.44
3:E:33:ARG:NH2	5:E:413:HOH:O	1.96	0.44
1:A:454:PHE:CE1	2:B:261:LEU:HD13	2.53	0.44
2:D:248:LYS:NZ	5:D:341:HOH:O	2.45	0.44
3:E:139:ARG:HG3	3:E:328:ASP:O	2.18	0.44
3:G:57:SER:CB	3:G:72:LEU:O	2.65	0.44
3:G:147:ASP:OD1	3:G:148:VAL:N	2.50	0.44
2:D:247:TYR:HB3	2:D:248:LYS:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:THR:HG22	1:C:540:ASP:CG	2.38	0.43
3:E:231:VAL:CG1	3:E:267:VAL:HG11	2.48	0.43
3:E:312:TYR:CZ	3:E:319:THR:HG21	2.53	0.43
2:D:247:TYR:O	2:D:249:GLU:N	2.40	0.43
2:D:221:LEU:HB2	2:D:223:GLU:N	2.26	0.43
2:B:294:LYS:NZ	5:B:303:HOH:O	2.50	0.43
3:G:315:TYR:O	3:G:316:ASP:C	2.55	0.43
3:G:62:ASP:OD2	3:G:62:ASP:C	2.55	0.43
3:G:68:PHE:N	5:G:567:HOH:O	2.52	0.43
3:E:120:ILE:O	3:E:120:ILE:HG13	2.18	0.43
3:E:182:VAL:O	3:E:187:MET:CE	2.67	0.43
3:G:316:ASP:HB3	3:G:319:THR:H	1.84	0.43
3:E:123:HIS:HB3	3:E:126:HIS:CG	2.54	0.43
3:E:294:VAL:HG12	3:E:300:LEU:HA	2.01	0.43
3:G:208:ILE:HA	3:G:211:LEU:HD12	2.01	0.43
1:C:504:PRO:O	1:C:508:ARG:HB2	2.19	0.43
3:E:280:PHE:HZ	3:E:313:ILE:HD11	1.81	0.43
3:G:178:ALA:O	3:G:181:ARG:HD3	2.19	0.43
2:D:251:GLN:CA	5:D:342:HOH:O	2.66	0.43
1:C:479:GLN:OE1	1:C:500:ARG:NH1	2.52	0.43
2:D:207:GLN:O	2:D:208:TYR:C	2.57	0.43
1:A:485:PRO:HG3	1:A:490:TYR:CE2	2.54	0.43
3:G:268:HIS:HE1	5:G:530:HOH:O	2.02	0.42
3:E:71:LEU:HD21	3:E:142:ARG:CG	2.42	0.42
3:E:231:VAL:HG12	3:E:267:VAL:HG11	2.00	0.42
3:G:319:THR:CG2	3:G:320:THR:HG23	2.46	0.42
2:D:221:LEU:HA	2:D:222:GLN:C	2.40	0.42
3:G:202:THR:N	5:G:595:HOH:O	2.52	0.42
3:G:316:ASP:OD2	3:G:317:LYS:HG3	2.18	0.42
3:E:13:LYS:HE2	5:E:447:HOH:O	2.20	0.42
1:A:475:ARG:NH1	5:A:650:HOH:O	2.50	0.42
3:G:139:ARG:HB2	5:G:583:HOH:O	2.19	0.42
1:C:450:ASN:H	1:C:450:ASN:HD22	1.68	0.42
1:C:539:LYS:NZ	1:C:540:ASP:O	2.39	0.42
1:C:539:LYS:HB3	1:C:539:LYS:HE3	1.89	0.42
2:D:214:ALA:O	2:D:217:THR:OG1	2.31	0.42
1:C:479:GLN:CD	1:C:500:ARG:HH12	2.21	0.42
1:C:492:SER:O	1:C:494:MET:N	2.52	0.42
1:C:532:ASP:OD1	2:D:264:HIS:CD2	2.57	0.42
2:D:283:TYR:CB	5:D:332:HOH:O	2.67	0.42
