Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 05:08 AM EDT

PDB ID	:	6AVH
Title	:	GH3.15 acyl acid amido synthetase
Authors	:	Sherp, A.M.; Jez, J.M.
Deposited on	:	2017-09-02
Resolution	:	3.01 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:

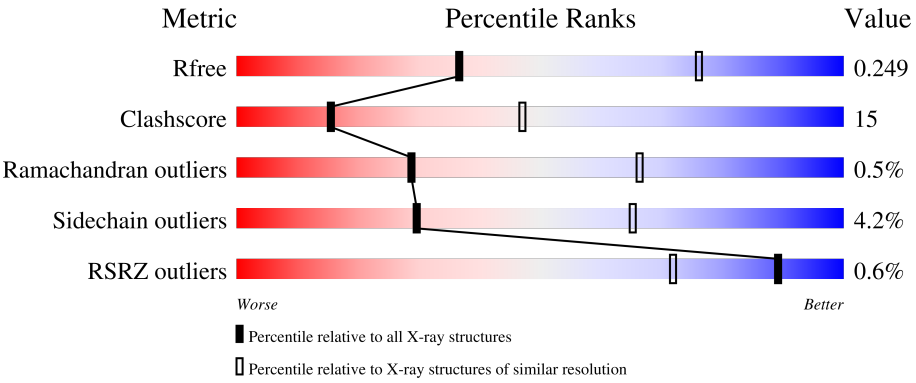
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	595	60% 29% • 8%
1	B	595	% 58% 31% • 9%
1	C	595	% 59% 32% • 7%
1	D	595	% 66% 25% • 8%

2 Entry composition

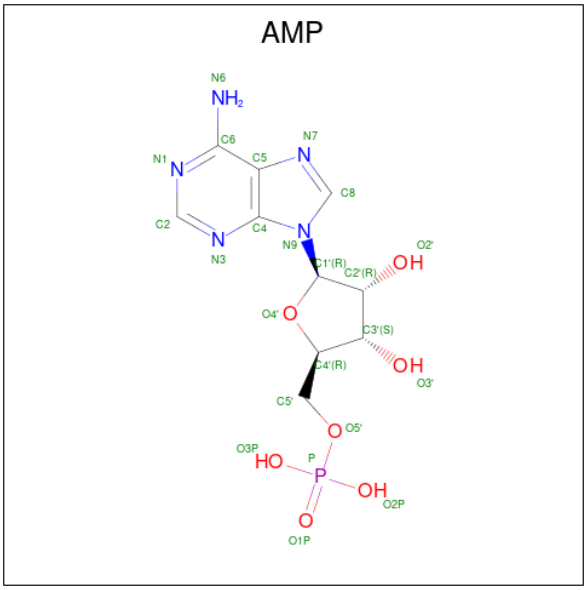
There are 2 unique types of molecules in this entry. The entry contains 17399 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GH3.15 acyl acid amido synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4331	2773	708	824	26			
1	B	541	Total	C	N	O	S	0	0	0
			4285	2743	699	817	26			
1	C	552	Total	C	N	O	S	0	0	0
			4353	2783	712	832	26			
1	D	549	Total	C	N	O	S	0	0	0
			4338	2777	707	828	26			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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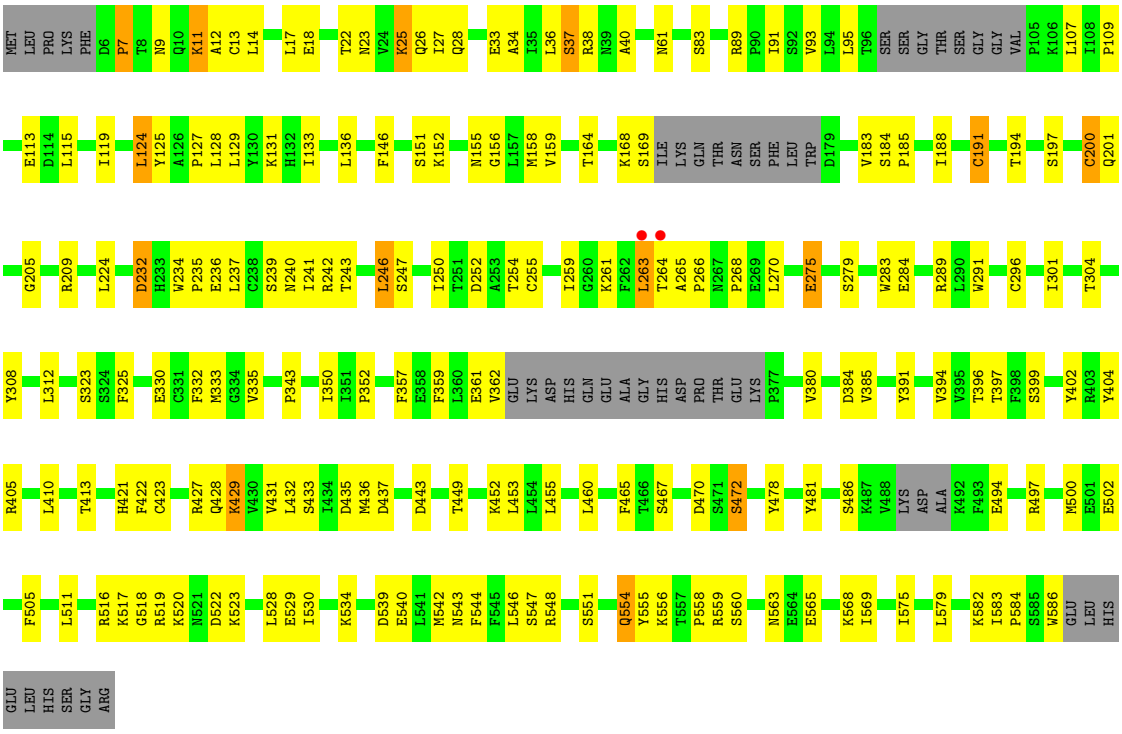
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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.

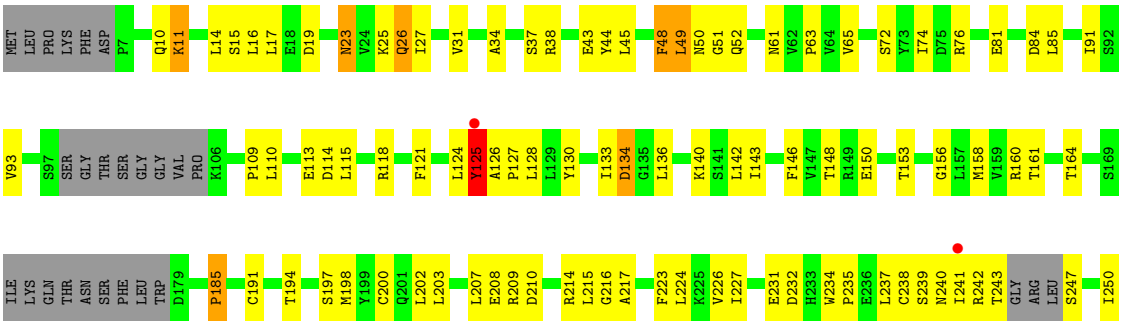
• Molecule 1: GH3.15 acyl acid amido synthetase

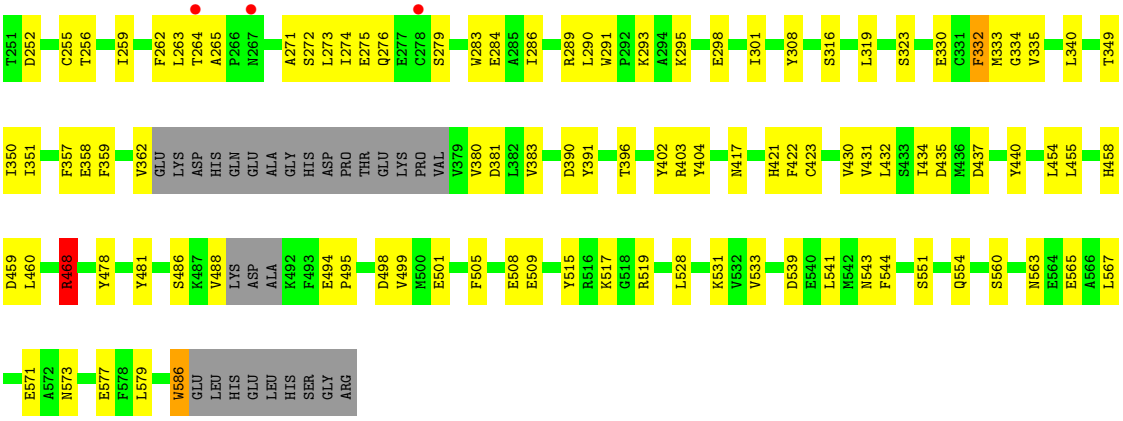
Chain A:



• Molecule 1: GH3.15 acyl acid amido synthetase

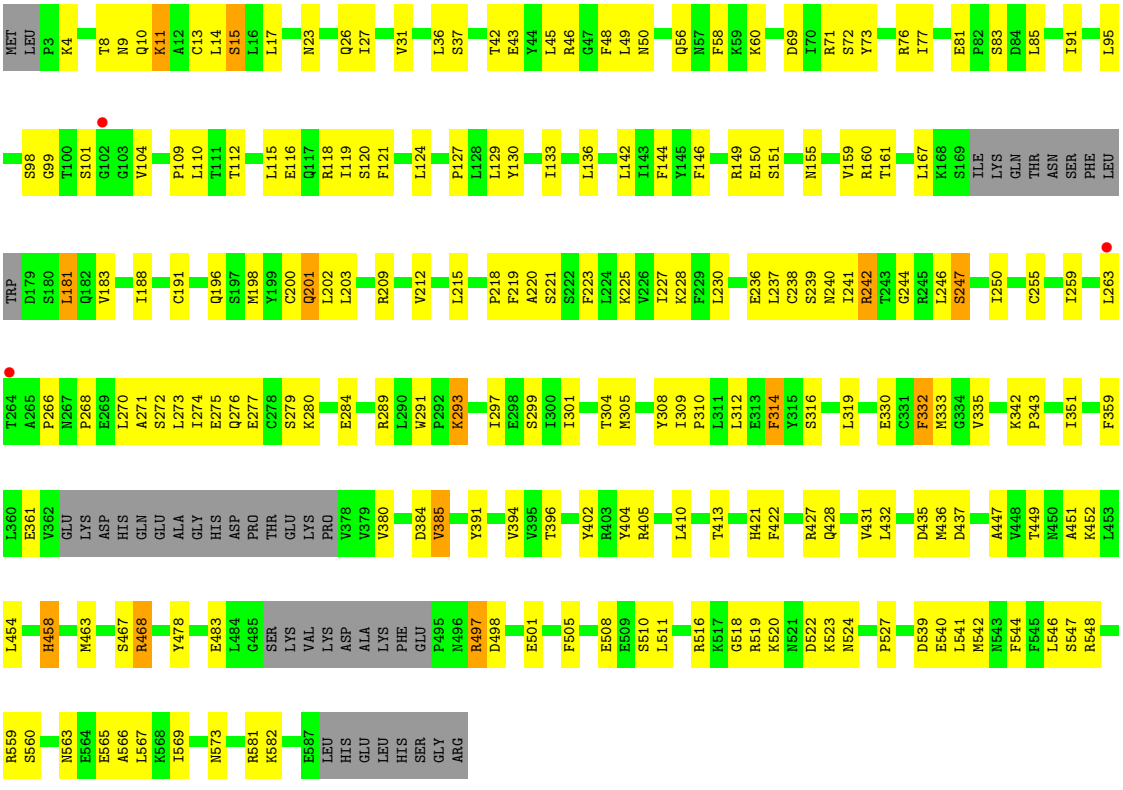
Chain B:





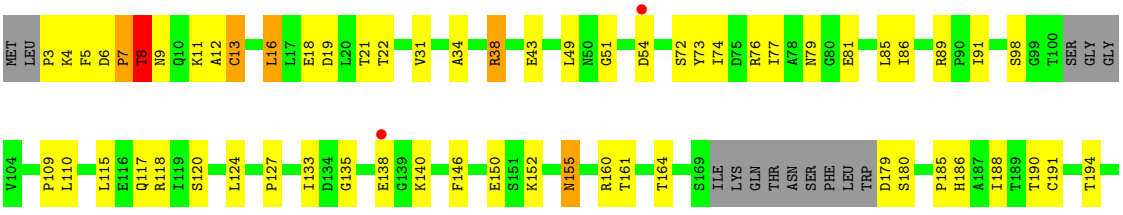
• Molecule 1: GH3.15 acyl acid amido synthetase

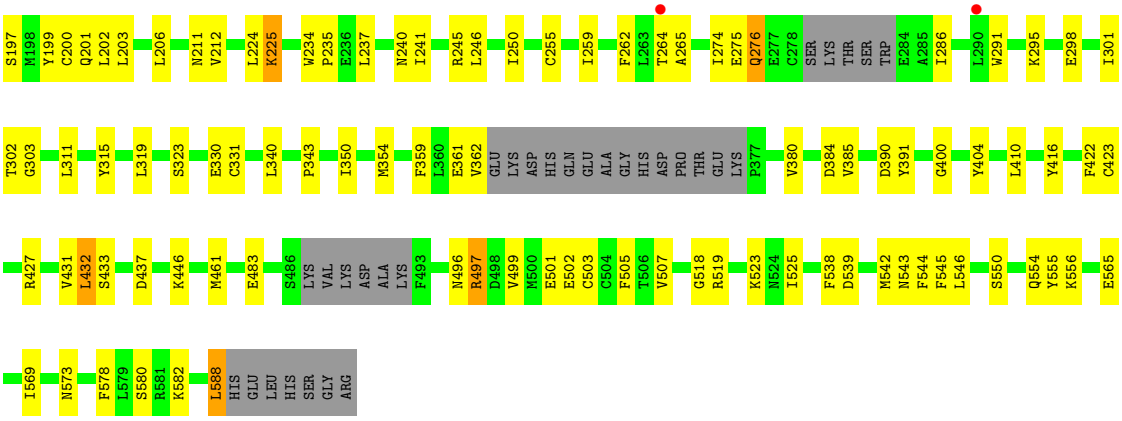
Chain C:



• Molecule 1: GH3.15 acyl acid amido synthetase

Chain D:




S197 M198 Y199 C200 Q201 L202 L203 L206 N211 V212 L224 K225 W234 P235 E236 L237 N240 I241 R245 L246 I250 C255 I259 F262 L263 T264 A265 I274 E275 Q276 E277 C278 SER LYS THR SER TRP E284 A285 I286 L290 W291 K295 E298 I301
T302 G303 L311 Y315 L319 S323 E330 C331 L340 P343 I350 M354 F359 L360 E361 V362 GLU LYS ASP HIS GLN GLU ALA GLY HIS ASP PRO THR GLU LYS P377 V380 D384 V385 D390 Y391 G400 Y404 L410 Y416 F422 C423
R427 V431 L432 S433 D437 K446 M461 E483 S486 LYS VAL LYS ASP ALA LYS F493 N496 R497 D498 V499 M500 E501 E502 C503 C504 F505 T506 V507 G518 R519 K523 N524 I525 F538 D539 M542 N543 F544 F545 L546 S550 Q554 Y555 K556 E565
I569 N573 F578 L579 S580 R581 K582 L588 HIS GLU LEU HIS SER GLY ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.91Å 191.60Å 319.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.53 – 3.01 46.53 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.53-3.01) 99.1 (46.53-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.185 , 0.249 0.185 , 0.249	Depositor DCC
R_{free} test set	1995 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.2	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	0.94	EDS
Total number of atoms	17399	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0705e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.73	2/4422 (0.0%)	0.89	4/5991 (0.1%)
1	B	0.65	0/4373	0.70	1/5922 (0.0%)
1	C	0.73	2/4445 (0.0%)	0.72	1/6024 (0.0%)
1	D	0.78	5/4428 (0.1%)	0.85	4/5999 (0.1%)
All	All	0.73	9/17668 (0.1%)	0.80	10/23936 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	1
1	D	0	4
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	218	PRO	N-CD	-16.83	1.24	1.47
1	D	276	GLN	CB-CG	12.64	1.86	1.52
1	D	276	GLN	CD-NE2	12.44	1.64	1.32
1	D	276	GLN	CG-CD	8.32	1.70	1.51
1	A	200	CYS	CB-SG	-5.77	1.72	1.81
1	D	385	VAL	CB-CG1	-5.76	1.40	1.52
1	A	13	CYS	CB-SG	-5.36	1.73	1.81
1	C	385	VAL	CB-CG1	-5.24	1.41	1.52
1	D	331	CYS	CB-SG	-5.20	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ASN	CB-CG-OD1	28.84	179.29	121.60
1	D	276	GLN	CG-CD-OE1	22.21	166.03	121.60
1	D	276	GLN	OE1-CD-NE2	-19.04	78.11	121.90
1	A	9	ASN	CB-CG-ND2	-18.37	72.60	116.70
1	A	124	LEU	CB-CG-CD2	-10.33	93.44	111.00
1	A	9	ASN	OD1-CG-ND2	-6.49	106.98	121.90
1	C	49	LEU	C-N-CA	-5.78	107.25	121.70
1	B	468	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	118	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	D	432	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	PRO	Peptide
1	B	125	TYR	Peptide
1	B	15	SER	Peptide
1	B	48	PHE	Peptide
1	B	52	GLN	Peptide
1	C	15	SER	Peptide
1	D	13	CYS	Peptide
1	D	523	LYS	Peptide
1	D	7	PRO	Peptide
1	D	8	THR	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	4331	0	4326	129	0
1	B	4285	0	4275	139	0
1	C	4353	0	4340	148	0
1	D	4338	0	4324	101	4
2	A	23	0	12	0	0
2	B	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	23	0	12	1	0
2	D	23	0	12	2	0
All	All	17399	0	17313	512	4

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 15.