3:E:326:GLN:O	3:E:327:THR:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:122:VAL:HG21	3:G:131:ALA:HB2	2.01	0.42
2:D:250:ASP:O	2:D:251:GLN:HB2	2.17	0.42
1:A:544:HIS:ND1	1:A:544:HIS:N	2.68	0.42
2:D:223:GLU:O	2:D:224:LEU:HD23	2.20	0.42
3:E:332:SER:HA	3:E:333:ALA:HB2	2.02	0.42
1:C:498:LYS:HB3	1:C:518:GLU:HG3	2.02	0.41
3:E:75:ALA:HB2	3:E:334:VAL:HG23	2.02	0.41
3:G:140:ALA:HB1	3:G:142:ARG:O	2.20	0.41
3:G:320:THR:C	3:G:322:GLY:H	2.24	0.41
1:C:513:THR:HA	1:C:540:ASP:HA	2.01	0.41
5:A:651:HOH:O	2:B:227:PRO:HD3	2.19	0.41
3:G:242:GLN:C	3:G:244:GLY:H	2.24	0.41
3:E:47:LEU:HD22	3:E:238:MET:HG3	2.03	0.41
3:E:140:ALA:CB	3:E:332:SER:HB3	2.44	0.41
1:A:539:LYS:HE2	1:A:541:ILE:HA	2.01	0.41
2:B:292:MET:HE3	3:G:61:TRP:CD1	2.55	0.41
1:A:539:LYS:HA	3:G:151:GLU:OE1	2.20	0.41
2:B:270:THR:O	2:B:271:GLN:HB2	2.20	0.41
3:G:85:TYR:HE2	3:G:249:LEU:HD13	1.86	0.41
2:D:221:LEU:HA	2:D:223:GLU:N	2.36	0.41
3:E:165:ARG:HH11	3:E:165:ARG:HG3	1.82	0.41
3:G:316:ASP:N	5:G:559:HOH:O	2.51	0.41
2:B:290:THR:HA	3:G:34:LEU:O	2.21	0.41
3:G:127:SER:C	5:G:561:HOH:O	2.60	0.41
3:G:257:LEU:HD12	3:G:257:LEU:HA	1.84	0.41
1:C:475:ARG:HH11	1:C:475:ARG:HG2	1.85	0.41
1:C:521:LEU:HD23	1:C:521:LEU:HA	1.90	0.41
3:E:143:ILE:O	3:E:143:ILE:HG23	2.21	0.41
3:E:208:ILE:HD11	3:E:249:LEU:HD22	2.03	0.41
3:E:181:ARG:HA	3:E:275:ARG:HG3	2.03	0.41
1:A:450:ASN:HD22	1:A:450:ASN:HA	1.67	0.40
1:C:521:LEU:HD22	1:C:529:PHE:HB3	2.02	0.40
2:D:295:ASN:ND2	3:E:40:THR:O	2.54	0.40
2:B:219:ASN:HB3	5:B:318:HOH:O	2.21	0.40
3:G:141:ARG:HB2	5:G:444:HOH:O	2.22	0.40
3:E:187:MET:CE	5:E:533:HOH:O	2.69	0.40
3:G:49:LEU:HA	3:G:52:LEU:HD22	2.03	0.40
3:E:20:ARG:NH2	5:E:516:HOH:O	2.55	0.40
3:E:187:MET:HE2	5:E:533:HOH:O	2.20	0.40
3:E:189:ILE:HG12	3:E:304:LEU:CD1	2.51	0.40
1:A:458:CYS:C	1:A:459:ARG:HG2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:252:SER:OG	3:G:255:GLU:HG3	2.22	0.40
3:E:165:ARG:HG2	3:E:165:ARG:NH1	2.35	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:434:HOH:O	5:E:408:HOH:O[2_554]	1.79	0.41
3:G:126:HIS:CD2	5:E:545:HOH:O[2_554]	2.10	0.10
5:G:430:HOH:O	5:E:406:HOH:O[2_554]	2.16	0.04