All (512) 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:D:276:GLN:CG	1:D:276:GLN:CB	1.86	1.48
1:C:236:GLU:O	1:C:240:ASN:ND2	1.98	0.97
1:A:284:GLU:O	1:A:289:ARG:NH1	1.97	0.96
1:D:133:ILE:HG13	1:D:340:LEU:HD11	1.49	0.94
1:A:502:GLU:OE2	1:A:582:LYS:NZ	2.01	0.94
1:B:240:ASN:HD21	1:B:247:SER:HB2	1.37	0.90
1:B:214:ARG:NH1	1:B:298:GLU:OE2	2.08	0.87
1:A:397:THR:HG22	1:A:399:SER:H	1.40	0.86
1:B:16:LEU:HA	1:B:19:ASP:HB3	1.55	0.86
1:D:250:ILE:HD11	1:D:255:CYS:HB3	1.58	0.85
1:B:544:PHE:HZ	1:B:565:GLU:HG3	1.40	0.85
1:C:272:SER:O	1:C:276:GLN:NE2	2.10	0.84
1:C:250:ILE:HD11	1:C:255:CYS:HB3	1.60	0.84
1:C:437:ASP:OD2	1:C:478:TYR:OH	1.97	0.82
1:A:236:GLU:O	1:A:240:ASN:ND2	2.13	0.82
1:B:43:GLU:OE2	1:B:76:ARG:NH2	2.11	0.81
1:B:508:GLU:HG2	1:B:515:TYR:HE2	1.46	0.80
1:C:284:GLU:HB3	1:C:314:PHE:HE1	1.45	0.80
1:B:275:GLU:O	1:B:279:SER:OG	1.98	0.80
1:B:544:PHE:CZ	1:B:565:GLU:HG3	2.16	0.80
1:B:481:TYR:OH	1:B:571:GLU:OE2	1.99	0.79
1:D:554:GLN:O	1:D:556:LYS:NZ	2.15	0.79
1:A:155:ASN:OD1	1:A:156:GLY:N	2.16	0.78
1:D:91:ILE:HD12	1:D:109:PRO:HB3	1.66	0.78
1:A:427:ARG:NH2	1:A:556:LYS:HD2	1.97	0.78
1:B:417:ASN:OD1	1:C:523:LYS:NZ	2.15	0.78
1:D:433:SER:OG	1:D:437:ASP:O	2.00	0.78
1:B:437:ASP:OD2	1:B:478:TYR:OH	2.00	0.77
1:A:437:ASP:OD2	1:A:478:TYR:OH	2.02	0.77
1:C:284:GLU:HB3	1:C:314:PHE:CE1	2.19	0.77
1:D:21:THR:HG21	1:D:416:TYR:HD1	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:VAL:HG21	1:D:291:TRP:CD1	2.21	0.76
1:A:14:LEU:HD21	1:A:127:PRO:HG2	1.67	0.76
1:B:430:VAL:HG22	1:B:440:TYR:HE1	1.50	0.75
1:B:264:THR:HG23	1:B:265:ALA:H	1.51	0.75
1:B:284:GLU:O	1:B:289:ARG:NH1	2.20	0.75
1:D:203:LEU:HD23	1:D:259:ILE:HD11	1.69	0.74
1:A:544:PHE:HZ	1:A:565:GLU:HB3	1.52	0.74
1:C:76:ARG:NH1	1:C:81:GLU:OE2	2.19	0.74
1:B:396:THR:HG23	1:B:402:TYR:HA	1.70	0.74
1:C:150:GLU:OE2	1:C:160:ARG:NH1	2.19	0.73
1:A:547:SER:OG	1:A:548:ARG:NH1	2.19	0.72
1:B:27:ILE:O	1:B:31:VAL:HG23	1.88	0.72
1:B:242:ARG:NH1	1:B:275:GLU:OE2	2.21	0.72
1:B:563:ASN:OD1	1:B:565:GLU:HG2	1.89	0.72
1:B:121:PHE:HE2	1:B:335:VAL:HG11	1.54	0.72
1:C:270:LEU:HD12	1:C:273:LEU:HD11	1.73	0.71
1:A:252:ASP:OD2	1:A:254:THR:OG1	2.08	0.71
1:C:129:LEU:O	1:C:133:ILE:HG22	1.90	0.71
1:B:49:LEU:HD12	1:B:61:ASN:ND2	2.06	0.71
1:B:350:ILE:HG12	1:B:422:PHE:HE1	1.55	0.70
1:D:7:PRO:O	1:D:8:THR:HG22	1.92	0.70
1:D:225:LYS:NZ	1:D:539:ASP:OD1	2.24	0.70
1:B:198:MET:O	1:B:202:LEU:HD13	1.92	0.70
1:B:239:SER:O	1:B:243:THR:HG22	1.91	0.69
1:C:144:PHE:CD2	1:C:201:GLN:HG2	2.27	0.69
1:B:133:ILE:HG13	1:B:340:LEU:HD11	1.73	0.69
1:B:143:ILE:HD13	1:B:216:GLY:HA3	1.75	0.69
1:A:304:THR:HB	1:A:559:ARG:HH21	1.57	0.68
1:A:470:ASP:OD1	1:A:472:SER:HB3	1.92	0.68
1:B:358:GLU:OE2	1:B:403:ARG:NH2	2.26	0.68
1:A:396:THR:HG23	1:A:402:TYR:HA	1.75	0.68
1:C:301:ILE:HB	1:C:309:ILE:HD11	1.75	0.68
1:C:183:VAL:HG21	1:C:212:VAL:HG22	1.75	0.68
1:C:242:ARG:O	1:C:266:PRO:HB3	1.94	0.68
1:B:494:GLU:HG2	1:B:495:PRO:HD2	1.76	0.66
1:D:380:VAL:HG22	1:D:384:ASP:HB2	1.77	0.66
1:C:133:ILE:HG21	1:C:136:LEU:HD12	1.77	0.66
1:B:17:LEU:HD13	1:B:125:TYR:CD2	2.30	0.66
1:D:199:TYR:OH	1:D:240:ASN:ND2	2.30	0.65
1:D:588:LEU:HD23	1:D:588:LEU:H	1.61	0.65
1:B:16:LEU:HA	1:B:19:ASP:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ILE:HD11	1:C:255:CYS:CB	2.27	0.64
1:A:91:ILE:HD12	1:A:109:PRO:HB3	1.78	0.64
1:D:185:PRO:HG3	1:D:262:PHE:HE1	1.62	0.64
1:D:502:GLU:OE2	1:D:582:LYS:NZ	2.22	0.64
1:A:529:GLU:HB2	1:A:579:LEU:HD23	1.79	0.63
1:A:359:PHE:HB3	1:A:391:TYR:HB3	1.80	0.63
1:B:271:ALA:O	1:B:275:GLU:HG3	1.99	0.63
1:D:146:PHE:HB3	1:D:194:THR:HG22	1.80	0.63
1:B:250:ILE:HD11	1:B:255:CYS:HB3	1.80	0.63
1:C:202:LEU:HD21	1:C:230:LEU:HB2	1.79	0.63
1:A:250:ILE:HD11	1:A:255:CYS:HB3	1.80	0.63
1:B:26:GLN:H	1:B:26:GLN:NE2	1.97	0.63
1:C:242:ARG:NH1	1:C:275:GLU:OE1	2.31	0.63
1:D:319:LEU:H	1:D:319:LEU:HD12	1.63	0.62
1:D:185:PRO:HG3	1:D:262:PHE:CE1	2.34	0.62
1:C:396:THR:HG23	1:C:402:TYR:HA	1.80	0.62
1:D:7:PRO:HG3	1:D:124:LEU:HG	1.82	0.62
1:A:28:GLN:NE2	1:A:352:PRO:O	2.33	0.62
1:D:34:ALA:O	1:D:38:ARG:HG2	1.99	0.62
1:C:380:VAL:CG1	1:C:384:ASP:HB2	2.30	0.61
1:C:45:LEU:O	1:C:48:PHE:O	2.17	0.61
1:A:380:VAL:HG13	1:A:384:ASP:HB2	1.81	0.61
1:A:275:GLU:O	1:A:279:SER:OG	2.17	0.61
1:A:301:ILE:HG12	1:A:323:SER:OG	2.00	0.61
1:C:14:LEU:HD12	1:C:127:PRO:HG2	1.81	0.61
1:C:246:LEU:HD13	1:C:250:ILE:HG21	1.81	0.61
1:A:14:LEU:HD12	1:A:14:LEU:O	2.01	0.61
1:D:431:VAL:HG12	1:D:432:LEU:HD12	1.83	0.61
1:B:434:ILE:HG13	1:B:478:TYR:HE1	1.64	0.60
1:A:89:ARG:HD3	1:A:113:GLU:HG3	1.83	0.60
1:A:264:THR:HG23	1:A:265:ALA:H	1.66	0.60
1:B:49:LEU:HD12	1:B:61:ASN:HD22	1.64	0.60
1:C:133:ILE:CG2	1:C:136:LEU:HD12	2.31	0.60
1:C:275:GLU:O	1:C:279:SER:OG	2.08	0.59
1:A:583:ILE:HD13	1:D:22:THR:HG23	1.83	0.59
1:B:43:GLU:HB3	1:B:85:LEU:HA	1.84	0.59
1:A:25:LYS:HE2	1:A:26:GLN:NE2	2.17	0.59
1:B:301:ILE:HG12	1:B:323:SER:OG	2.02	0.59
1:B:544:PHE:HZ	1:B:565:GLU:CG	2.13	0.59
1:D:124:LEU:O	1:D:127:PRO:HD2	2.01	0.59
1:B:110:LEU:HD21	1:B:115:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:HB3	1:D:85:LEU:HA	1.85	0.59
1:A:361:GLU:HG3	1:A:362:VAL:N	2.17	0.59
1:B:455:LEU:HD12	1:B:460:LEU:HB2	1.85	0.59
1:A:301:ILE:HD12	1:A:343:PRO:HB3	1.86	0.58
1:B:224:LEU:HD11	1:B:308:TYR:HB3	1.85	0.58
1:B:350:ILE:CG1	1:B:422:PHE:HE1	2.15	0.58
1:D:544:PHE:CZ	1:D:565:GLU:HB2	2.38	0.58
1:A:125:TYR:CE2	1:A:129:LEU:HD13	2.38	0.58
1:D:264:THR:HG23	1:D:265:ALA:H	1.68	0.58
1:A:544:PHE:HZ	1:A:565:GLU:CB	2.16	0.58
1:C:10:GLN:HB3	1:C:13:CYS:SG	2.44	0.57
1:C:112:THR:O	1:C:116:GLU:HG3	2.04	0.57
1:C:497:ARG:O	1:C:501:GLU:HG3	2.04	0.57
1:A:544:PHE:CZ	1:A:565:GLU:HB3	2.36	0.57
1:D:286:ILE:HD12	1:D:286:ILE:H	1.69	0.57
1:A:242:ARG:O	1:A:266:PRO:HB3	2.05	0.57
1:A:467:SER:OG	1:A:559:ARG:O	2.23	0.57
1:B:359:PHE:HB3	1:B:391:TYR:HB3	1.86	0.57
1:C:468:ARG:HD2	1:C:567:LEU:HD22	1.87	0.57
1:C:569:ILE:O	1:C:573:ASN:ND2	2.28	0.57
1:A:200:CYS:SG	1:A:250:ILE:HD13	2.44	0.57
1:A:433:SER:OG	1:A:437:ASP:O	2.14	0.57
1:A:511:LEU:O	1:A:516:ARG:NH1	2.36	0.57
1:B:25:LYS:HB2	1:B:383:VAL:HG21	1.85	0.56
1:B:72:SER:O	1:B:76:ARG:HG3	2.05	0.56
1:D:497:ARG:HG2	1:D:578:PHE:HE1	1.70	0.56
1:C:188:ILE:O	1:C:191:CYS:HB2	2.05	0.56
1:D:117:GLN:HG2	1:D:354:MET:HE1	1.86	0.56
1:A:240:ASN:OD1	1:A:247:SER:N	2.39	0.56
1:B:531:LYS:HE3	1:B:577:GLU:HG2	1.87	0.56
1:C:359:PHE:HB3	1:C:391:TYR:HB3	1.88	0.56
1:D:237:LEU:O	1:D:241:ILE:HG13	2.05	0.56
1:A:330:GLU:HG2	1:A:404:TYR:CE2	2.41	0.56
1:C:380:VAL:HG12	1:C:384:ASP:HB2	1.88	0.56
1:A:505:PHE:CD1	1:A:582:LYS:HB2	2.40	0.56
1:C:196:GLN:HB3	1:C:250:ILE:CD1	2.35	0.56
1:B:76:ARG:HD2	1:B:81:GLU:OE1	2.06	0.56
1:B:210:ASP:O	1:B:293:LYS:HD2	2.05	0.56
1:D:110:LEU:HD21	1:D:115:LEU:HB2	1.85	0.56
1:C:11:LYS:HD2	1:C:11:LYS:N	2.20	0.56
1:B:468:ARG:NH2	1:B:567:LEU:HD13	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TYR:HE1	1:B:136:LEU:HD12	1.71	0.55
1:B:498:ASP:OD1	1:B:499:VAL:HG23	2.07	0.55
1:B:136:LEU:HD21	1:B:214:ARG:HG3	1.89	0.55
1:B:501:GLU:HG2	1:B:579:LEU:O	2.06	0.55
1:C:43:GLU:OE2	1:C:76:ARG:NH2	2.40	0.55
1:C:26:GLN:CD	1:C:26:GLN:H	2.09	0.55
1:A:385:VAL:HG22	1:A:391:TYR:CE2	2.42	0.55
1:C:8:THR:OG1	1:C:9:ASN:N	2.35	0.55
1:B:539:ASP:O	1:B:543:ASN:ND2	2.37	0.55
1:D:150:GLU:OE2	1:D:160:ARG:HD3	2.07	0.55
1:C:98:SER:HB3	2:C:600:AMP:O2P	2.07	0.54
1:D:234:TRP:HZ3	1:D:275:GLU:HG3	1.71	0.54
1:A:410:LEU:HB3	1:A:422:PHE:HB3	1.90	0.54
1:B:185:PRO:HG3	1:B:262:PHE:HE2	1.73	0.54
1:D:302:THR:HB	2:D:600:AMP:N1	2.23	0.54
1:C:17:LEU:HD13	1:C:124:LEU:HD22	1.89	0.54
1:B:330:GLU:HG2	1:B:404:TYR:CE2	2.43	0.54
1:B:10:GLN:HG2	1:B:11:LYS:HG2	1.89	0.54
1:B:358:GLU:CD	1:B:403:ARG:HH21	2.10	0.54
1:D:542:MET:HG3	1:D:555:TYR:CE2	2.43	0.54
1:C:215:LEU:O	1:C:297:ILE:HA	2.08	0.53
1:D:543:ASN:HA	1:D:546:LEU:HD22	1.90	0.53
1:B:458:HIS:N	1:B:459:ASP:HA	2.22	0.53
1:A:397:THR:CG2	1:A:399:SER:H	2.18	0.53
1:A:185:PRO:HG2	1:A:188:ILE:HG13	1.90	0.53
1:C:91:ILE:HD12	1:C:109:PRO:HB3	1.90	0.53
1:D:234:TRP:CZ3	1:D:275:GLU:HG3	2.44	0.53
1:A:224:LEU:HD11	1:A:308:TYR:HB3	1.89	0.53
1:A:544:PHE:O	1:A:548:ARG:HD3	2.09	0.53
1:A:517:LYS:HG3	1:A:586:TRP:CZ2	2.44	0.53
1:D:18:GLU:O	1:D:22:THR:OG1	2.22	0.53
1:B:91:ILE:HD12	1:B:109:PRO:HB2	1.91	0.53
1:B:478:TYR:HB2	1:B:528:LEU:HD12	1.91	0.53
1:C:223:PHE:CE2	1:C:227:ILE:HD11	2.43	0.53
1:D:206:LEU:HD22	1:D:274:ILE:HD13	1.90	0.53
1:D:496:ASN:HB3	1:D:499:VAL:HG12	1.91	0.53
1:A:544:PHE:CZ	1:A:565:GLU:CB	2.92	0.53
1:B:148:THR:HG21	1:B:551:SER:HB3	1.90	0.53
1:C:121:PHE:HE2	1:C:335:VAL:HG11	1.73	0.53
1:C:237:LEU:O	1:C:241:ILE:HG13	2.09	0.53
1:A:237:LEU:O	1:A:241:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG12	1:B:158:MET:HB2	1.91	0.52
1:B:93:VAL:HG23	1:B:110:LEU:HB3	1.90	0.52
1:B:16:LEU:O	1:B:17:LEU:HB2	2.09	0.52
1:C:130:TYR:HE1	1:C:136:LEU:HD22	1.73	0.52
1:A:11:LYS:O	1:A:11:LYS:HG3	2.08	0.52
1:B:200:CYS:SG	1:B:250:ILE:CD1	2.97	0.52
1:C:273:LEU:HD12	1:C:274:ILE:N	2.24	0.52
1:C:277:GLU:HA	1:C:280:LYS:NZ	2.24	0.52
1:B:118:ARG:HD3	1:B:332:PHE:HB2	1.90	0.52
1:C:508:GLU:CD	1:C:519:ARG:HH11	2.12	0.52
1:D:264:THR:HG23	1:D:265:ALA:N	2.25	0.52
1:A:164:THR:O	1:A:168:LYS:HG2	2.09	0.52
1:B:350:ILE:HG12	1:B:422:PHE:CE1	2.42	0.52
1:A:200:CYS:SG	1:A:250:ILE:CD1	2.98	0.52
1:A:563:ASN:HB3	1:A:565:GLU:HG3	1.91	0.52
1:C:247:SER:O	1:C:250:ILE:HG22	2.10	0.52
1:D:133:ILE:CG1	1:D:340:LEU:HD11	2.31	0.52
1:D:188:ILE:O	1:D:191:CYS:HB2	2.10	0.52
1:B:140:LYS:NZ	1:B:208:GLU:OE2	2.36	0.52
1:D:86:ILE:HD12	1:D:400:GLY:HA3	1.92	0.52
1:D:497:ARG:O	1:D:501:GLU:HG3	2.10	0.51
1:A:234:TRP:CG	1:A:235:PRO:HD3	2.45	0.51
1:C:508:GLU:OE1	1:C:519:ARG:NH1	2.43	0.51
1:A:124:LEU:C	1:A:124:LEU:HD23	2.31	0.51
1:B:161:THR:HG23	1:B:554:GLN:OE1	2.10	0.51
1:A:17:LEU:CD1	1:A:124:LEU:HD21	2.41	0.51
1:A:168:LYS:O	1:A:169:SER:OG	2.20	0.51
1:D:569:ILE:O	1:D:573:ASN:ND2	2.38	0.51
1:B:150:GLU:HG2	1:B:160:ARG:HG2	1.92	0.51
1:C:316:SER:HB2	1:C:319:LEU:HB2	1.92	0.51
1:C:271:ALA:O	1:C:275:GLU:HG3	2.11	0.51
1:C:519:ARG:NH1	1:C:527:PRO:HA	2.26	0.51
1:D:186:HIS:CE1	1:D:190:THR:HG21	2.46	0.51
1:D:197:SER:O	1:D:201:GLN:HG3	2.11	0.51
1:C:225:LYS:NZ	1:C:539:ASP:OD1	2.31	0.51
1:B:125:TYR:CD2	1:B:128:LEU:HB2	2.46	0.50
1:B:430:VAL:HG22	1:B:440:TYR:CE1	2.39	0.50
1:A:197:SER:O	1:A:201:GLN:HG3	2.11	0.50
1:B:498:ASP:OD1	1:B:499:VAL:N	2.43	0.50
1:C:196:GLN:OE1	1:C:250:ILE:HD12	2.11	0.50
1:C:219:PHE:HB3	1:C:305:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:PHE:O	1:D:550:SER:HB2	2.12	0.50
1:A:34:ALA:O	1:A:38:ARG:HG3	2.12	0.50
1:B:126:ALA:N	1:B:127:PRO:HD2	2.25	0.50
1:B:146:PHE:HB3	1:B:194:THR:HG22	1.92	0.50
1:B:283:TRP:CE3	1:B:286:ILE:HD13	2.47	0.50
1:C:385:VAL:HG21	1:C:422:PHE:HZ	1.77	0.50
1:C:505:PHE:CD1	1:C:582:LYS:HB2	2.46	0.50
1:D:49:LEU:O	1:D:51:GLY:N	2.43	0.50
1:B:14:LEU:HD12	1:B:127:PRO:HG2	1.94	0.50
1:C:413:THR:OG1	1:C:421:HIS:HB3	2.12	0.50
1:D:3:PRO:HD3	1:D:31:VAL:HG22	1.94	0.50
1:A:333:MET:HE3	1:A:357:PHE:HE1	1.77	0.50
1:C:361:GLU:HG3	1:C:391:TYR:CE1	2.47	0.50
1:D:350:ILE:HD12	1:D:422:PHE:CE1	2.47	0.50
1:D:362:VAL:N	1:D:390:ASP:O	2.43	0.50
1:D:301:ILE:HG13	1:D:323:SER:HB2	1.94	0.50
1:B:209:ARG:HH12	1:B:273:LEU:HD22	1.77	0.49
1:D:135:GLY:O	1:D:138:GLU:HB2	2.12	0.49
1:D:286:ILE:HD13	1:D:315:TYR:HD1	1.77	0.49
1:A:431:VAL:HG12	1:A:432:LEU:HG	1.93	0.49
1:B:125:TYR:CG	1:B:128:LEU:HB2	2.47	0.49
1:B:17:LEU:HD11	1:B:124:LEU:HG	1.94	0.49
1:D:330:GLU:HG2	1:D:404:TYR:CE2	2.48	0.49
1:A:432:LEU:HD21	1:A:467:SER:HB2	1.94	0.49
1:B:224:LEU:CD1	1:B:308:TYR:HB3	2.41	0.49
1:B:543:ASN:H	1:B:543:ASN:HD22	1.59	0.49
1:B:127:PRO:HA	1:B:130:TYR:CD2	2.47	0.49
1:C:467:SER:OG	1:C:559:ARG:O	2.28	0.49
1:C:144:PHE:CE2	1:C:201:GLN:HG2	2.47	0.49
1:D:544:PHE:HE1	1:D:565:GLU:OE1	1.95	0.49
1:B:130:TYR:CE1	1:B:136:LEU:HD12	2.47	0.49
1:D:72:SER:O	1:D:76:ARG:HG3	2.12	0.49
1:A:558:PRO:HB2	1:A:560:SER:O	2.13	0.48
1:D:497:ARG:HG2	1:D:578:PHE:CE1	2.48	0.48
1:B:541:LEU:O	1:B:544:PHE:HB3	2.14	0.48
1:A:455:LEU:HD21	1:A:500:MET:HE2	1.95	0.48
1:B:237:LEU:O	1:B:241:ILE:HG13	2.13	0.48
1:C:221:SER:HB3	1:C:308:TYR:CE2	2.47	0.48
1:D:224:LEU:HD13	1:D:311:LEU:HD23	1.96	0.48
1:D:302:THR:HG22	1:D:303:GLY:H	1.79	0.48
1:C:146:PHE:CZ	1:C:198:MET:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ASP:OD1	1:D:6:ASP:N	2.47	0.48
1:C:43:GLU:HB3	1:C:85:LEU:HA	1.96	0.48
1:A:242:ARG:HG2	1:A:268:PRO:HA	1.95	0.48
1:B:49:LEU:HD22	1:B:51:GLY:HA3	1.96	0.48
1:C:431:VAL:HG12	1:C:432:LEU:HG	1.95	0.48
1:B:49:LEU:O	1:B:50:ASN:HB3	2.13	0.48
1:C:130:TYR:CD1	1:C:136:LEU:HB3	2.49	0.48
1:A:17:LEU:HD11	1:A:124:LEU:CD2	2.43	0.48
1:A:497:ARG:NH2	1:D:384:ASP:OD1	2.45	0.48
1:B:283:TRP:CE3	1:B:286:ILE:HG21	2.49	0.48
1:D:200:CYS:SG	1:D:250:ILE:HD12	2.54	0.48
1:B:63:PRO:O	1:B:65:VAL:HG13	2.13	0.47
1:B:256:THR:O	1:B:259:ILE:HG22	2.14	0.47
1:B:334:GLY:HA2	1:B:349:THR:O	2.13	0.47
1:C:76:ARG:HD2	1:C:81:GLU:OE2	2.14	0.47
1:C:116:GLU:HA	1:C:119:ILE:HG12	1.95	0.47
1:C:142:LEU:HD23	1:C:215:LEU:HD23	1.96	0.47
1:D:76:ARG:HB3	1:D:81:GLU:HG3	1.97	0.47
1:B:23:ASN:O	1:B:27:ILE:HG13	2.14	0.47
1:A:547:SER:C	1:A:548:ARG:HD2	2.34	0.47
1:B:517:LYS:HG2	1:B:586:TRP:O	2.13	0.47
1:C:4:LYS:HE3	1:C:4:LYS:HB2	1.47	0.47
1:C:4:LYS:NZ	1:C:121:PHE:HA	2.30	0.47
1:C:27:ILE:O	1:C:31:VAL:HG23	2.14	0.47
1:C:238:CYS:O	1:C:241:ILE:N	2.45	0.47
1:B:333:MET:HG2	1:B:357:PHE:HE1	1.79	0.47
1:C:273:LEU:O	1:C:276:GLN:HB2	2.14	0.47
1:C:270:LEU:CD1	1:C:273:LEU:HD11	2.43	0.47
1:A:17:LEU:HD11	1:A:124:LEU:HD21	1.97	0.47
1:B:143:ILE:HD13	1:B:216:GLY:CA	2.43	0.47
1:B:240:ASN:HD21	1:B:247:SER:CB	2.17	0.47
1:C:449:THR:HA	1:C:452:LYS:HD3	1.97	0.47
1:A:540:GLU:HG2	1:A:569:ILE:HG21	1.96	0.47
1:C:56:GLN:O	1:C:60:LYS:HB3	2.15	0.47
1:A:38:ARG:NH1	1:A:89:ARG:HH21	2.12	0.47
1:A:224:LEU:CD1	1:A:308:TYR:HB3	2.44	0.47
1:A:232:ASP:N	1:A:232:ASP:OD1	2.48	0.47
1:B:227:ILE:O	1:B:231:GLU:HG3	2.15	0.47
1:C:518:GLY:HA2	1:C:522:ASP:HB2	1.96	0.47
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.68	0.47
1:C:463:MET:HB2	1:C:483:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:O	1:A:266:PRO:HG3	2.15	0.46
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.64	0.46
1:A:350:ILE:HG12	1:A:422:PHE:CE1	2.50	0.46
1:C:118:ARG:HD3	1:C:332:PHE:HB2	1.97	0.46
1:D:234:TRP:CD2	1:D:235:PRO:HD3	2.50	0.46
1:A:478:TYR:HB2	1:A:528:LEU:HD12	1.97	0.46
1:A:542:MET:HG2	1:A:546:LEU:HD13	1.97	0.46
1:D:179:ASP:OD1	1:D:180:SER:N	2.43	0.46
1:D:234:TRP:CG	1:D:235:PRO:HD3	2.51	0.46
1:B:234:TRP:CG	1:B:235:PRO:HD3	2.50	0.46
1:C:246:LEU:HD11	1:C:259:ILE:HG21	1.97	0.46
1:B:274:ILE:HG23	1:B:290:LEU:HD21	1.97	0.46
1:C:14:LEU:HB3	1:C:124:LEU:HD23	1.96	0.46
1:B:508:GLU:OE2	1:B:519:ARG:HD2	2.16	0.46
1:A:33:GLU:O	1:A:37:SER:HB2	2.16	0.46
1:B:431:VAL:HG12	1:B:432:LEU:HG	1.98	0.46
1:C:410:LEU:HB3	1:C:422:PHE:HB3	1.97	0.46
1:D:16:LEU:HD23	1:D:16:LEU:HA	1.80	0.46
1:C:225:LYS:HD3	1:C:542:MET:SD	2.56	0.46
1:C:240:ASN:O	1:C:244:GLY:N	2.39	0.46
1:D:301:ILE:HD13	1:D:343:PRO:HB3	1.98	0.46
1:C:98:SER:OG	1:C:99:GLY:N	2.49	0.45
1:C:101:SER:O	1:C:104:VAL:HG12	2.16	0.45