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 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	126/137 (92%)	112 (89%)	9 (7%)	5 (4%)	3	3
1	C	126/137 (92%)	103 (82%)	12 (10%)	11 (9%)	1	0
2	B	91/97 (94%)	74 (81%)	6 (7%)	11 (12%)	0	0
2	D	91/97 (94%)	65 (71%)	15 (16%)	11 (12%)	0	0
3	E	331/333 (99%)	305 (92%)	16 (5%)	10 (3%)	4	7
3	G	323/333 (97%)	303 (94%)	11 (3%)	9 (3%)	5	7
All	All	1088/1134 (96%)	962 (88%)	69 (6%)	57 (5%)	2	2

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	207	GLN
2	B	224	LEU
2	B	225	LYS
2	B	227	PRO

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Mol	Chain	Res	Type
2	B	244	ASN
3	G	140	ALA
3	G	215	ASN
3	G	316	ASP
3	G	320	THR
3	G	324	PRO
1	C	498	LYS
1	C	546	GLU
1	C	547	ARG
1	C	551	HIS
1	C	553	MET
2	D	207	GLN
2	D	247	TYR
2	D	248	LYS
3	E	321	PRO
3	E	323	VAL
3	E	327	THR
2	B	206	GLU
2	B	218	SER
2	B	226	LEU
2	B	249	GLU
3	G	21	SER
1	C	542	TYR
1	C	550	ASP
2	D	206	GLU
2	D	217	THR
2	D	219	ASN
2	D	223	GLU
2	D	226	LEU
2	D	251	GLN
3	E	319	THR
1	A	550	ASP
1	A	556	LEU
2	B	220	THR
2	B	296	PHE
3	G	3	ASP
3	G	321	PRO
1	C	493	ASP
2	D	236	LEU
1	A	543	SER
1	A	553	MET
3	G	117	PRO

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Mol	Chain	Res	Type
3	E	117	PRO
3	E	318	THR
1	A	557	LYS
1	C	540	ASP
1	C	545	PRO
2	D	216	LEU
3	E	264	PHE
3	E	322	GLY
3	E	333	ALA
3	E	296	GLU
1	C	552	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 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	107/120 (89%)	91 (85%)	16 (15%)	3 5
1	C	102/120 (85%)	87 (85%)	15 (15%)	3 5
2	B	84/88 (96%)	71 (84%)	13 (16%)	2 4
2	D	84/88 (96%)	72 (86%)	12 (14%)	3 5
3	E	286/296 (97%)	259 (91%)	27 (9%)	8 17
3	G	287/296 (97%)	249 (87%)	38 (13%)	4 7
All	All	950/1008 (94%)	829 (87%)	121 (13%)	4 8

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	458	CYS
1	A	482	VAL
1	A	484	LYS
1	A	492	SER
1	A	498	LYS
1	A	513	THR

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	521	LEU
1	A	534	LYS
1	A	544	HIS
1	A	556	LEU
1	A	557	LYS
1	A	565	LEU
1	A	568	MET
1	A	569	LEU
2	B	217	THR
2	B	219	ASN
2	B	222	GLN
2	B	223	GLU
2	B	224	LEU
2	B	226	LEU
2	B	232	LEU
2	B	248	LYS
2	B	249	GLU
2	B	262	LEU
2	B	271	GLN
2	B	281	THR
2	B	290	THR
3	G	3	ASP
3	G	9	LYS
3	G	20	ARG
3	G	21	SER
3	G	30	THR
3	G	39	VAL
3	G	52	LEU
3	G	80	VAL
3	G	84	TYR
3	G	85	TYR
3	G	92	GLU
3	G	102	LEU
3	G	120	ILE
3	G	137	LYS
3	G	139	ARG
3	G	146	ILE
3	G	154	SER
3	G	162	THR
3	G	163	GLN
3	G	165	ARG

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Mol	Chain	Res	Type
3	G	181	ARG
3	G	184	LEU
3	G	185	ASN
3	G	186	GLN
3	G	217	SER
3	G	227	THR
3	G	228	LEU
3	G	231	VAL
3	G	243	ASP
3	G	257	LEU
3	G	275	ARG
3	G	276	LEU
3	G	287	ARG
3	G	299	LYS
3	G	305	SER
3	G	310	LEU
3	G	317	LYS
3	G	319	THR
1	C	450	ASN
1	C	459	ARG
1	C	475	ARG
1	C	486	VAL
1	C	498	LYS
1	C	500	ARG
1	C	508	ARG
1	C	511	LYS
1	C	512	ASN
1	C	521	LEU
1	C	536	ASN
1	C	539	LYS
1	C	555	ASP
1	C	565	LEU
1	C	569	LEU
2	D	219	ASN
2	D	221	LEU
2	D	225	LYS
2	D	226	LEU
2	D	232	LEU
2	D	248	LYS
2	D	249	GLU
2	D	259	HIS
2	D	261	LEU

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Mol	Chain	Res	Type
2	D	262	LEU
2	D	290	THR
2	D	297	ASP
3	E	3	ASP
3	E	5	GLN
3	E	39	VAL
3	E	44	LYS
3	E	52	LEU
3	E	66	ASN
3	E	92	GLU
3	E	102	LEU
3	E	107	GLU
3	E	115	ILE
3	E	126	HIS
3	E	163	GLN
3	E	165	ARG
3	E	181	ARG
3	E	184	LEU
3	E	185	ASN
3	E	223	ASN
3	E	227	THR
3	E	228	LEU
3	E	243	ASP
3	E	257	LEU
3	E	275	ARG
3	E	276	LEU
3	E	286	SER
3	E	287	ARG
3	E	316	ASP
3	E	318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	474	GLN
1	A	479	GLN
1	A	505	HIS
2	B	219	ASN
2	B	235	HIS
2	B	259	HIS
2	B	284	HIS

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Mol	Chain	Res	Type
3	G	86	GLN
3	G	123	HIS
3	G	185	ASN
3	G	194	ASN
1	C	450	ASN
1	C	474	GLN
1	C	505	HIS
1	C	520	GLN
2	D	207	GLN
2	D	219	ASN
2	D	264	HIS
2	D	269	ASN
2	D	295	ASN
3	E	5	GLN
3	E	66	ASN
3	E	163	GLN
3	E	185	ASN
3	E	186	GLN
3	E	215	ASN
3	E	223	ASN
3	E	242	GLN
3	E	263	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)

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	$\#\|Z\| > 2$
4	AMP	G	401	-	22,25,25	1.21	1 (4%)	25,38,38	1.40	4 (16%)
4	AMP	E	401	-	22,25,25	1.05	2 (9%)	25,38,38	1.71	7 (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
4	AMP	G	401	-	-	3/6/26/26	0/3/3/3
4	AMP	E	401	-	-	5/6/26/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	401	AMP	C5-C4	2.63	1.47	1.40
4	E	401	AMP	C5-C4	2.28	1.47	1.40
4	E	401	AMP	O4'-C1'	2.06	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401	AMP	P-O5'-C5'	4.29	130.12	118.30
4	E	401	AMP	N3-C2-N1	-3.55	123.13	128.68
4	G	401	AMP	C3'-C2'-C1'	3.19	105.78	100.98
4	G	401	AMP	P-O5'-C5'	2.55	125.32	118.30
4	G	401	AMP	N3-C2-N1	-2.43	124.88	128.68
4	E	401	AMP	O4'-C4'-C5'	2.24	116.74	109.37
4	E	401	AMP	O3P-P-O2P	2.23	116.16	107.64
4	E	401	AMP	C3'-C2'-C1'	2.13	104.18	100.98
4	E	401	AMP	N6-C6-N1	2.06	122.84	118.57
4	G	401	AMP	C4-C5-N7	-2.05	107.27	109.40
4	E	401	AMP	O5'-C5'-C4'	2.02	115.94	108.99

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	AMP	C5'-O5'-P-O2P
4	G	401	AMP	C5'-O5'-P-O3P
4	E	401	AMP	C5'-O5'-P-O1P
4	E	401	AMP	C5'-O5'-P-O2P
4	E	401	AMP	C5'-O5'-P-O3P
4	G	401	AMP	C5'-O5'-P-O1P
4	E	401	AMP	O4'-C4'-C5'-O5'
4	E	401	AMP	C3'-C4'-C5'-O5'