1:C:181:LEU:HD23	1:C:181:LEU:H	1.81	0.45
1:B:114:ASP:O	1:B:118:ARG:HG3	2.17	0.45
1:C:42:THR:OG1	1:C:45:LEU:HB2	2.16	0.45
1:C:188:ILE:HD13	1:C:200:CYS:HB3	1.98	0.45
1:B:200:CYS:SG	1:B:250:ILE:HD12	2.57	0.45
1:D:410:LEU:HB3	1:D:422:PHE:HB3	1.99	0.45
1:A:304:THR:CG2	1:A:559:ARG:HE	2.29	0.45
1:C:333:MET:O	1:C:351:ILE:HG13	2.16	0.45
1:D:152:LYS:HB3	1:D:152:LYS:HE3	1.77	0.45
1:C:309:ILE:HB	1:C:310:PRO:HD3	1.97	0.45
1:D:505:PHE:CD1	1:D:582:LYS:HB2	2.51	0.45
1:A:83:SER:HB3	1:A:91:ILE:HG12	1.99	0.45
1:A:520:LYS:O	1:A:523:LYS:NZ	2.50	0.45
1:A:543:ASN:HA	1:A:546:LEU:HD22	1.98	0.45
1:B:209:ARG:NH1	1:B:273:LEU:HD22	2.32	0.45
1:A:146:PHE:HB3	1:A:194:THR:HG22	1.97	0.45
1:A:518:GLY:HA2	1:A:522:ASP:HB2	1.98	0.45
1:B:283:TRP:HE3	1:B:286:ILE:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:VAL:HG12	1:B:381:ASP:O	2.16	0.45
1:B:434:ILE:HG13	1:B:478:TYR:CE1	2.50	0.45
1:B:458:HIS:H	1:B:459:ASP:HA	1.81	0.44
1:C:151:SER:HB2	1:C:159:VAL:HB	1.99	0.44
1:C:196:GLN:HB3	1:C:250:ILE:HD12	1.99	0.44
1:D:206:LEU:HB3	1:D:274:ILE:CD1	2.47	0.44
1:A:89:ARG:H	1:A:89:ARG:HG3	1.39	0.44
1:D:73:TYR:O	1:D:77:ILE:HG12	2.17	0.44
1:D:74:ILE:HD13	1:D:109:PRO:HD3	1.98	0.44
1:D:155:ASN:OD1	1:D:155:ASN:N	2.50	0.44
1:D:518:GLY:HA3	1:D:525:ILE:HD12	1.99	0.44
1:C:72:SER:O	1:C:76:ARG:HG3	2.18	0.44
1:C:458:HIS:ND1	1:C:458:HIS:N	2.61	0.44
1:C:511:LEU:O	1:C:516:ARG:NH1	2.50	0.44
1:A:460:LEU:HD23	1:A:486:SER:HB2	2.00	0.44
1:C:240:ASN:ND2	1:C:240:ASN:H	2.14	0.44
1:C:563:ASN:OD1	1:C:565:GLU:HB2	2.18	0.44
1:A:95:LEU:O	1:A:107:LEU:HA	2.17	0.44
1:B:335:VAL:HG13	1:B:351:ILE:HD11	2.00	0.44
1:C:542:MET:O	1:C:546:LEU:HG	2.16	0.44
1:D:234:TRP:N	1:D:235:PRO:HD2	2.33	0.44
1:A:361:GLU:HG3	1:A:362:VAL:H	1.81	0.44
1:B:74:ILE:HD12	1:B:109:PRO:HD3	2.00	0.44
1:C:431:VAL:HG13	1:C:560:SER:OG	2.18	0.44
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.72	0.44
1:C:394:VAL:HG22	1:C:405:ARG:HG2	1.99	0.44
1:C:447:ALA:HB2	1:C:510:SER:HB2	2.00	0.44
1:C:273:LEU:HD12	1:C:274:ILE:H	1.83	0.43
1:B:134:ASP:O	1:B:295:LYS:HD2	2.17	0.43
1:D:496:ASN:HB3	1:D:499:VAL:CG1	2.47	0.43
1:D:503:CYS:O	1:D:507:VAL:HG23	2.18	0.43
1:A:449:THR:HA	1:A:452:LYS:HD3	2.00	0.43
1:A:547:SER:O	1:A:548:ARG:HD2	2.18	0.43
1:C:73:TYR:O	1:C:77:ILE:HG12	2.18	0.43
1:C:95:LEU:HD11	1:C:110:LEU:HD22	1.99	0.43
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.64	0.43
1:C:581:ARG:HA	1:C:581:ARG:HD3	1.84	0.43
1:A:18:GLU:O	1:A:22:THR:OG1	2.18	0.43
1:B:349:THR:OG1	1:B:421:HIS:HB3	2.17	0.43
1:A:234:TRP:HZ3	1:A:275:GLU:HG2	1.84	0.43
1:A:330:GLU:OE1	1:A:330:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.79	0.43
1:A:542:MET:HG3	1:A:555:TYR:CE2	2.52	0.43
1:A:304:THR:HG22	1:A:559:ARG:HE	1.84	0.43
1:A:494:GLU:OE1	1:C:458:HIS:CD2	2.71	0.43
1:A:517:LYS:HG3	1:A:586:TRP:CE2	2.54	0.43
1:C:540:GLU:HG2	1:C:569:ILE:HG21	2.00	0.43
1:A:209:ARG:HA	1:A:291:TRP:CD1	2.54	0.43
1:B:142:LEU:HB3	1:B:215:LEU:HD23	2.01	0.43
1:B:316:SER:O	1:B:319:LEU:HD12	2.19	0.43
1:D:359:PHE:HB3	1:D:391:TYR:HB3	2.01	0.43
1:B:44:TYR:O	1:B:48:PHE:HD1	2.01	0.43
1:A:443:ASP:OD1	1:A:443:ASP:N	2.49	0.43
1:C:198:MET:O	1:C:202:LEU:HB2	2.18	0.43
1:C:498:ASP:OD1	1:C:498:ASP:N	2.51	0.43
1:B:240:ASN:ND2	1:B:247:SER:HB2	2.18	0.42
1:C:202:LEU:HA	1:C:202:LEU:HD12	1.74	0.42
1:C:209:ARG:HA	1:C:291:TRP:CD1	2.54	0.42
1:C:273:LEU:HD12	1:C:274:ILE:HG13	2.00	0.42
1:C:330:GLU:HG2	1:C:404:TYR:CE2	2.53	0.42
1:D:161:THR:CG2	1:D:554:GLN:OE1	2.67	0.42
1:D:544:PHE:CE1	1:D:565:GLU:OE1	2.72	0.42
1:B:93:VAL:CG2	1:B:110:LEU:HB3	2.49	0.42
1:B:238:CYS:SG	1:B:275:GLU:HG2	2.60	0.42
1:B:486:SER:C	1:B:488:VAL:H	2.23	0.42
1:D:140:LYS:HG3	1:D:211:ASN:OD1	2.19	0.42
1:A:239:SER:O	1:A:243:THR:OG1	2.20	0.42
1:B:161:THR:HB	1:B:164:THR:OG1	2.19	0.42
1:C:435:ASP:CG	1:C:436:MET:H	2.22	0.42
1:A:246:LEU:HD11	1:A:259:ILE:HG21	2.01	0.42
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.77	0.42
1:B:430:VAL:CG2	1:B:440:TYR:HE1	2.26	0.42
1:C:42:THR:O	1:C:46:ARG:HB2	2.19	0.42
1:D:161:THR:HB	1:D:164:THR:OG1	2.19	0.42
1:A:115:LEU:O	1:A:119:ILE:HG13	2.19	0.42
1:B:84:ASP:OD1	1:B:84:ASP:N	2.50	0.42
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.78	0.42
1:D:4:LYS:HZ1	1:D:120:SER:HB3	1.84	0.42
1:D:519:ARG:HH11	1:D:519:ARG:HD2	1.72	0.42
1:A:325:PHE:CE1	1:A:335:VAL:HG12	2.54	0.42
1:C:268:PRO:O	1:C:272:SER:OG	2.37	0.42
1:D:200:CYS:SG	1:D:250:ILE:CD1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LYS:HA	1:A:575:ILE:HD11	2.01	0.42
1:A:23:ASN:O	1:A:27:ILE:HG13	2.20	0.42
1:A:397:THR:HG22	1:A:399:SER:N	2.20	0.42
1:A:494:GLU:OE1	1:C:458:HIS:HD2	2.03	0.42
1:C:277:GLU:HA	1:C:280:LYS:HZ2	1.84	0.42
1:B:202:LEU:HD11	1:B:226:VAL:CG1	2.50	0.42
1:C:203:LEU:HD23	1:C:259:ILE:HD11	2.02	0.42
1:A:188:ILE:O	1:A:191:CYS:HB2	2.19	0.41
1:B:185:PRO:HG3	1:B:262:PHE:CE2	2.53	0.41
1:B:209:ARG:HA	1:B:291:TRP:HD1	1.84	0.41
1:C:23:ASN:O	1:C:27:ILE:HG13	2.20	0.41
1:C:196:GLN:HB3	1:C:250:ILE:HD13	2.02	0.41
1:B:34:ALA:O	1:B:38:ARG:HG3	2.20	0.41
1:B:272:SER:O	1:B:276:GLN:HG3	2.19	0.41
1:B:454:LEU:N	1:B:454:LEU:HD23	2.35	0.41
1:A:25:LYS:HE2	1:A:26:GLN:HE21	1.82	0.41
1:A:455:LEU:HD21	1:A:500:MET:CE	2.50	0.41
1:A:530:ILE:HG21	1:A:530:ILE:HD13	1.79	0.41
1:C:110:LEU:HD21	1:C:115:LEU:HB2	2.01	0.41
1:D:11:LYS:C	1:D:13:CYS:H	2.23	0.41
1:D:202:LEU:HD23	1:D:202:LEU:HA	1.79	0.41
1:A:125:TYR:CE2	1:A:129:LEU:CD1	3.03	0.41
1:A:133:ILE:CD1	1:A:296:CYS:HB3	2.50	0.41
1:A:551:SER:OG	1:A:554:GLN:HB2	2.21	0.41
1:C:121:PHE:CE2	1:C:351:ILE:HD13	2.56	0.41
1:C:220:ALA:HA	1:C:299:SER:OG	2.21	0.41
1:C:451:ALA:O	1:C:454:LEU:HG	2.21	0.41
1:A:151:SER:HB2	1:A:159:VAL:HB	2.03	0.41
1:B:126:ALA:H	1:B:127:PRO:HD2	1.83	0.41
1:B:191:CYS:CB	1:B:255:CYS:SG	3.06	0.41
1:B:563:ASN:OD1	1:B:565:GLU:CG	2.64	0.41
1:D:361:GLU:HG2	1:D:362:VAL:N	2.35	0.41
1:D:483:GLU:OE1	1:D:538:PHE:HB2	2.21	0.41
1:C:36:LEU:HD11	1:C:58:PHE:HB2	2.02	0.41
1:C:293:LYS:O	1:C:293:LYS:HG3	2.20	0.41
1:C:351:ILE:HG13	1:C:351:ILE:H	1.64	0.41
1:C:522:ASP:HB3	1:C:524:ASN:ND2	2.36	0.41
1:D:295:LYS:HA	1:D:295:LYS:HD3	1.71	0.41
1:A:452:LYS:O	1:A:455:LEU:HB2	2.21	0.41
1:C:541:LEU:HD11	1:C:566:ALA:HB1	2.02	0.41
1:A:183:VAL:HG11	1:A:205:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:HG22	1:A:405:ARG:HG2	2.02	0.41
1:A:413:THR:OG1	1:A:421:HIS:HB3	2.21	0.41
1:A:427:ARG:HB3	1:A:429:LYS:HD3	2.03	0.41
1:B:153:THR:O	1:B:156:GLY:N	2.53	0.41
1:B:217:ALA:HB3	1:B:223:PHE:HB2	2.02	0.41
1:B:362:VAL:HB	1:B:390:ASP:HB2	2.02	0.41
1:B:505:PHE:CZ	1:B:509:GLU:HG2	2.56	0.41
1:C:14:LEU:CD1	1:C:127:PRO:HG2	2.51	0.41
1:C:160:ARG:HB2	1:C:161:THR:H	1.74	0.41
1:C:228:LYS:NZ	1:C:539:ASP:OD2	2.54	0.41
1:C:541:LEU:O	1:C:544:PHE:HB3	2.21	0.41
1:B:533:VAL:HA	1:B:573:ASN:O	2.21	0.41
1:C:301:ILE:HD13	1:C:343:PRO:HB3	2.02	0.41
1:D:98:SER:HB3	2:D:600:AMP:O3P	2.21	0.41
1:A:93:VAL:HG12	1:A:158:MET:HB2	2.03	0.40
1:B:203:LEU:O	1:B:207:LEU:HG	2.21	0.40
1:C:273:LEU:O	1:C:277:GLU:OE1	2.38	0.40
1:D:76:ARG:NH2	1:D:81:GLU:OE1	2.54	0.40
1:A:333:MET:HE3	1:A:357:PHE:CE1	2.56	0.40
1:A:465:PHE:HA	1:A:481:TYR:O	2.22	0.40
1:C:119:ILE:HG13	1:C:120:SER:N	2.35	0.40
1:D:5:PHE:CD1	1:D:5:PHE:N	2.85	0.40
1:C:83:SER:HB3	1:C:91:ILE:HG12	2.03	0.40
1:C:304:THR:HB	1:C:559:ARG:HH21	1.86	0.40
1:C:547:SER:HB2	1:C:548:ARG:NH1	2.37	0.40
1:D:519:ARG:HD3	1:D:525:ILE:HG22	2.04	0.40
1:A:36:LEU:O	1:A:40:ALA:HB2	2.21	0.40
1:A:133:ILE:CG2	1:A:136:LEU:HD22	2.52	0.40
1:A:209:ARG:HD3	1:A:270:LEU:HD11	2.03	0.40
1:D:446:LYS:HE3	1:D:446:LYS:HB2	1.78	0.40

All (4) 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)
1:D:276:GLN:CD	1:D:276:GLN:OE1[8_545]	1.19	1.01
1:D:276:GLN:CD	1:D:276:GLN:CD[8_545]	1.26	0.94
1:D:276:GLN:OE1	1:D:276:GLN:NE2[8_545]	1.81	0.39
1:D:276:GLN:CD	1:D:276:GLN:NE2[8_545]	1.90	0.30

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	537/595 (90%)	508 (95%)	24 (4%)	5 (1%)	17 53
1	B	529/595 (89%)	508 (96%)	19 (4%)	2 (0%)	34 71
1	C	544/595 (91%)	522 (96%)	21 (4%)	1 (0%)	47 81
1	D	537/595 (90%)	524 (98%)	11 (2%)	2 (0%)	34 71
All	All	2147/2380 (90%)	2062 (96%)	75 (4%)	10 (0%)	29 66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	7	PRO
1	B	49	LEU
1	D	8	THR
1	B	435	ASP
1	C	15	SER
1	A	12	ALA
1	A	435	ASP
1	D	12	ALA
1	A	584	PRO

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	494/535 (92%)	470 (95%)	24 (5%)	25 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	489/535 (91%)	472 (96%)	17 (4%)	36 70
1	C	496/535 (93%)	473 (95%)	23 (5%)	27 62
1	D	495/535 (92%)	477 (96%)	18 (4%)	35 69
All	All	1974/2140 (92%)	1892 (96%)	82 (4%)	30 65

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	37	SER
1	A	61	ASN
1	A	128	LEU
1	A	131	LYS
1	A	152	LYS
1	A	184	SER
1	A	191	CYS
1	A	232	ASP
1	A	246	LEU
1	A	261	LYS
1	A	263	LEU
1	A	275	GLU
1	A	283	TRP
1	A	332	PHE
1	A	423	CYS
1	A	428	GLN
1	A	429	LYS
1	A	436	MET
1	A	472	SER
1	A	519	ARG
1	A	539	ASP
1	A	554	GLN
1	A	568	LYS
1	B	11	LYS
1	B	23	ASN
1	B	26	GLN
1	B	37	SER
1	B	113	GLU
1	B	125	TYR
1	B	134	ASP
1	B	185	PRO
1	B	197	SER

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Mol	Chain	Res	Type
1	B	232	ASP
1	B	252	ASP
1	B	263	LEU
1	B	332	PHE
1	B	423	CYS
1	B	468	ARG
1	B	560	SER
1	B	586	TRP
1	C	11	LYS
1	C	37	SER
1	C	50	ASN
1	C	69	ASP
1	C	71	ARG
1	C	149	ARG
1	C	155	ASN
1	C	181	LEU
1	C	201	GLN
1	C	239	SER
1	C	242	ARG
1	C	247	SER
1	C	289	ARG
1	C	293	LYS
1	C	314	PHE
1	C	332	PHE
1	C	342	LYS
1	C	427	ARG
1	C	428	GLN
1	C	458	HIS
1	C	468	ARG
1	C	497	ARG
1	C	520	LYS
1	D	9	ASN
1	D	16	LEU
1	D	19	ASP
1	D	38	ARG
1	D	54	ASP
1	D	79	ASN
1	D	89	ARG
1	D	155	ASN
1	D	225	LYS
1	D	245	ARG
1	D	246	LEU

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Mol	Chain	Res	Type
1	D	298	GLU
1	D	423	CYS
1	D	427	ARG
1	D	461	MET
1	D	497	ARG
1	D	580	SER
1	D	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	B	26	GLN
1	B	240	ASN
1	C	240	ASN
1	C	276	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\|>2$
2	AMP	D	600	-	22,25,25	1.18	2 (9%)	25,38,38	1.35	2 (8%)
2	AMP	A	600	-	22,25,25	1.01	1 (4%)	25,38,38	1.54	5 (20%)
2	AMP	C	600	-	22,25,25	0.86	1 (4%)	25,38,38	1.33	3 (12%)
2	AMP	B	600	-	22,25,25	1.03	2 (9%)	25,38,38	1.18	1 (4%)

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
2	AMP	D	600	-	-	4/6/26/26	0/3/3/3
2	AMP	A	600	-	-	5/6/26/26	0/3/3/3
2	AMP	C	600	-	-	0/6/26/26	0/3/3/3
2	AMP	B	600	-	-	2/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	AMP	C5-C4	2.99	1.48	1.40
2	D	600	AMP	C2-N3	2.77	1.36	1.32
2	B	600	AMP	C5-C4	2.70	1.48	1.40
2	B	600	AMP	C2-N3	2.64	1.36	1.32
2	D	600	AMP	C5-C4	2.59	1.47	1.40
2	C	600	AMP	C5-C4	2.23	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	AMP	N3-C2-N1	-4.43	121.76	128.68
2	C	600	AMP	N3-C2-N1	-3.52	123.18	128.68
2	D	600	AMP	N3-C2-N1	-3.39	123.37	128.68
2	B	600	AMP	C4-C5-N7	-3.18	106.08	109.40
2	D	600	AMP	C4-C5-N7	-3.07	106.20	109.40
2	A	600	AMP	O3P-P-O2P	3.06	119.33	107.64
2	A	600	AMP	C2-N1-C6	2.70	123.38	118.75
2	A	600	AMP	O3P-P-O5'	-2.28	100.67	106.73
2	A	600	AMP	O2P-P-O5'	-2.17	100.95	106.73
2	C	600	AMP	C2-N1-C6	2.07	122.30	118.75
2	C	600	AMP	O3P-P-O2P	2.04	115.45	107.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	AMP	C5'-O5'-P-O2P
2	A	600	AMP	C5'-O5'-P-O3P
2	A	600	AMP	C3'-C4'-C5'-O5'
2	B	600	AMP	C3'-C4'-C5'-O5'
2	D	600	AMP	C5'-O5'-P-O1P
2	D	600	AMP	C5'-O5'-P-O2P
2	D	600	AMP	C5'-O5'-P-O3P
2	A	600	AMP	O4'-C4'-C5'-O5'
2	B	600	AMP	O4'-C4'-C5'-O5'
2	A	600	AMP	C5'-O5'-P-O1P
2	D	600	AMP	O4'-C4'-C5'-O5'

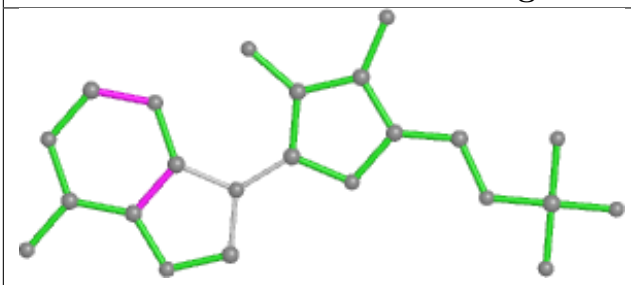
There are no ring outliers.