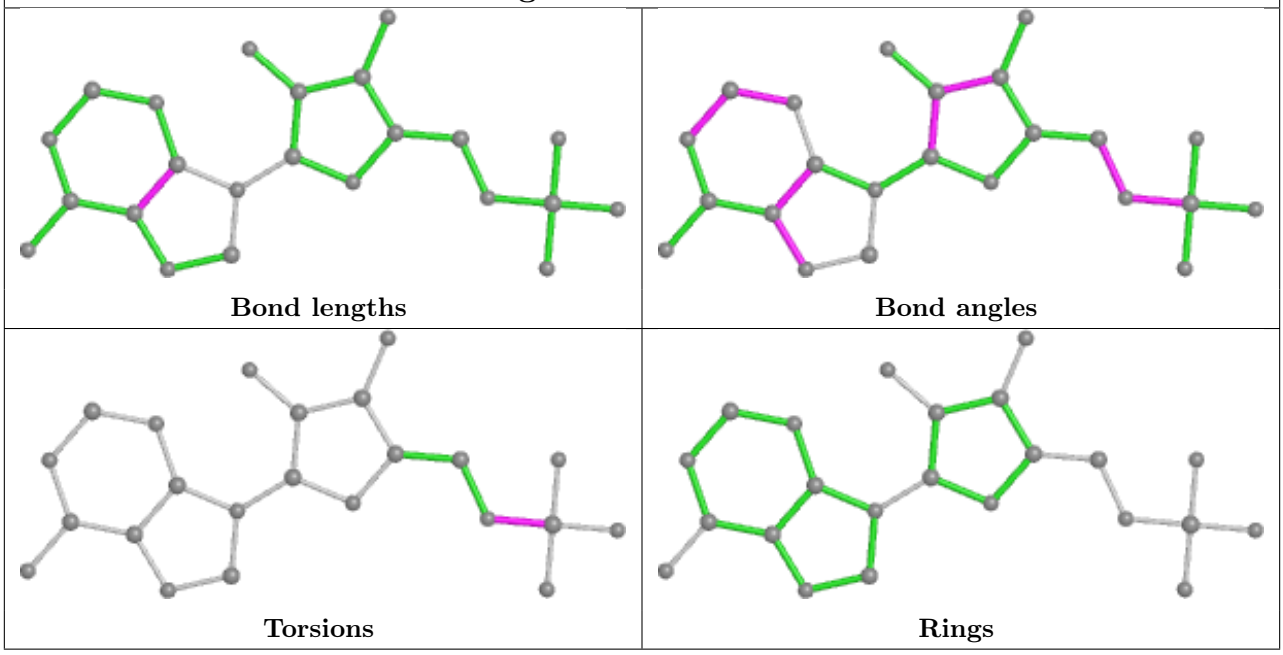
There are no ring outliers.

1 monomer is involved in 2 short contacts:

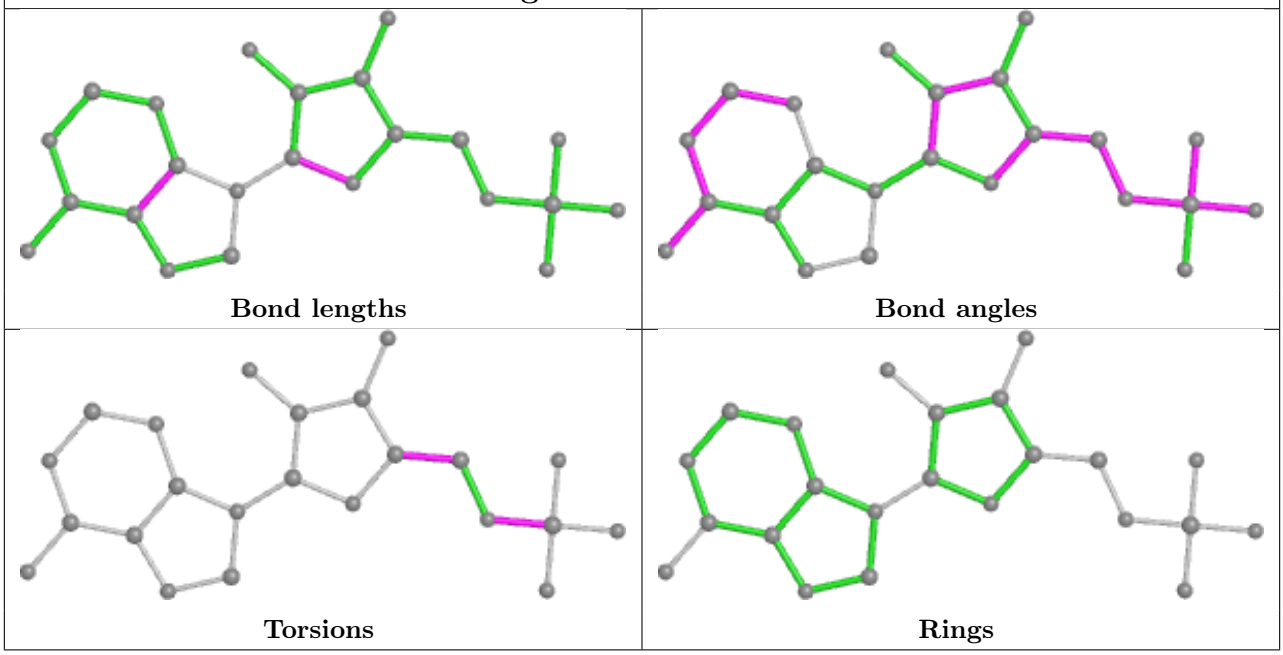
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	AMP	2	0

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 then 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.

Ligand AMP G 401



Ligand AMP E 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	286:LYS	C	287:TYR	N	1.14
1	C	481:THR	C	482:VAL	N	1.10

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	128/137 (93%)	-0.01	14 (10%)	5	3	12, 26, 74, 85	2 (1%)
1	C	128/137 (93%)	0.85	22 (17%)	1	0	19, 42, 86, 94	0
2	B	93/97 (95%)	0.27	12 (12%)	3	2	12, 31, 68, 73	0
2	D	93/97 (95%)	0.56	12 (12%)	3	2	18, 51, 81, 89	1 (1%)
3	E	333/333 (100%)	-0.20	19 (5%)	23	18	10, 27, 61, 123	0
3	G	324/333 (97%)	-0.40	13 (4%)	38	31	8, 24, 49, 81	3 (0%)
All	All	1099/1134 (96%)	-0.01	92 (8%)	11	7	8, 28, 72, 123	6 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	547	ARG	11.7
1	C	548	THR	9.2
3	E	329	ASN	9.0
1	C	549	ALA	8.4
3	E	332	SER	7.1
1	C	544	HIS	6.9
3	E	322	GLY	6.8
2	B	247	TYR	6.7
3	E	333	ALA	6.6
1	C	545	PRO	6.6
3	E	318	THR	6.5
1	C	486	VAL	6.5
1	A	449	ARG	6.3
3	G	318	THR	6.0
3	E	326	GLN	5.9
1	A	450	ASN	5.9
1	C	546	GLU	5.7
3	E	321	PRO	5.6
3	E	319	THR	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	205	SER	5.2
3	G	323	VAL	5.1
2	D	224	LEU	5.1
3	E	327	THR	4.8
1	C	551	HIS	4.8
3	E	334	VAL	4.7
1	C	553	MET	4.7
1	C	449	ARG	4.7
1	C	543	SER	4.5
3	E	330	PHE	4.5
1	C	542	TYR	4.3
2	D	221	LEU	4.2
2	D	218	SER	4.2
2	D	247	TYR	4.2
2	B	220	THR	4.1
3	G	325	GLU	4.0
2	D	234	PRO	3.9
2	B	246	ALA	3.9
1	C	448	ARG	3.9
3	E	328	ASP	3.8
3	E	324	PRO	3.8
1	A	553	MET	3.8
3	G	117	PRO	3.7
1	C	552	GLY	3.7
2	B	218	SER	3.6
3	E	323	VAL	3.6
2	D	244	ASN	3.5
2	D	220	THR	3.4
2	B	206	GLU	3.4
3	G	321	PRO	3.4
2	B	245	THR	3.3
1	C	554	ASP	3.3
3	E	331	GLU	3.3
3	E	117	PRO	3.3
1	C	510	GLY	3.2
1	A	487	ASN	3.2
2	B	223	GLU	3.1
2	B	248	LYS	3.1
3	G	322	GLY	3.1
1	A	547	ARG	3.1
3	G	324	PRO	3.0
2	D	222	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	320	THR	3.0
1	C	491	ARG	2.9
3	G	85	TYR	2.9
1	A	551	HIS	2.8
3	G	317	LYS	2.8
2	B	219	ASN	2.7
2	B	221	LEU	2.7
1	C	487	ASN	2.7
3	G	140	ALA	2.6
1	A	505	HIS	2.6
2	D	245	THR	2.6
2	D	210	THR	2.5
1	A	545	PRO	2.5
1	A	550	ASP	2.4
1	C	485	PRO	2.4
1	C	550	ASP	2.4
3	E	317	LYS	2.4
2	D	261	LEU	2.4
3	G	118	GLU	2.4
2	D	219	ASN	2.3
1	A	544	HIS	2.3
3	G	83	TYR	2.3
1	A	549	ALA	2.2
3	E	3	ASP	2.2
1	C	450	ASN	2.2
1	C	541	ILE	2.2
1	A	576	ALA	2.2
1	A	486	VAL	2.1
2	B	244	ASN	2.1
1	A	555	ASP	2.1
3	E	4	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