2 monomers are involved in 3 short contacts:

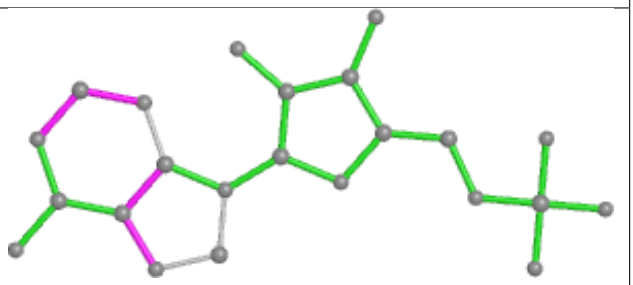
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	AMP	2	0
2	C	600	AMP	1	0

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 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.

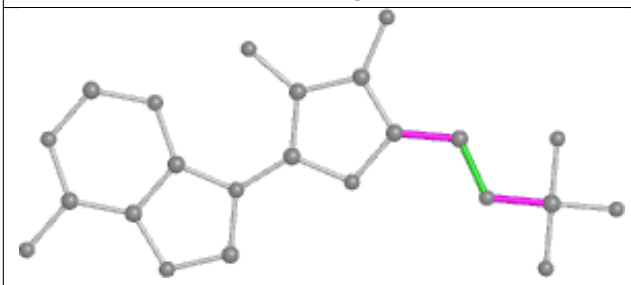
Ligand AMP D 600



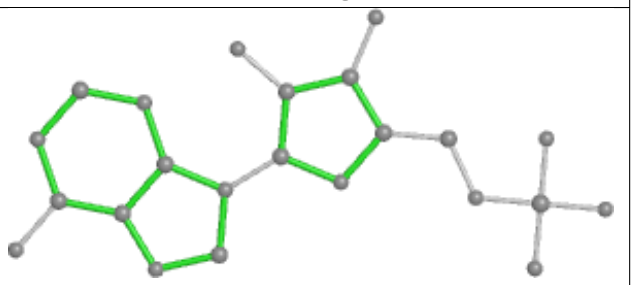
Bond lengths



Bond angles

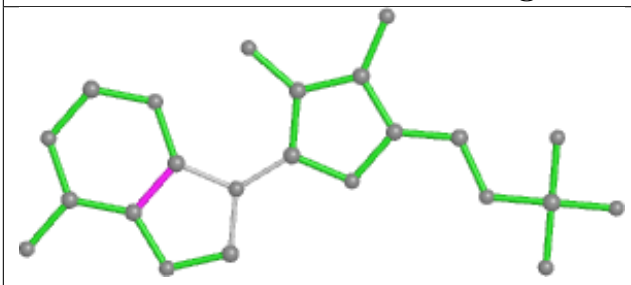


Torsions

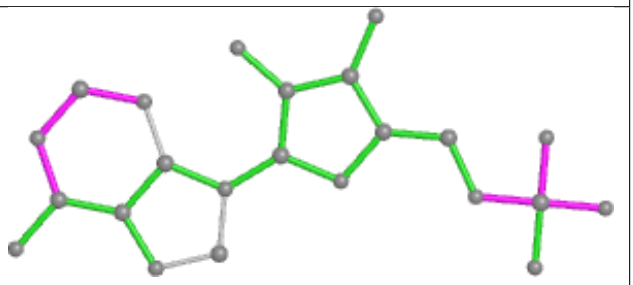


Rings

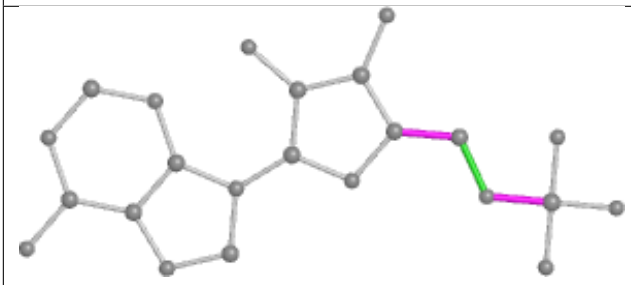
Ligand AMP A 600



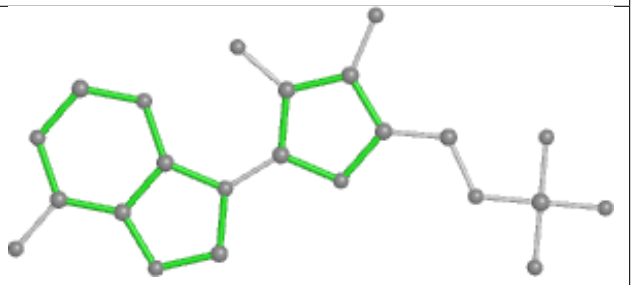
Bond lengths



Bond angles

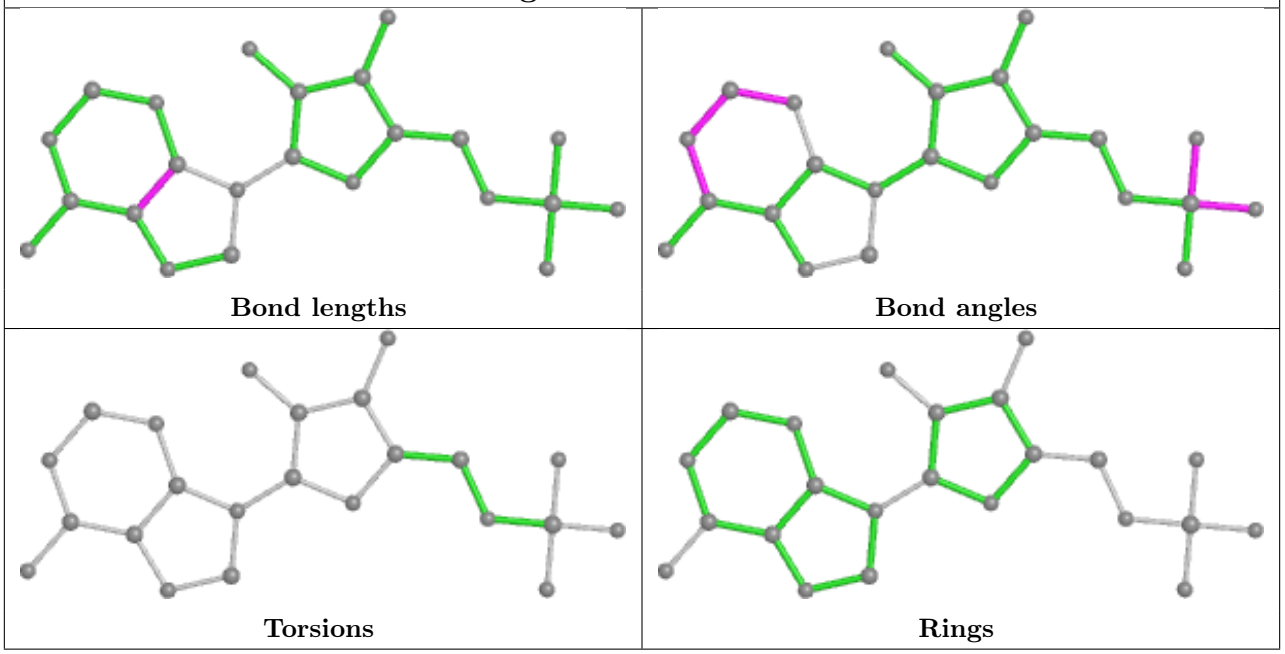


Torsions

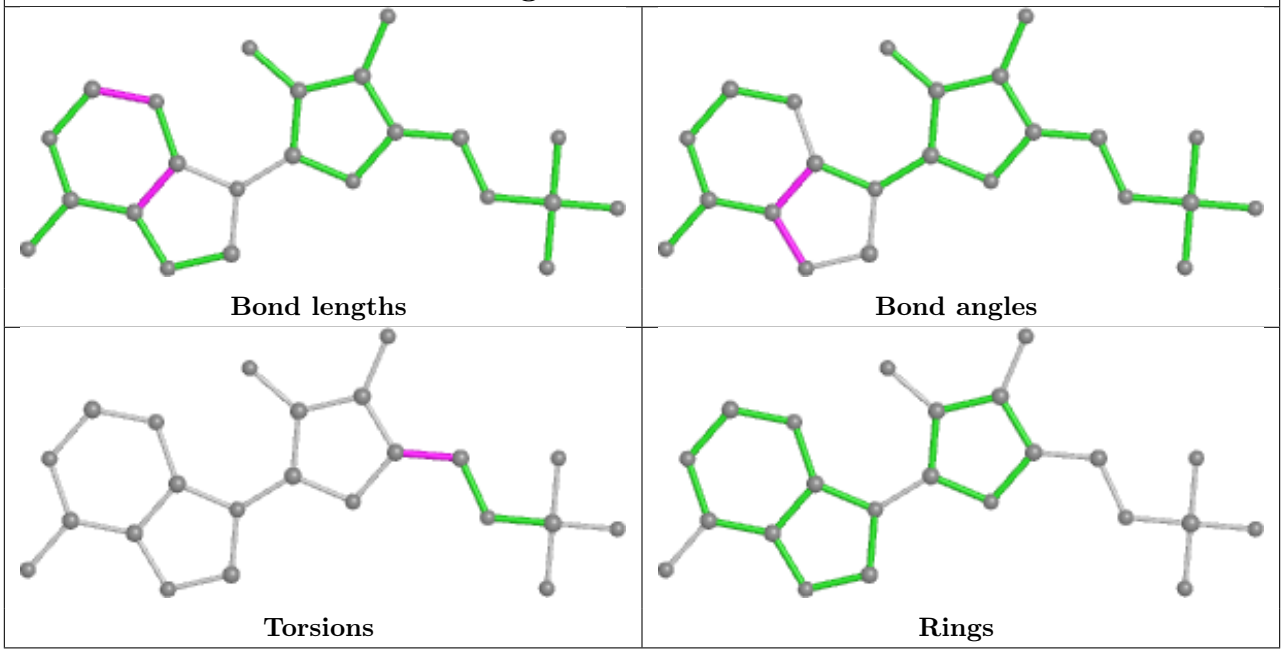


Rings

Ligand AMP C 600



Ligand AMP B 600



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	547/595 (91%)	-0.40	2 (0%)	92	78	27, 45, 81, 104	1 (0%)
1	B	541/595 (90%)	-0.28	5 (0%)	84	62	30, 54, 89, 122	1 (0%)
1	C	552/595 (92%)	-0.37	3 (0%)	91	75	30, 51, 90, 118	1 (0%)
1	D	549/595 (92%)	-0.43	4 (0%)	87	68	27, 46, 81, 115	1 (0%)
All	All	2189/2380 (91%)	-0.37	14 (0%)	89	72	27, 49, 87, 122	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	TYR	4.3
1	C	102	GLY	3.8
1	A	264	THR	3.5
1	B	241	ILE	2.9
1	C	263	LEU	2.8
1	B	264	THR	2.8
1	A	263	LEU	2.6
1	D	264	THR	2.5
1	B	278	CYS	2.5
1	C	264	THR	2.4
1	B	267	ASN	2.3
1	D	290	LEU	2.1
1	D	54	ASP	2.1
1	D	138	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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)