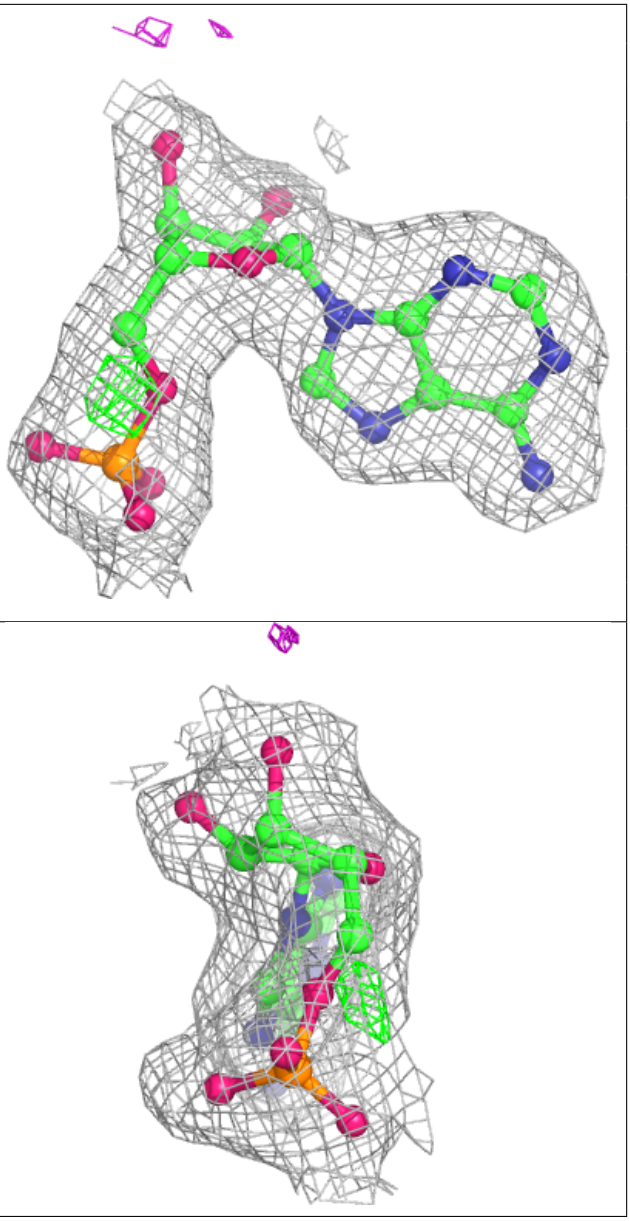
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AMP	G	401	23/23	0.97	0.13	19,21,29,31	0
4	AMP	E	401	23/23	0.97	0.11	20,22,31,32	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.