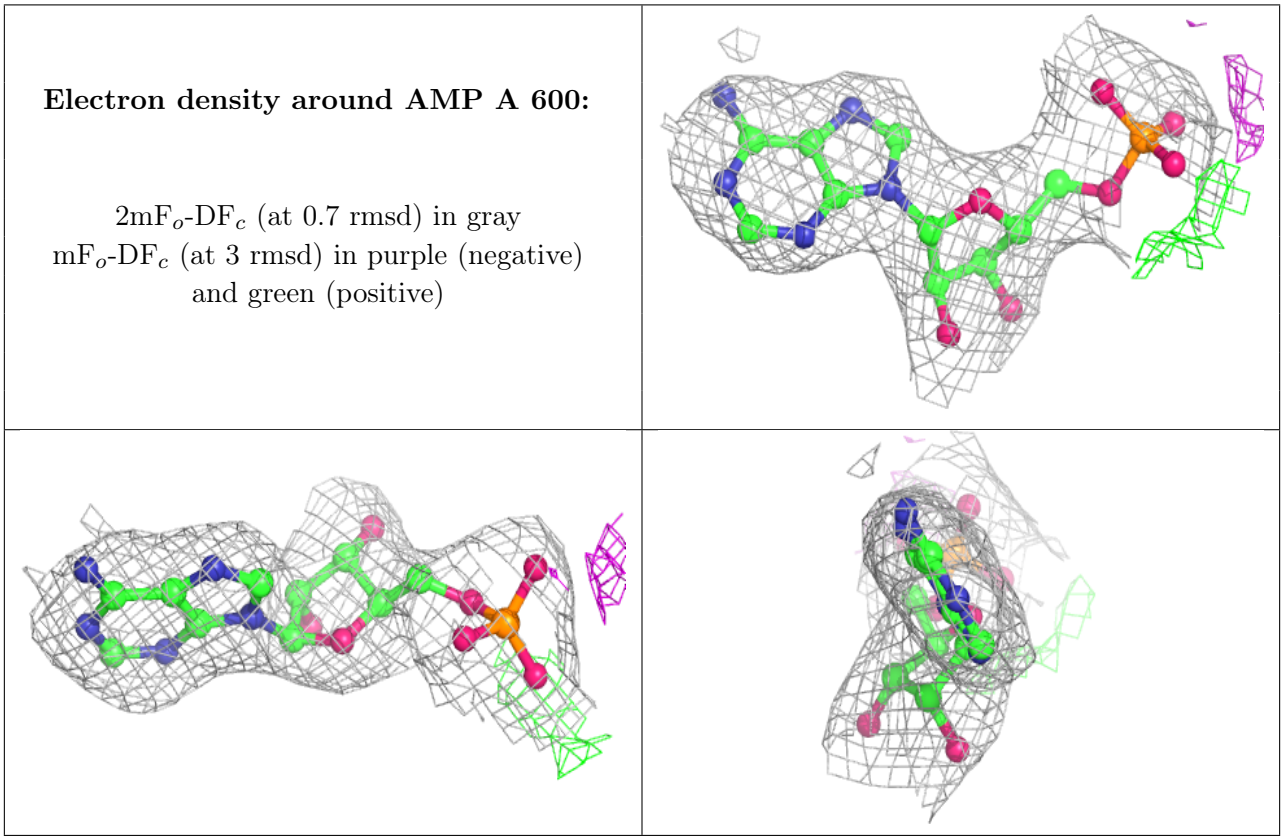
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	AMP	A	600	23/23	0.96	0.16	18,30,83,97	0
2	AMP	D	600	23/23	0.96	0.17	12,27,57,74	0
2	AMP	C	600	23/23	0.97	0.17	20,35,68,84	0
2	AMP	B	600	23/23	0.97	0.14	21,32,68,87	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.

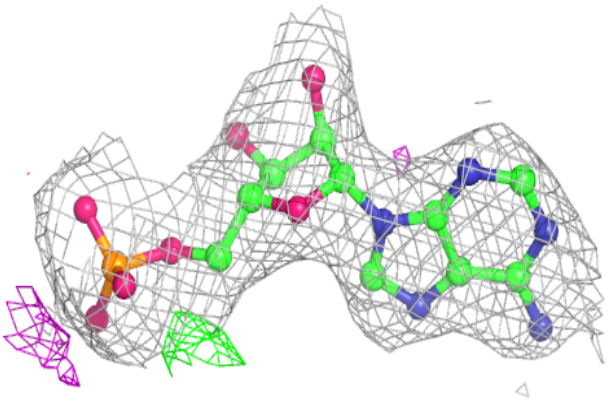
Electron density around AMP A 600:

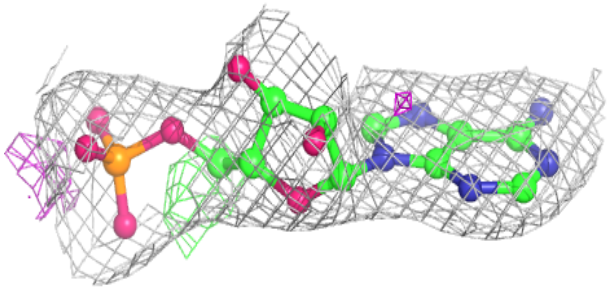
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

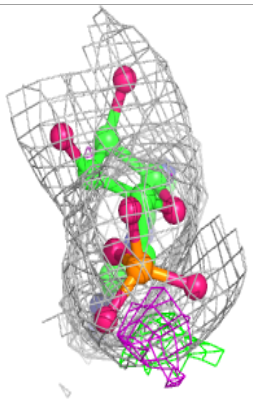


Electron density around AMP D 600:

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

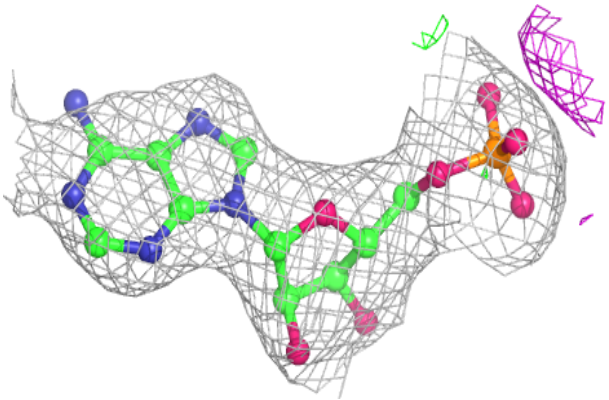


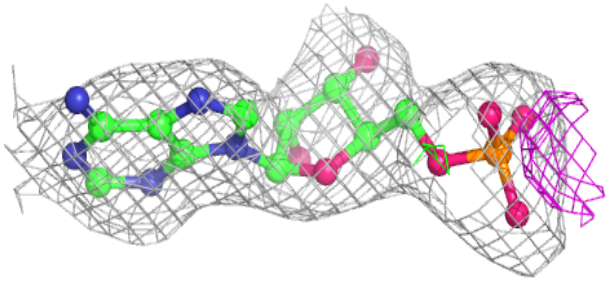


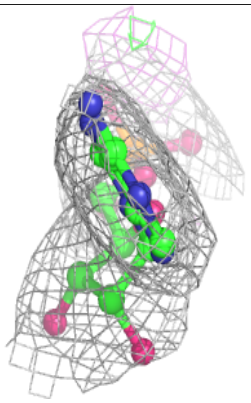


Electron density around AMP C 600:

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

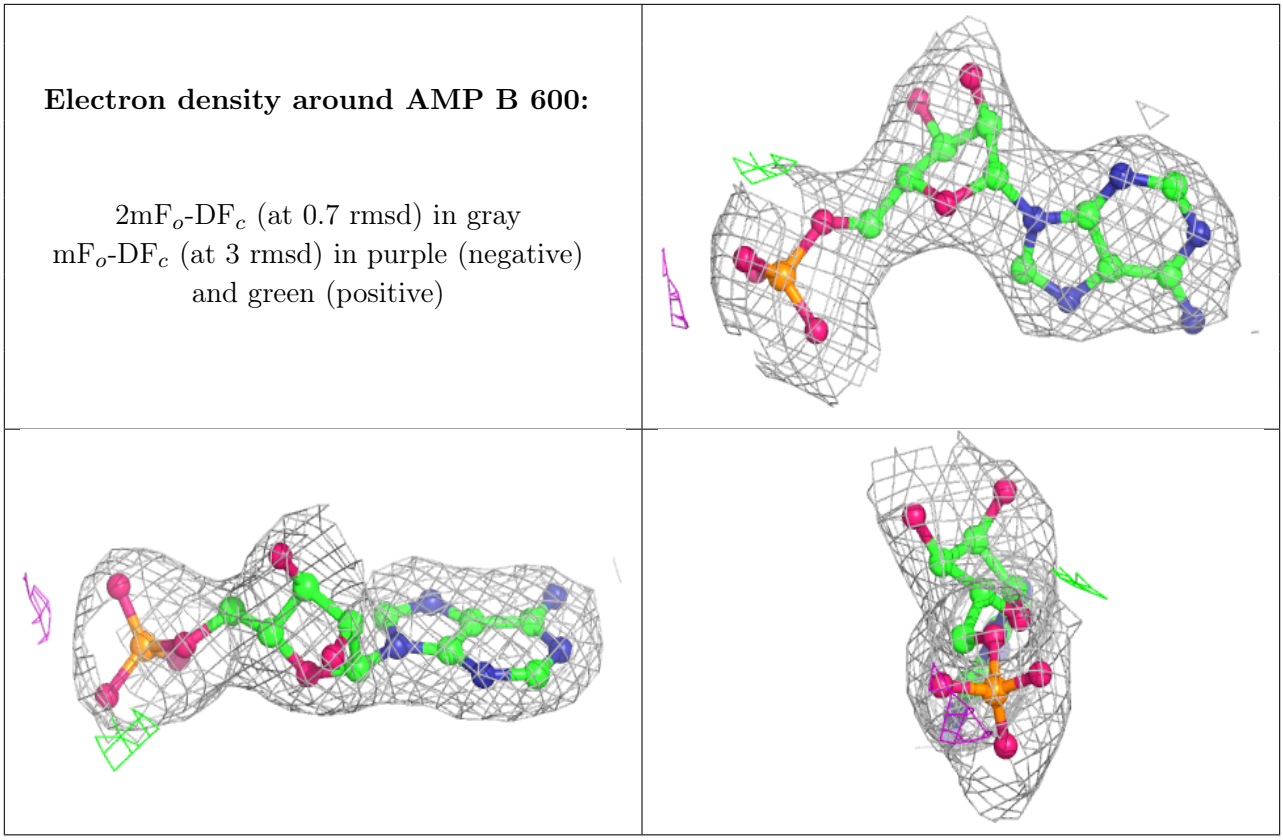






Electron density around AMP B 600:

$2mF_o$-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.