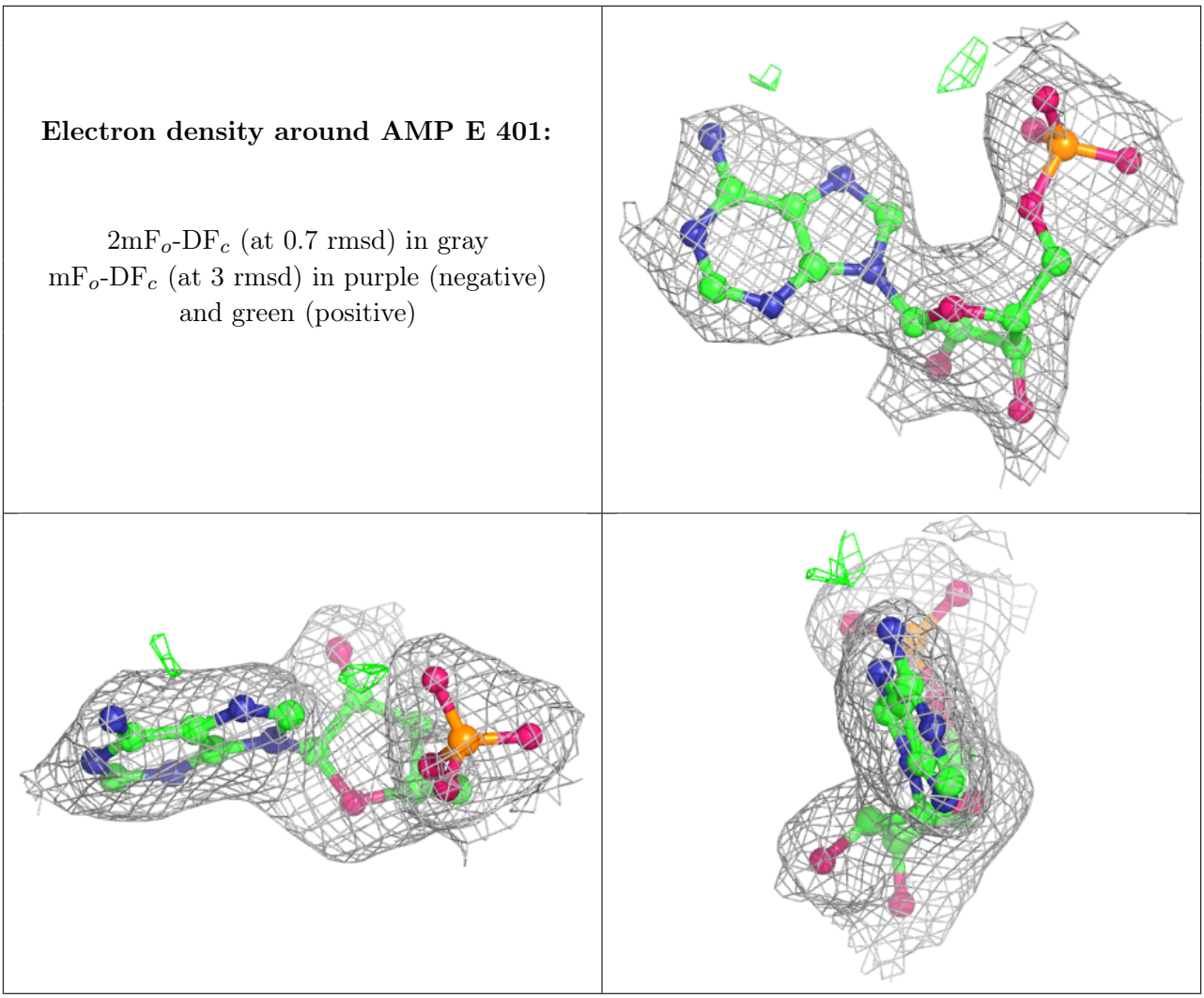
Electron density around AMP G 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP E 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.